Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary Information

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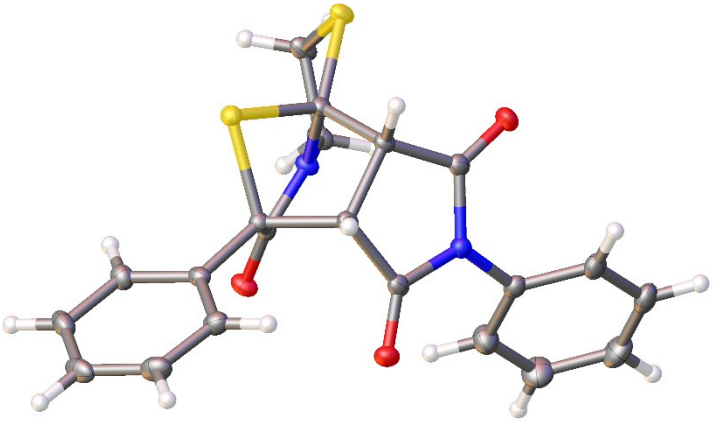
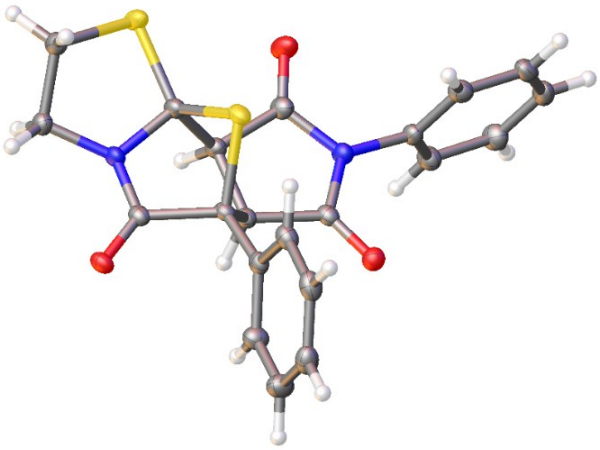


Experimental. Single crystals of $C_{21}H_{16}N_2O_3S_2$ **8** were grown from ethyl acetate. A suitable crystal (0.24×0.20×0.03 mm^3) was selected and mounted on a MITIGEN holder in perflourotether oil on a Rigaku FRE+ diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program, using the Charge Flipping solution method. The model was refined with the ShelXL [3] refinement package using Least Squares minimisation.

Crystal Data. $C_{21}H_{16}N_2O_3S_2$, M = 408.50, monoclinic, $P2_1/c$ (No. 14, a = 11.0765 Å, b = 18.7037 Å, c = 17.8788 Å, b = 91.808˚, a = g = 90˚,V = 3702.1(6) $Å^3$, T = 100(2) K, Z = 8, m (Mo K_a) = 0.314, 33998 reflections measured, 8515 unique (R_{int} = 0.0376) which were used in all calculations. The final wR_2 was 0.0829 (all data) and R_1 was 0.0315 (I > 2(I)).

[1] Olex2 (Dolomanov et al., 2009)
[2] olex2.solve (Bourhis et al., 2013)
[3] ShelXL (Sheldrick, 2008)

Compound	**8**
Code	VD-1
Formula	$C_{21}H_{16}N_2O_3S_2$
D calc./g cm^{-3}	1.466
m/mm^{-1}	0.314
Formula Weight	408.50
Colour	clear colourless
Shape	Prism
Size/mm^3	0.24×0.20×0.03
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	11.0765(11)
b/Å	18.7037(19)
c/Å	17.8788(18)
a/˚	90
b/˚	91.808(2)
g/˚	90
V/Å^3	3702.1(6)
Z	8 (Z'=2)
Theta min/°	2.279
Theta max/°	27.522
Measured Refl.	33998
Independent Refl.	8515
Reflections Used	7402
R(int)	0.0376
Parameters	505
Restraints	0
Largest Peak	0.821
Deepest Hole	-0.276
GooF	1.049
wR_2(all data)	0.0829
wR_2	0.0805
R_1(all data)	0.0373
R_1	0.0315



Experimental. Single crystals of $C_{21}H_{16}N_2O_3S_2$ (**9**) were obtained by recrystallisation from dichloromethane. A suitable crystal (0.13×0.12×0.08 mm^3) was selected and mounted on a MITIGEN holder in perflourotether oil on a Rigaku FRE+ diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program, using the Charge Flipping solution method. The model was refined with the ShelXL [3] refinement package using Least Squares minimisation.

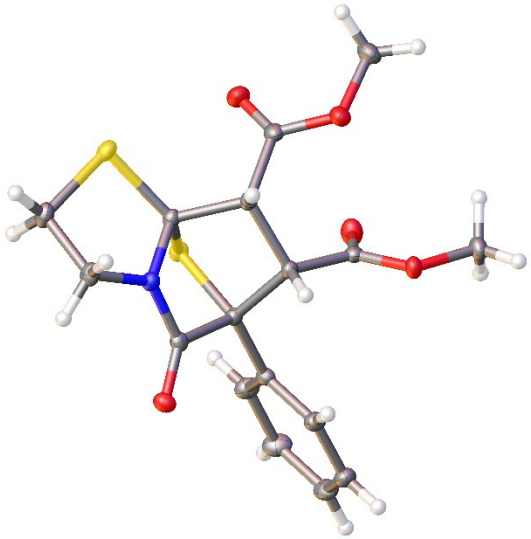
Crystal Data. $C_{21}H_{16}N_2O_3S_2$, M = 408.48, monoclinic, $P2_1/c$ (No. 14, a = 11.8815 Å, b = 6.2795 Å, c = 23.859 Å, b = 95.94˚, a = g = 90˚,V = 1770.6(3) $Å^3$, T = 100(2) K, Z = 4, m (Mo K_a) = 0.328, 15920 reflections measured, 4058 unique (R_{int} = 0.0299) which were used in all calculations. The final wR_2 was 0.0810 (all data) and R_1 was 0.0294 (I > 2(I)).

[1] Olex2 (Dolomanov et al., 2009)

[2] olex2.solve (Bourhis et al., 2013)

[3] ShelXL (Sheldrick, 2008)

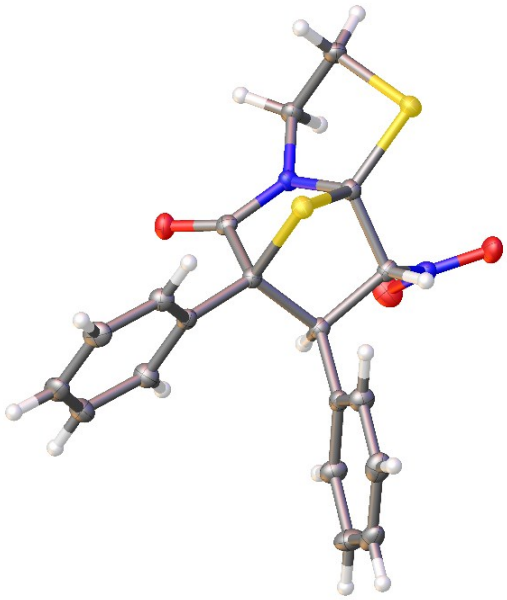
Compound	**9**
Code	VD-2
Formula	$C_{21}H_{16}N_2O_3S_2$
D calc./g cm^{-3}	1.532
m/mm^{-1}	0.328
Formula Weight	408.48
Colour	clear colourless
Shape	block
Size/mm^3	0.13×0.12×0.08
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	11.8815(12)
b/Å	6.2795(6)
c/Å	23.859(3)
a/˚	90
b/˚	95.940(3)
g/˚	90
V/Å^3	1770.6(3)
Z	4
Theta min/°	2.555
Theta max/°	27.531
Measured Refl.	15920
Independent Refl.	4058
Reflections Used	3608
R(int)	0.0299
Parameters	253
Restraints	0
Largest Peak	0.369
Deepest Hole	-0.224
GooF	1.058
wR_2(all data)	0.0810
wR_2	0.0793
R_1(all data)	0.0328
R_1	0.0294



Experimental. Single clear colourless block-shaped crystals of **11** were obtained by recrystallisation from toluene. A suitable crystal (0.62 × 0.50 × 0.25 mm^3) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku R-AXIS Spider diffractometer. The crystal was kept at T = 120 K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the ShelXT (Sheldrick, 2008) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{17}H_{17}NO_5S_2$, M_r = 379.43, orthorhombic, $P2_12_12_1$ (No. 19), a = 5.84070(10) Å, b = 14.9477(4) Å, c = 19.3104(6) Å, □ = □ = □ = 90 °, V = 1685.90(7) $Å^3$, T = 120 K, Z = 4, Z' = 1, □ ($MoK_□$) = 0.345, 21760 reflections measured, 4321 unique (R_{int} = 0.0300) which were used in all calculations. The final wR_2 was 0.0602 (all data) and R_1 was 0.0226 (I > 2(I)).

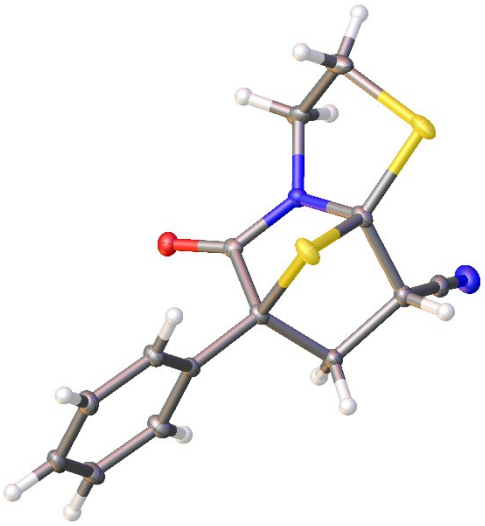
Compound	**11**
Formula	$C_{17}H_{17}NO_5S_2$
$D_{calc.}$/ g cm^{-3}	1.495
□/mm^{-1}	0.345
Formula Weight	379.43
Colour	clear colourless
Shape	block
Max Size/mm	0.62
Mid Size/mm	0.50
Min Size/mm	0.25
T/K	120
Crystal System	orthorhombic
Flack Parameter	0.030(12)
Hooft Parameter	0.038(17)
Space Group	$P2_12_12_1$
a/Å	5.84070(10)
b/Å	14.9477(4)
c/Å	19.3104(6)
□/°	90
□/°	90
□/°	90
V/Å^3	1685.90(7)
Z	4
Z'	1
□$_{min}$/°	2.923
□$_{max}$/°	28.695
Measured Refl.	21760
Independent Refl.	4321
Reflections Used	4287
R_{int}	0.0300
Parameters	228
Restraints	0
Largest Peak	0.301
Deepest Hole	-0.201
GooF	1.112
wR_2 (all data)	0.0602
wR_2	0.0600
R_1 (all data)	0.0228
R_1	0.0226



Experimental. Single clear colourless block-shaped crystals of **14** were obtained by recrystallisation from ethyl acetate. A suitable crystal (0.12×0.09×0.03) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{19}H_{16}N_2O_3S_2$, M_r = 384.46, orthorhombic, Pbca (No. 61), a = 10.4140(3) Å, b = 15.8099(4) Å, c = 21.1096(5) Å, □ = □ = □ = 90°, V = 3475.57(15) Å^3, T = 100(2) K, Z = 8, Z' = 1, □(MoK□) = 0.329, 18670 reflections measured, 4978 unique (R_{int} = 0.0401) which were used in all calculations. The final wR_2 was 0.0948 (all data) and R_1 was 0.0410 (I > 2(I)).

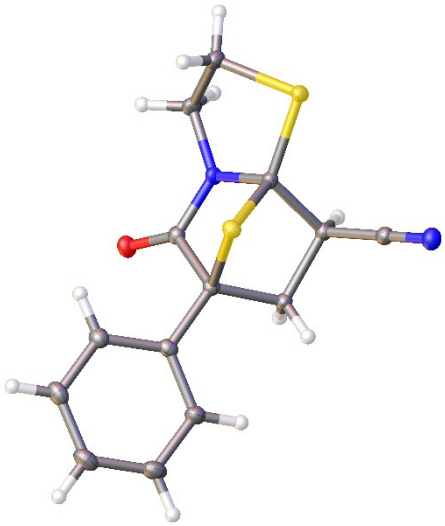
Compound	**14**
Formula	$C_{19}H_{16}N_2O_3S_2$
$D_{calc.}$/ g cm^{-3}	1.469
□/mm^{-1}	0.329
Formula Weight	384.46
Colour	clear colourless
Shape	block
Max Size/mm	0.12
Mid Size/mm	0.09
Min Size/mm	0.03
T/K	100(2)
Crystal System	orthorhombic
Space Group	Pbca
a/Å	10.4140(3)
b/Å	15.8099(4)
c/Å	21.1096(5)
□/°	90
□/°	90
□/°	90
V/Å^3	3475.57(15)
Z	8
Z'	1
□$_{min}$/°	1.929
□$_{max}$/°	30.811
Measured Refl.	18670
Independent Refl.	4978
Reflections Used	4044
R_{int}	0.0401
Parameters	235
Restraints	0
Largest Peak	0.424
Deepest Hole	-0.293
GooF	1.032
wR_2 (all data)	0.0948
wR_2	0.0886
R_1 (all data)	0.0552
R_1	0.0410



Experimental. Single clear colourless rod-shaped crystals of **16** were obtained by recrystallisation from ethyl acetate. A suitable crystal (0.22×0.04×0.04) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-VHF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the ShelXT (Sheldrick, 2015) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{14}H_{12}N_2OS_2$, M_r = 288.38, triclinic, P-1 (No. 2), a = 5.6439(3) Å, b = 10.3733(3) Å, c = 11.1733(4) Å, □ = 88.811(3)°, □ = 76.205(4)°, □ = 88.281(3)°, V = 634.93(4) Å^3, T = 100(2) K, Z = 2, Z' = 1, □(MoK□) = 0.411, 12461 reflections measured, 4143 unique (R_{int} = 0.0192) which were used in all calculations. The final wR_2 was 0.0864 (all data) and R_1 was 0.0313 (I > 2(I)).

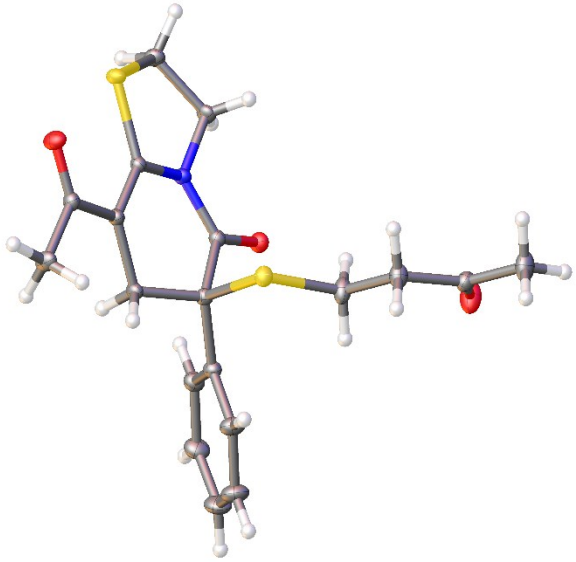
Compound	**16**
Formula	$C_{14}H_{12}N_2OS_2$
$D_{calc.}$/ g cm^{-3}	1.508
□/mm^{-1}	0.411
Formula Weight	288.38
Colour	clear colourless
Shape	?
Max Size/mm	0.22
Mid Size/mm	0.04
Min Size/mm	0.04
T/K	100(2)
Crystal System	triclinic
Space Group	P-1
a/Å	5.6439(3)
b/Å	10.3733(3)
c/Å	11.1733(4)
□/°	88.811(3)
□/°	76.205(4)
□/°	88.281(3)
V/Å^3	634.93(4)
Z	2
Z'	1
□$_{min}$/°	2.698
□$_{max}$/°	32.334
Measured Refl.	12461
Independent Refl.	4143
Reflections Used	3796
R_{int}	0.0192
Parameters	172
Restraints	0
Largest Peak	0.584
Deepest Hole	-0.240
GooF	1.043
wR_2 (all data)	0.0864
wR_2	0.0845
R_1 (all data)	0.0341
R_1	0.0313



Experimental. Single clear colourless prism-shaped crystals of **17** were obtained by recrystallisation from ethyl acetate. A suitable crystal (0.13×0.10×0.05) was selected and mounted on a MITIGEN holder in perfluoroether oil on a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the ShelXT (Sheldrick, 2015) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{14}H_{12}N_2OS_2$, M_r = 288.38, orthorhombic, Pbca (No. 61), a = 10.3634 Å, b = 12.0468 Å, c = 21.0449 Å, □ = □ = □ = 90°, V = 2627.36(10) Å^3, T = 100(2) K, Z = 8, Z' = 1, □(Mo□) = 0.397, 24439 reflections measured, 4330 unique (R_{int} = 0.0320) which were used in all calculations. The final wR_2 was 0.0798 (all data) and R_1 was 0.0298 (I > 2(I)).

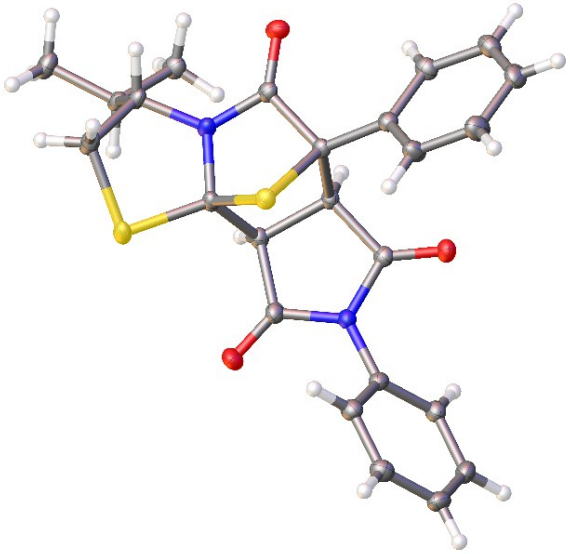
Compound	**17**
Formula	$C_{14}H_{12}N_2OS_2$
$D_{calc.}$/ g cm^{-3}	1.458
□/mm^{-1}	0.397
Formula Weight	288.38
Colour	clear colourless
Shape	prism
Max Size/mm	0.13
Mid Size/mm	0.10
Min Size/mm	0.05
T/K	100(2)
Crystal System	orthorhombic
Space Group	Pbca
a/Å	10.3634(2)
b/Å	12.0468(3)
c/Å	21.0449(4)
□/°	90
□/°	90
□/°	90
V/Å^3	2627.36(10)
Z	8
Z'	1
□$_{min}$/°	1.935
□$_{max}$/°	31.984
Measured Refl.	24439
Independent Refl.	4330
Reflections Used	3840
R_{int}	0.0320
Parameters	172
Restraints	0
Largest Peak	0.460
Deepest Hole	-0.225
GooF	1.019
wR_2 (all data)	0.0798
wR_2	0.0770
R_1 (all data)	0.0346
R_1	0.0298



Experimental. Single clear colourless slab-shaped crystals of (**18**) were obtained by recrystallisation from ethyl acetate. A suitable crystal (0.20 × 0.16 × 0.03 mm^3) was selected and mounted on a MITIGEN holder in perfluoroether oil a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the ShelXT (Sheldrick, 2008) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{19}H_{21}NO_3S_2$, M_r = 375.49, orthorhombic, Pbca (No. 61), a = 9.13571(13) Å, b = 13.38135(18) Å, c = 30.0335(4) Å, □ = □ = □ = 90 °, V = 3671.54(9) $Å^3$, T = 100(2) K, Z = 8, Z' = 1, □ ($MoK_□$) = 0.308, 40740 reflections measured, 6097 unique (R_{int} = 0.0232) which were used in all calculations. The final wR_2 was 0.0815 (all data) and R_1 was 0.0296 (I > 2(I)).

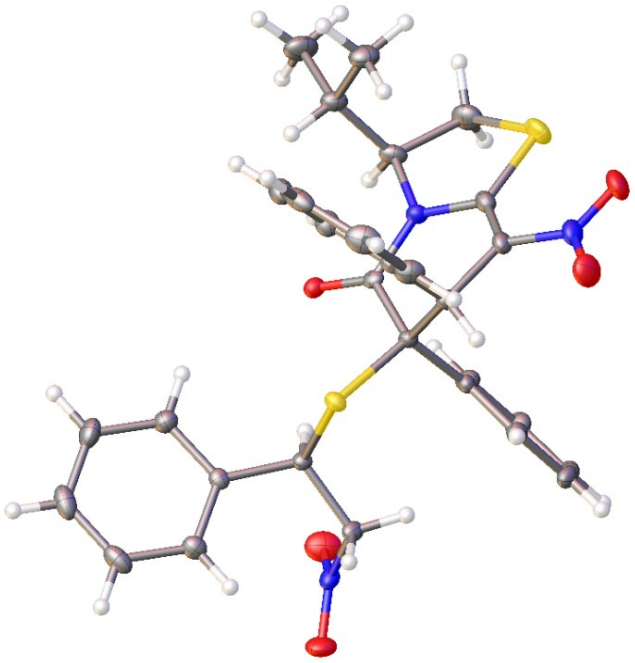
Compound	**2014acc0006**
Formula	$C_{19}H_{21}NO_3S_2$
$D_{calc.}$/ g cm^{-3}	1.359
□/mm^{-1}	0.308
Formula Weight	375.49
Colour	clear colourless
Shape	slab
Max Size/mm	0.20
Mid Size/mm	0.16
Min Size/mm	0.03
T/K	100(2)
Crystal System	orthorhombic
Space Group	Pbca
a/Å	9.13571(13)
b/Å	13.38135(18)
c/Å	30.0335(4)
□/°	90
□/°	90
□/°	90
V/Å^3	3671.54(9)
Z	8
Z'	1
□$_{min}$/°	2.713
□$_{max}$/°	31.963
Measured Refl.	40740
Independent Refl.	6097
Reflections Used	5697
R_{int}	0.0232
Parameters	228
Restraints	0
Largest Peak	0.550
Deepest Hole	-0.226
GooF	1.042
wR_2 (all data)	0.0815
wR_2	0.0798
R_1 (all data)	0.0323
R_1	0.0296



Experimental. Single clear colourless rod-shaped crystals of (**21**) were obtained by recrystallisation from diethyl ether. A suitable crystal (0.22 × 0.06 × 0.05 mm^3) was selected and mounted on a MITIGEN holder in perfluoroether oil a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the ShelXT (Sheldrick, 2008) structure solution program, using the Direct Methods solution method. The model was refined with version of **ShelXL** (Sheldrick, 2008) using Least Squares minimisation.

Crystal Data. $C_{24}H_{22}N_2O_3S_2$, M_r = 450.55, monoclinic, $P2_1$ (No. 4), a = 14.3941(2) Å, b = 6.92520(11) Å, c = 21.6163(4) Å, □ = 94.3263(15)°, □ = □ = 90°, V = 2148.62(6) $Å^3$, T = 100(2) K, Z = 4, Z' = 2, □ ($MoK_□$) = 0.277, 26689 reflections measured, 9824 unique (R_{int} = 0.0179) which were used in all calculations. The final wR_2 was 0.0657 (all data) and R_1 was 0.0253 (I > 2(I)).

Compound	**21**
Formula	$C_{17}H_{17}NO_5S_2$
$D_{calc.}$/ g cm^{-3}	1.495
□/mm^{-1}	0.345
Formula Weight	379.43
Colour	clear colourless
Shape	block
Max Size/mm	0.62
Mid Size/mm	0.50
Min Size/mm	0.25
T/K	120
Crystal System	orthorhombic
Flack Parameter	0.030(12)
Hooft Parameter	0.038(17)
Space Group	$P2_12_12_1$
a/Å	5.84070(10)
b/Å	14.9477(4)
c/Å	19.3104(6)
□/°	90
□/°	90
□/°	90
V/Å^3	1685.90(7)
Z	4
Z'	1
□$_{min}$/°	2.923
□$_{max}$/°	28.695
Measured Refl.	21760
Independent Refl.	4321
Reflections Used	4287
R_{int}	0.0300
Parameters	228
Restraints	0
Largest Peak	0.301
Deepest Hole	-0.201
GooF	1.112
wR_2 (all data)	0.0602
wR_2	0.0600
R_1 (all data)	0.0228
R_1	0.0226



Experimental. Single clear colourless prism-shaped crystals of (**25**) were recrystallised from methanol by slow evaporation. A suitable crystal (0.30×0.20×0.20) mm^3 was selected and mounted on a MITIGEN holder silicon oil on a Rigaku AFC12 FRE-HF diffractometer. The crystal was kept at T = 100(2) K during data collection. Using **Olex2** (Dolomanov et al., 2009), the structure was solved with the **ShelXT** (Sheldrick, 2015) structure solution program, using the Intrinsic Phasing solution method. The model was refined with version 2016/6 of **ShelXL** (Sheldrick, 2015) using Least Squares minimisation.

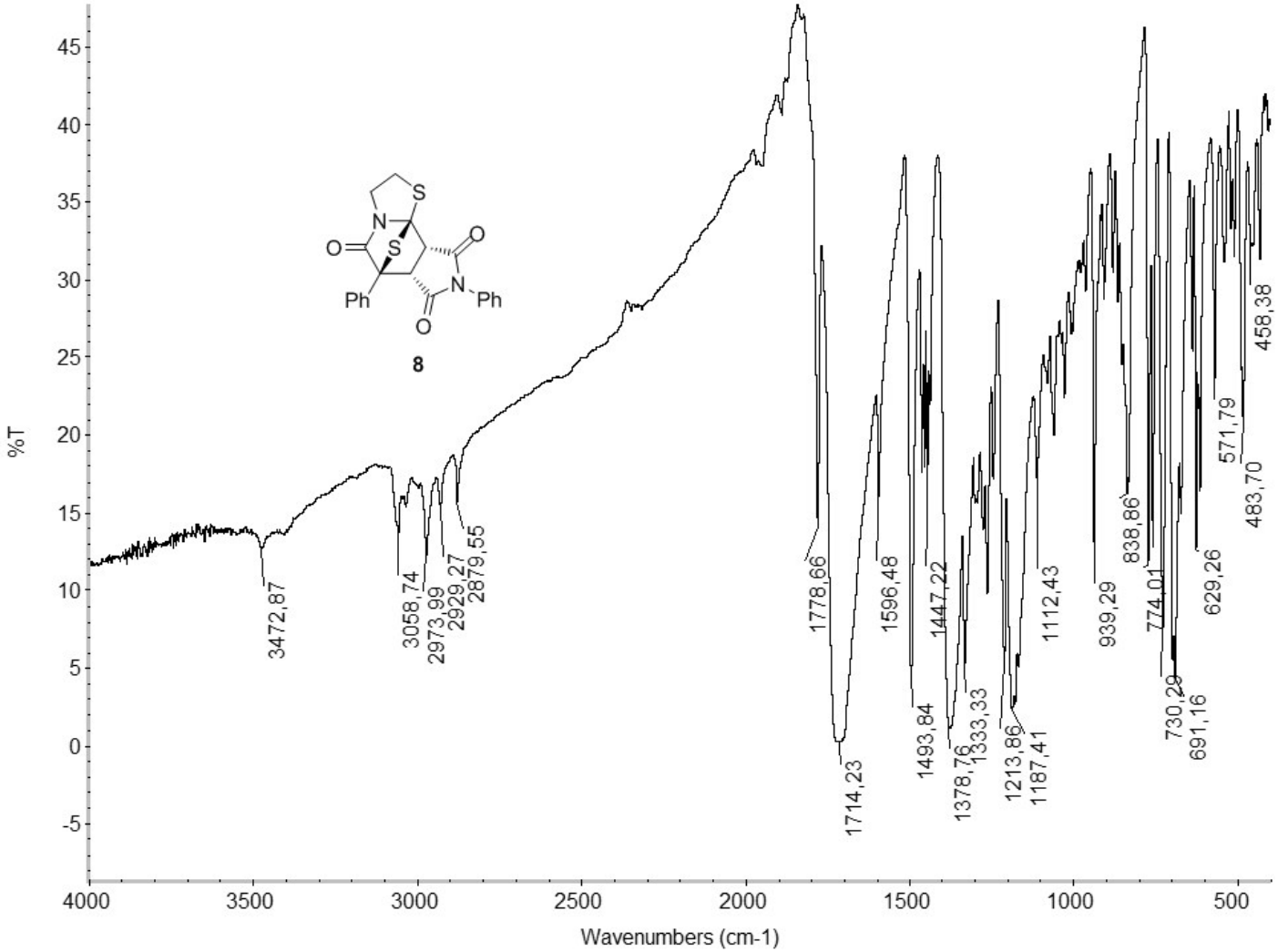
Crystal Data. $C_{30}H_{29}N_3O_5S_2$, M_r = 575.68, monoclinic, $P2_1$ (No. 4), a = 8.60010(10) Å, b = 17.1655(2) Å, c = 9.58080(10) Å, □ = 94.4730(10)°, □ = □ = 90°, V = 1410.06(3) $Å^3$, T = 100(2) K, Z = 2, Z' = 1, □(MoK□) = 0.234, 17745 reflections measured, 7251 unique (R_{int} = 0.0259) which were used in all calculations. The final wR_2 was 0.0704 (all data) and R_1 was 0.0310 (I > 2(I)).

Compound	**25**
Formula	$C_{30}H_{29}N_3O_5S_2$
$D_{calc.}$/ g cm^{-3}	1.356
□/mm^{-1}	0.234
Formula Weight	575.68
Colour	clear colourless
Shape	prism
Size/mm^3	0.30×0.20×0.20
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	-0.01(2)
Hooft Parameter	-0.01(2)
Space Group	$P2_1$
a/Å	8.60010(10)
b/Å	17.1655(2)
c/Å	9.58080(10)
□/°	90
□/°	94.4730(10)
□/°	90
V/Å^3	1410.06(3)
Z	2
Z'	1
Wavelength/Å	0.71073
Radiation type	MoK□
□$_{min}$/°	3.879
□$_{max}$/°	28.694
Measured Refl.	17745
Independent Refl.	7251
Reflections Used	7054
R_{int}	0.0259
Parameters	363
Restraints	1
Largest Peak	0.295
Deepest Hole	-0.163
GooF	1.042
wR_2 (all data)	0.0704
wR_2	0.0697
R_1 (all data)	0.0321
R_1	0.0310

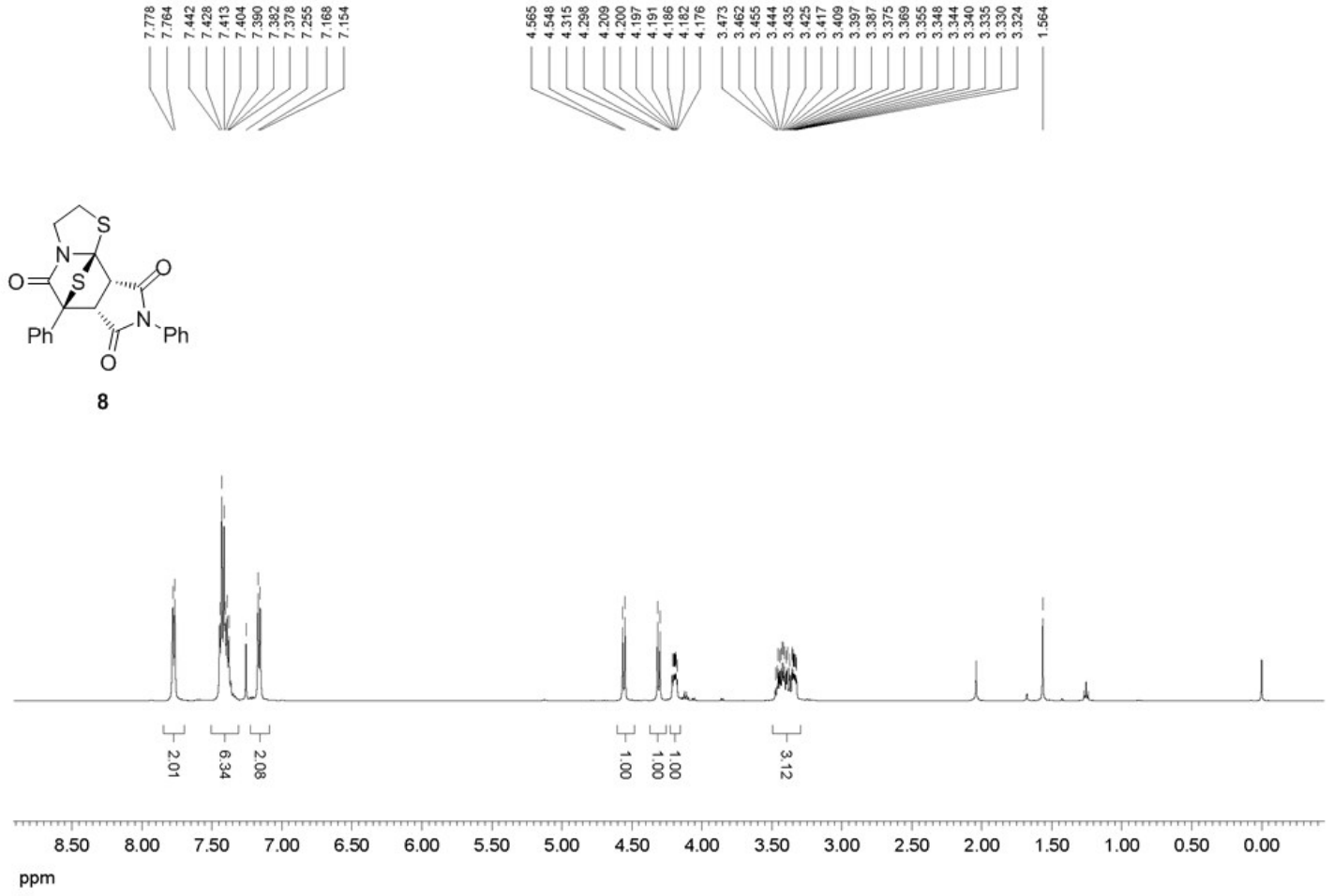
Copies of FT-IR, ^{1}H NMR and ^{13}C NMR spectra for all synthetic products.

All NMR data were recorded in $CDCl_3$ (500 MHz for ^{1}H and 125 MHz for ^{13}C).
All FT-IR spectra were registered in the 4000-6000 cm^{-1} range, in potassium bromide disks.

Compound **8**: FT-IR spectrum

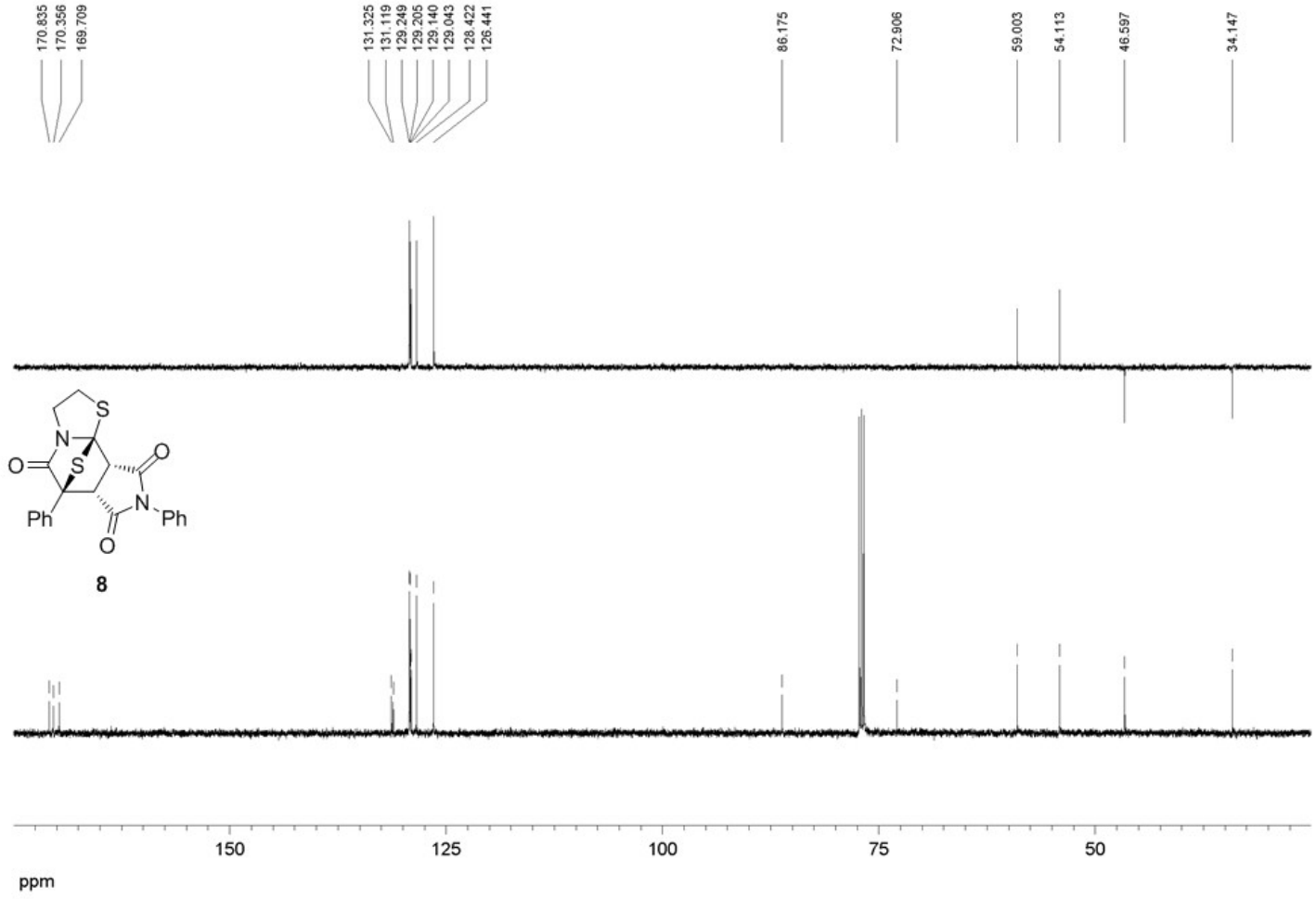


Compound **8**: ^{1}H NMR spectrum

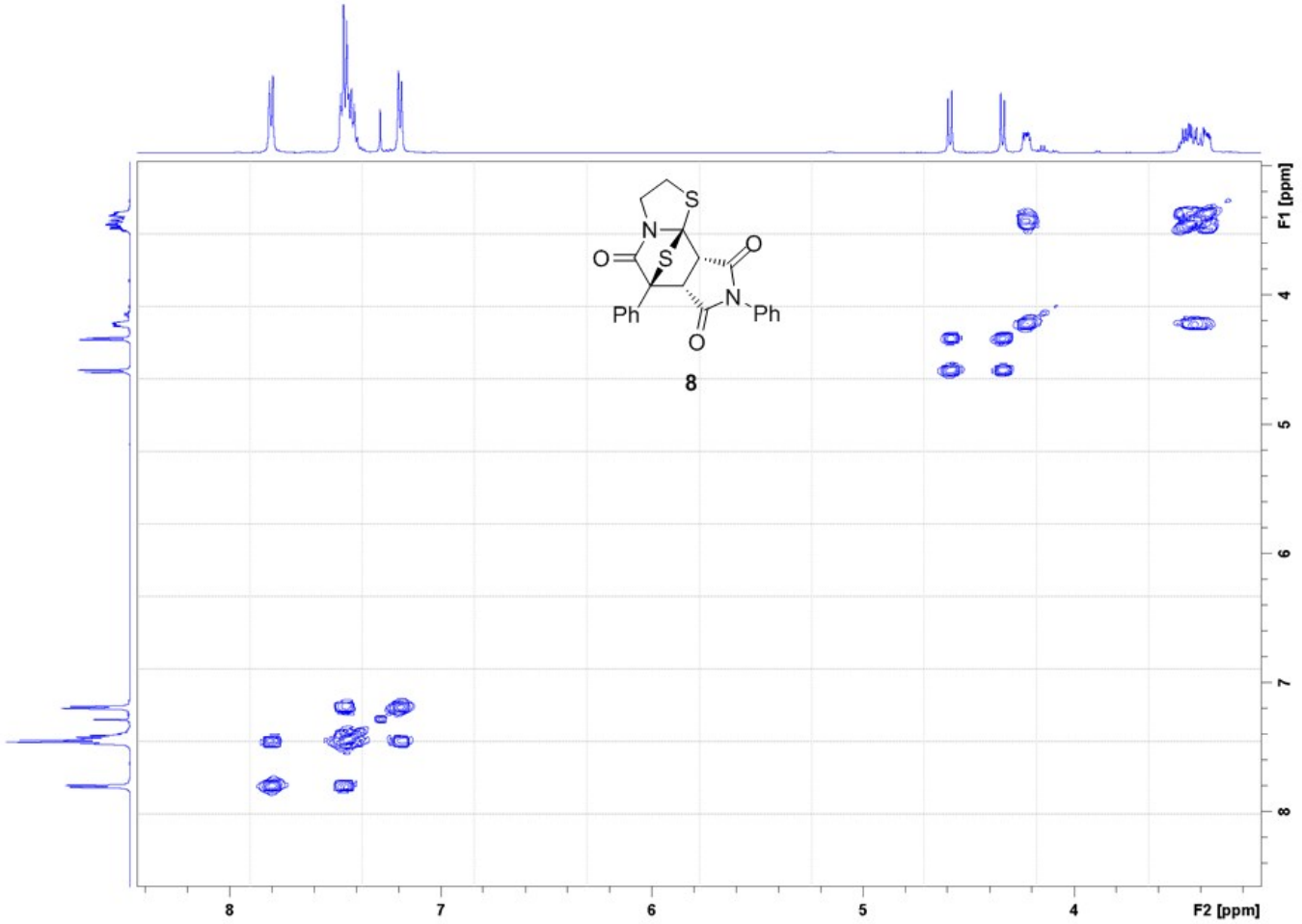


8

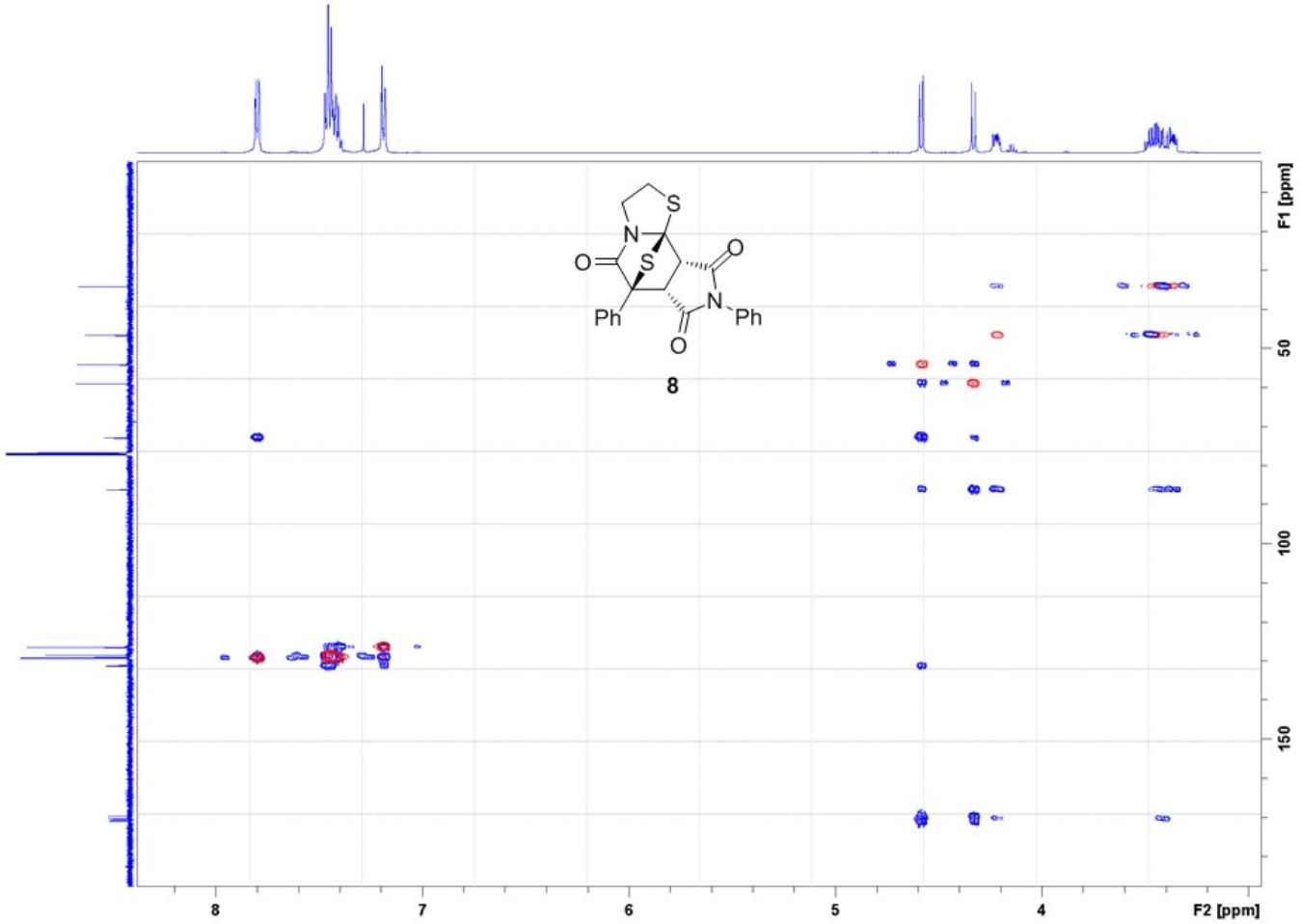
Compound **8**: ^{13}C NMR spectrum recorded in $CDCl_3$ at 125 MHz



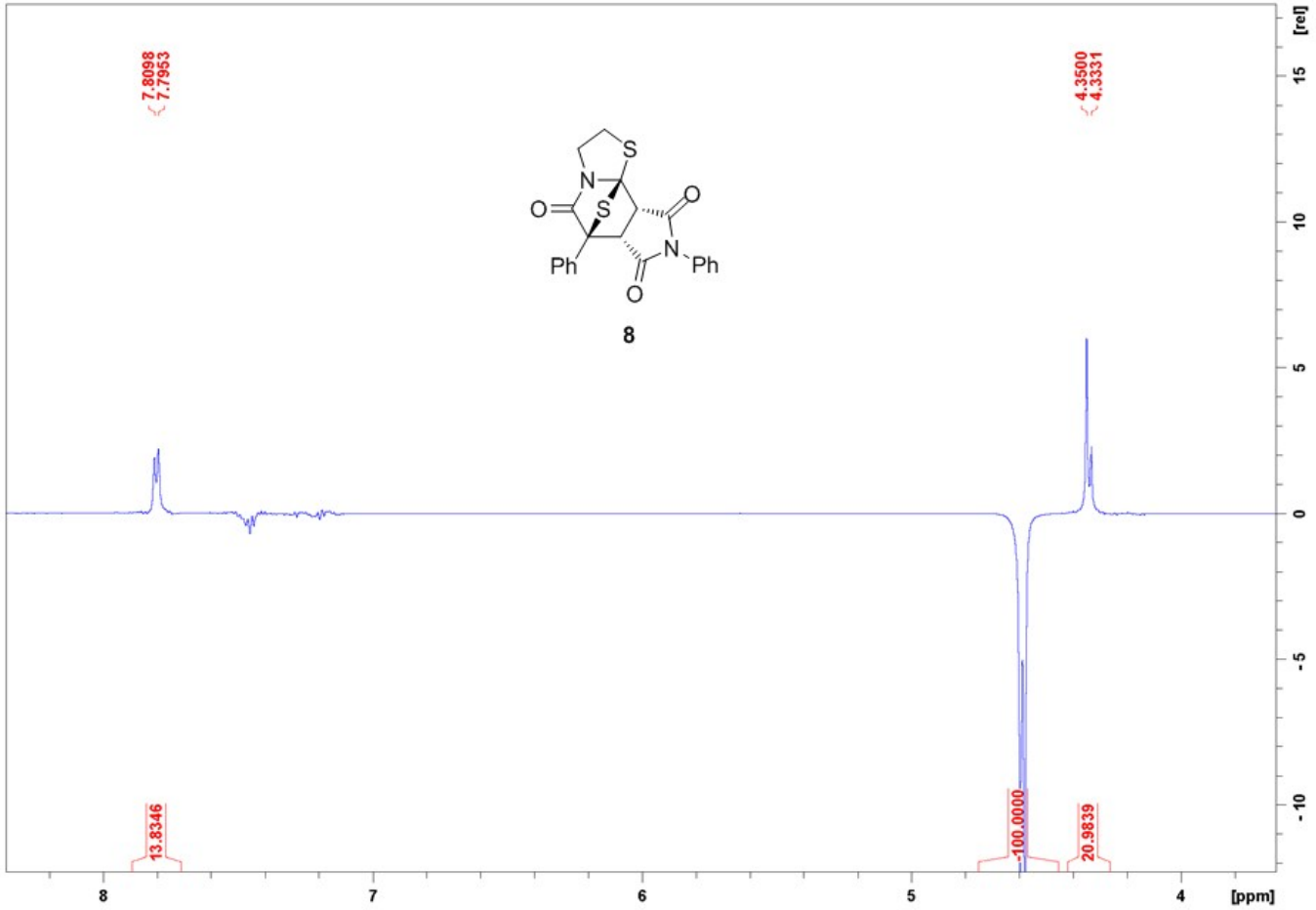
Compound **8**: COSY spectrum



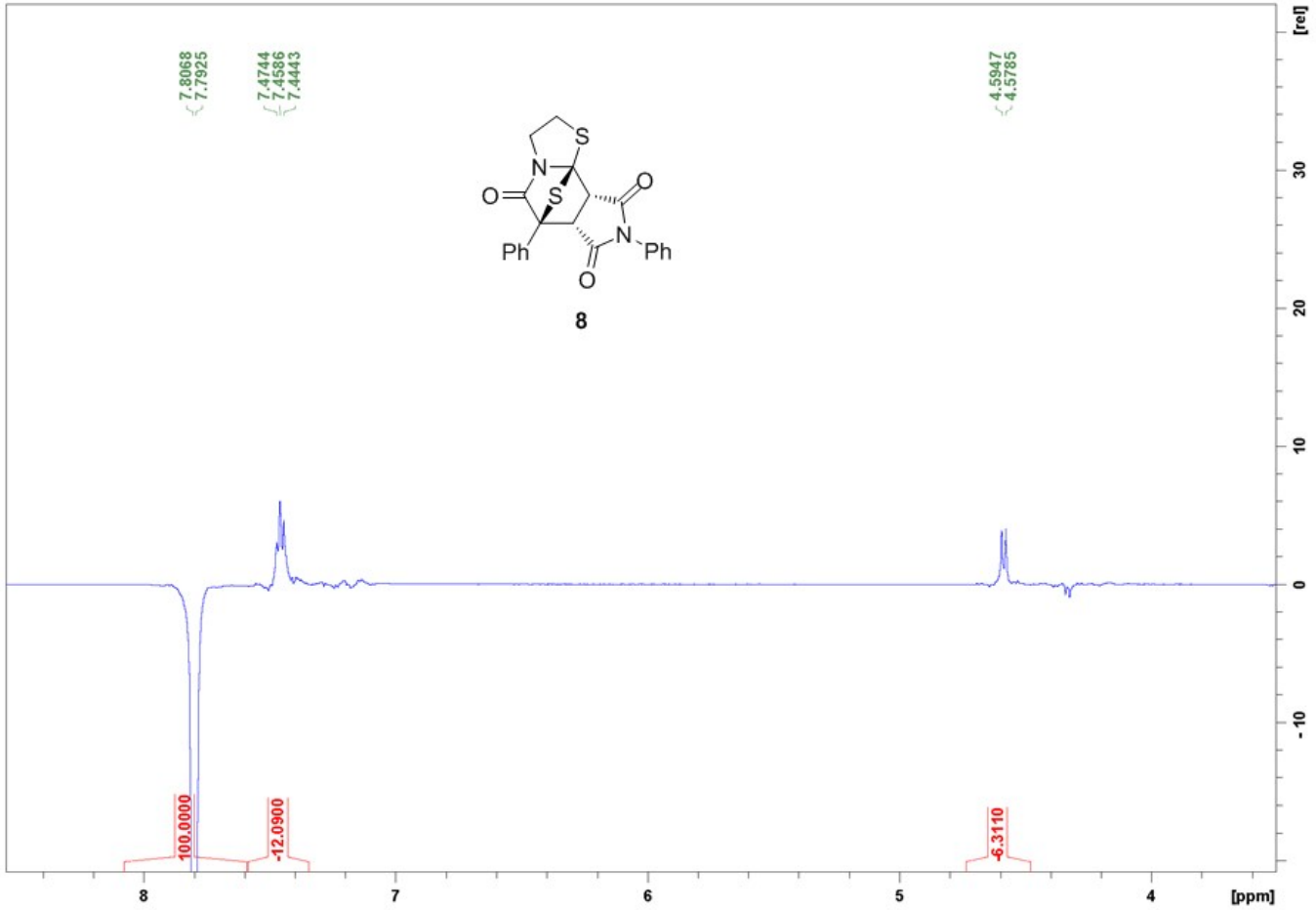
Compound **14**: HSQC and HMBC spectra



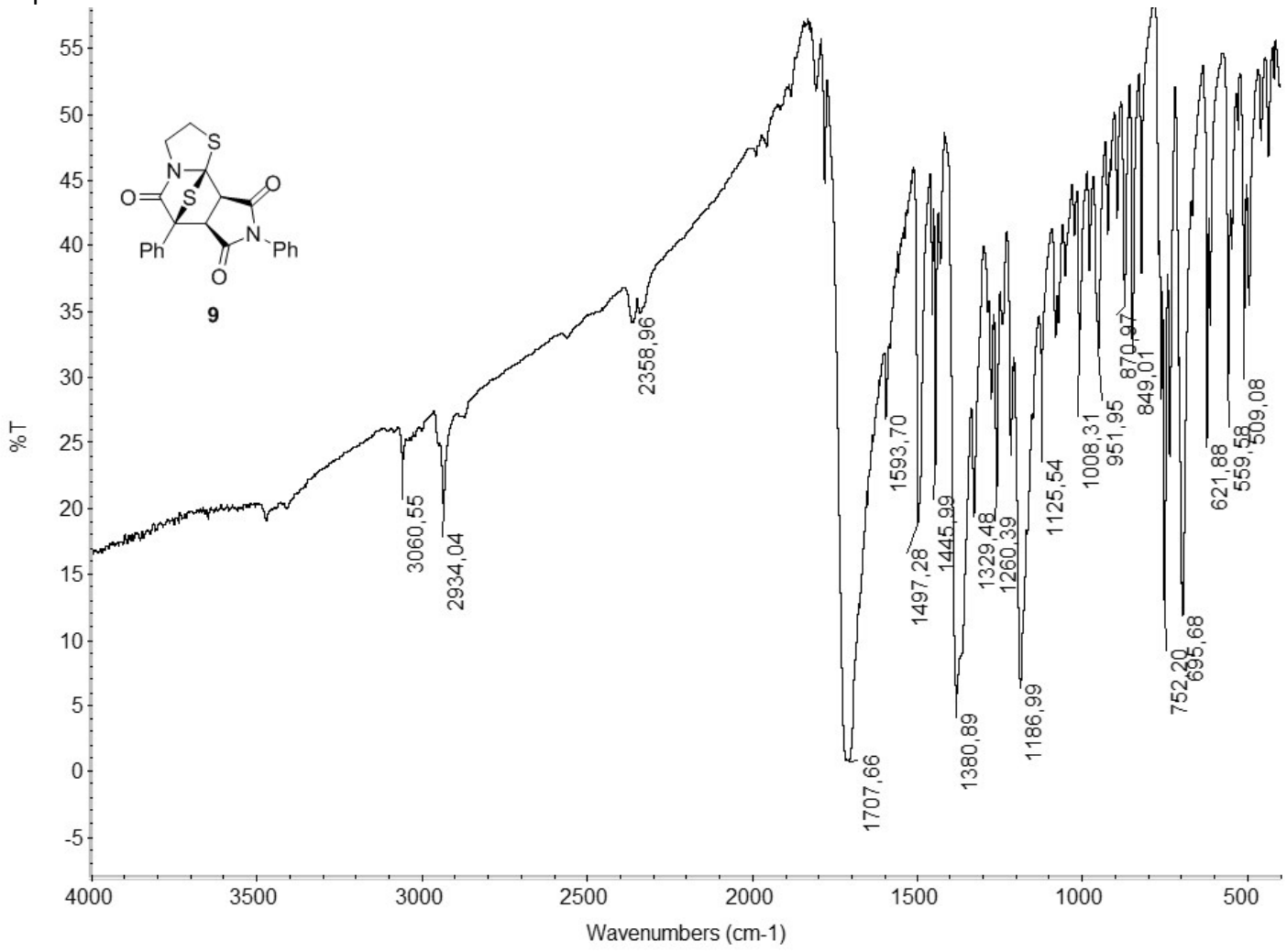
Compound **8**: NOE spectrum



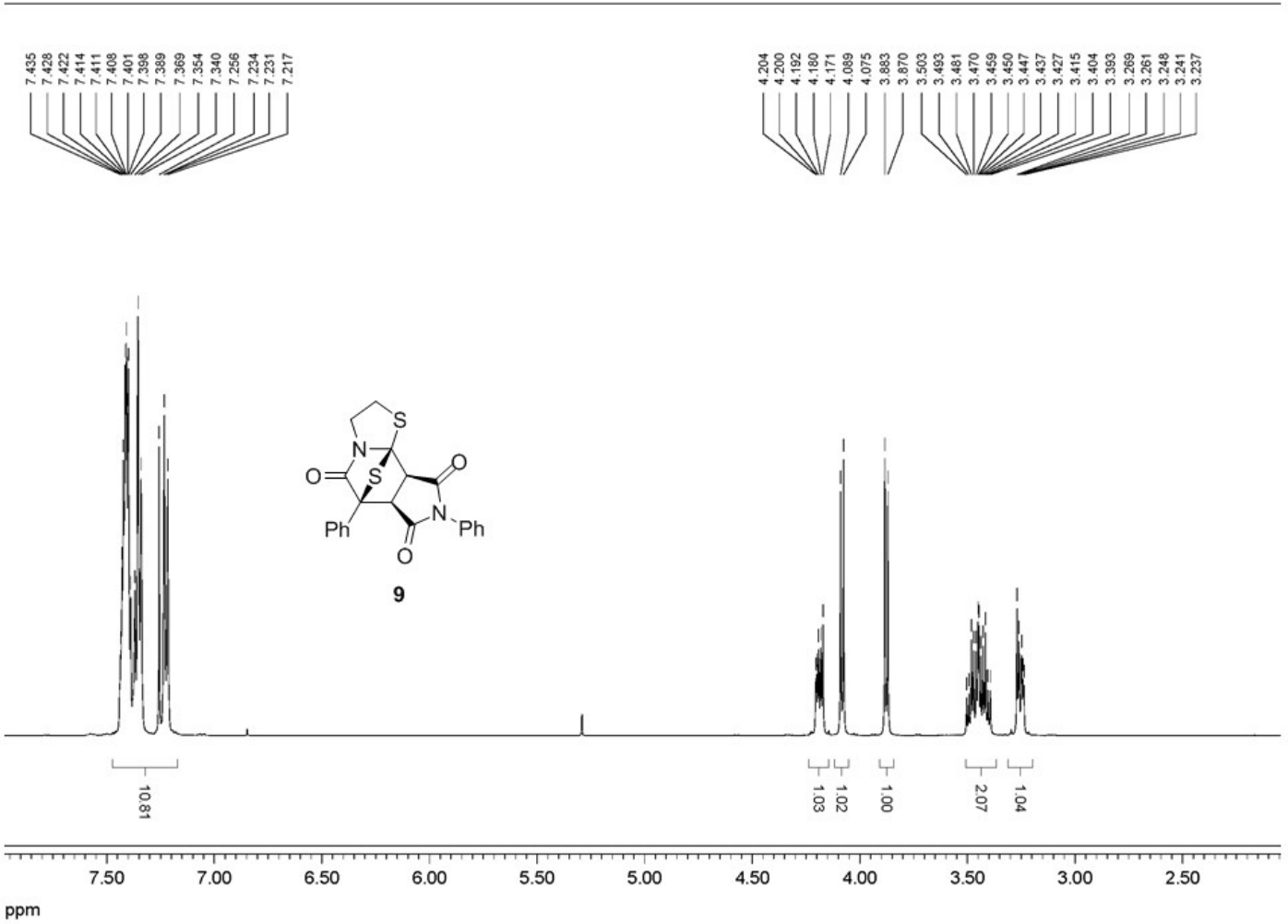
Compound **8**: NOE spectrum



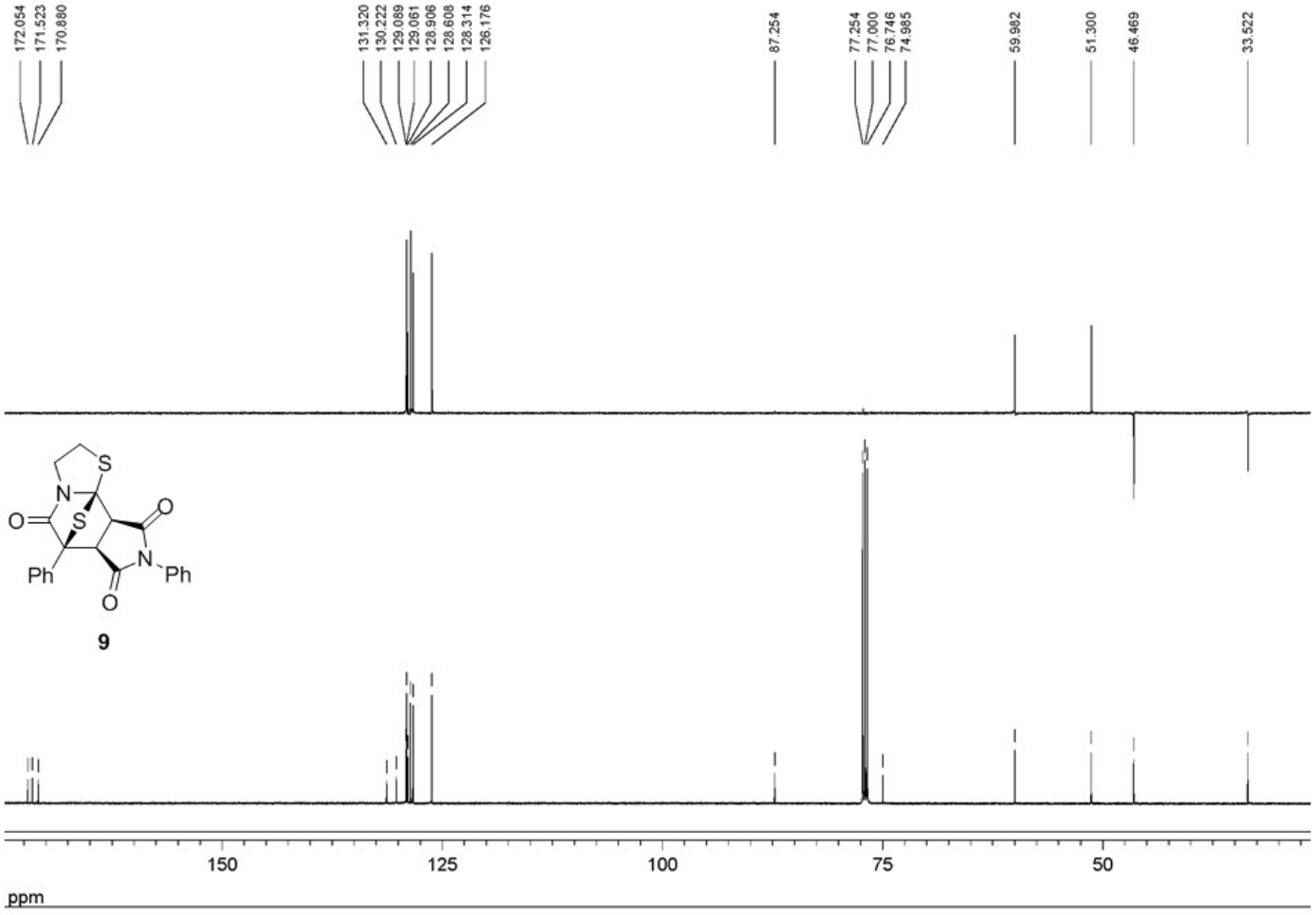
Compound **9**: FT-IR spectrum



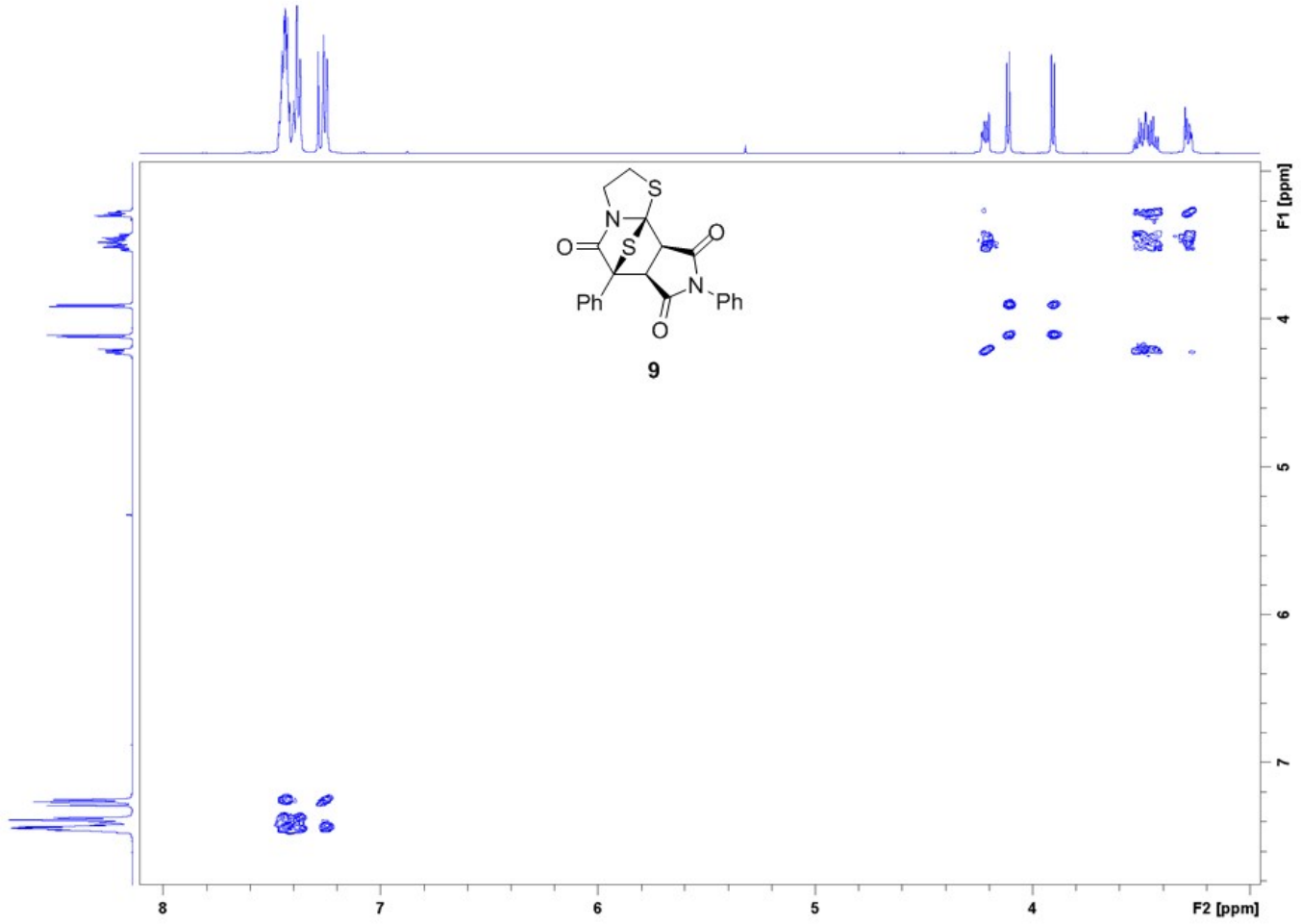
Compound **9**: ^{1}H NMR spectrum



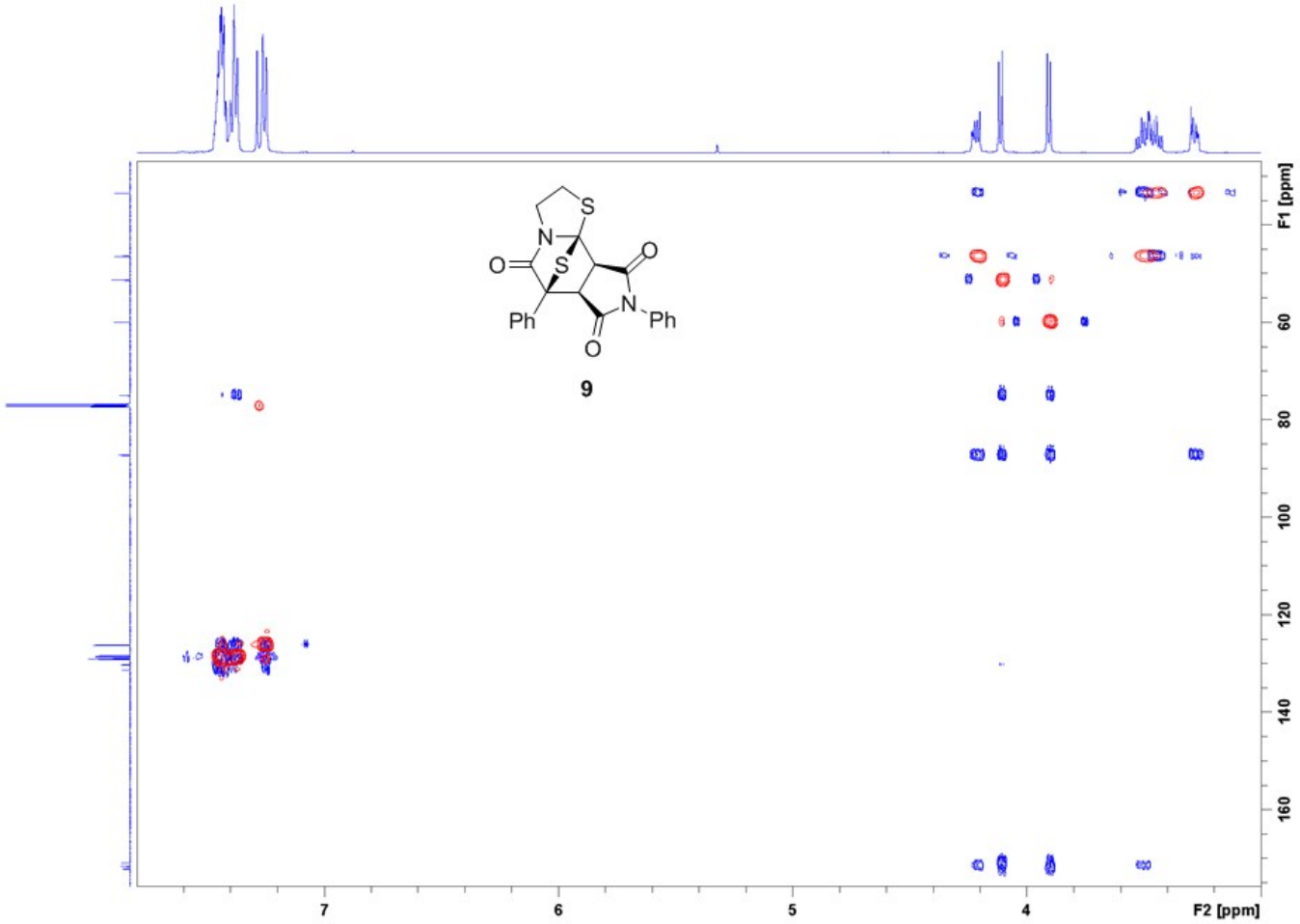
Compound **9**: ^{13}C NMR spectrum



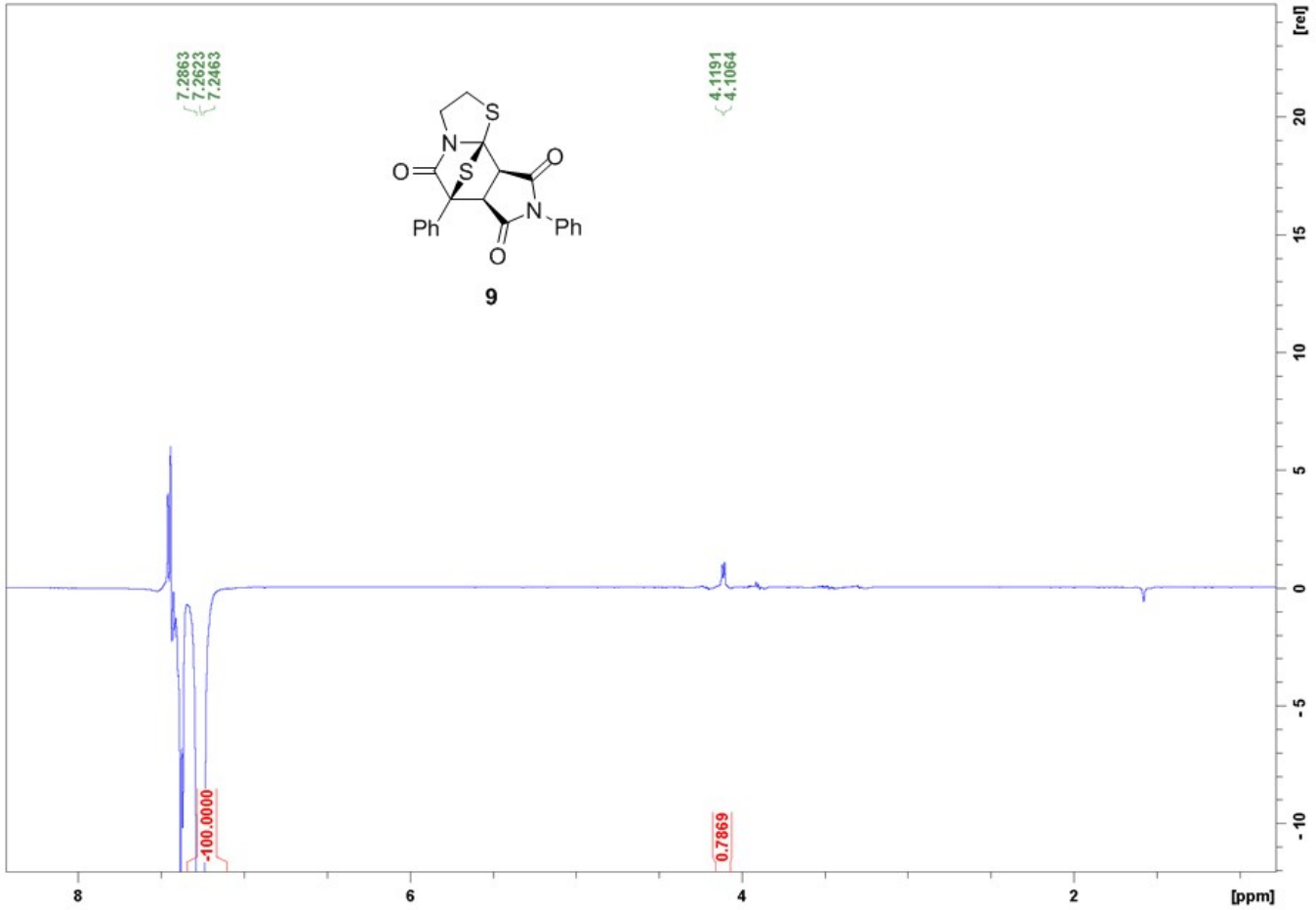
Compound **9**: COSY spectrum



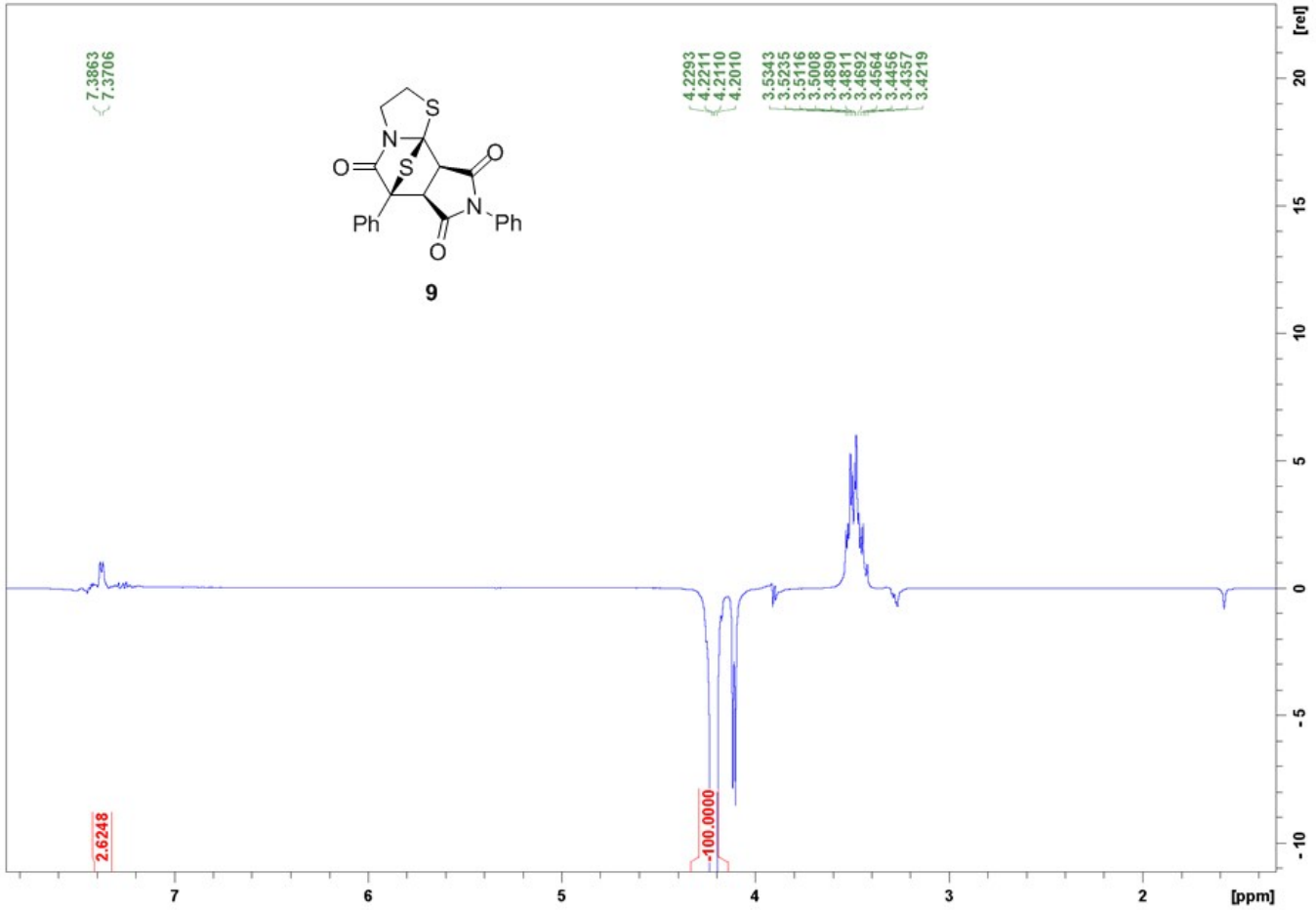
Compound **9**: HSQC and HMBC spectra



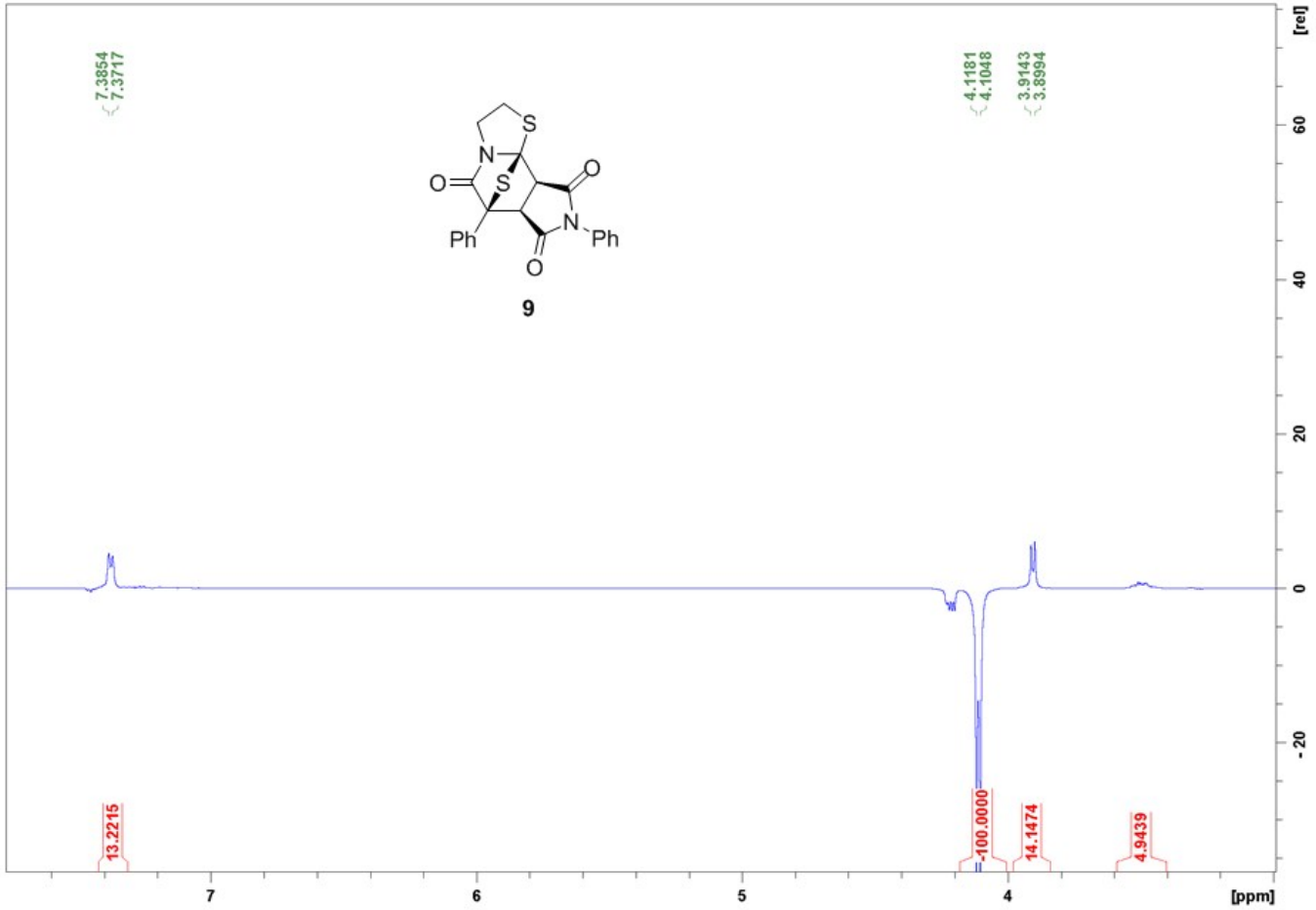
Compound **9**: NOE spectrum



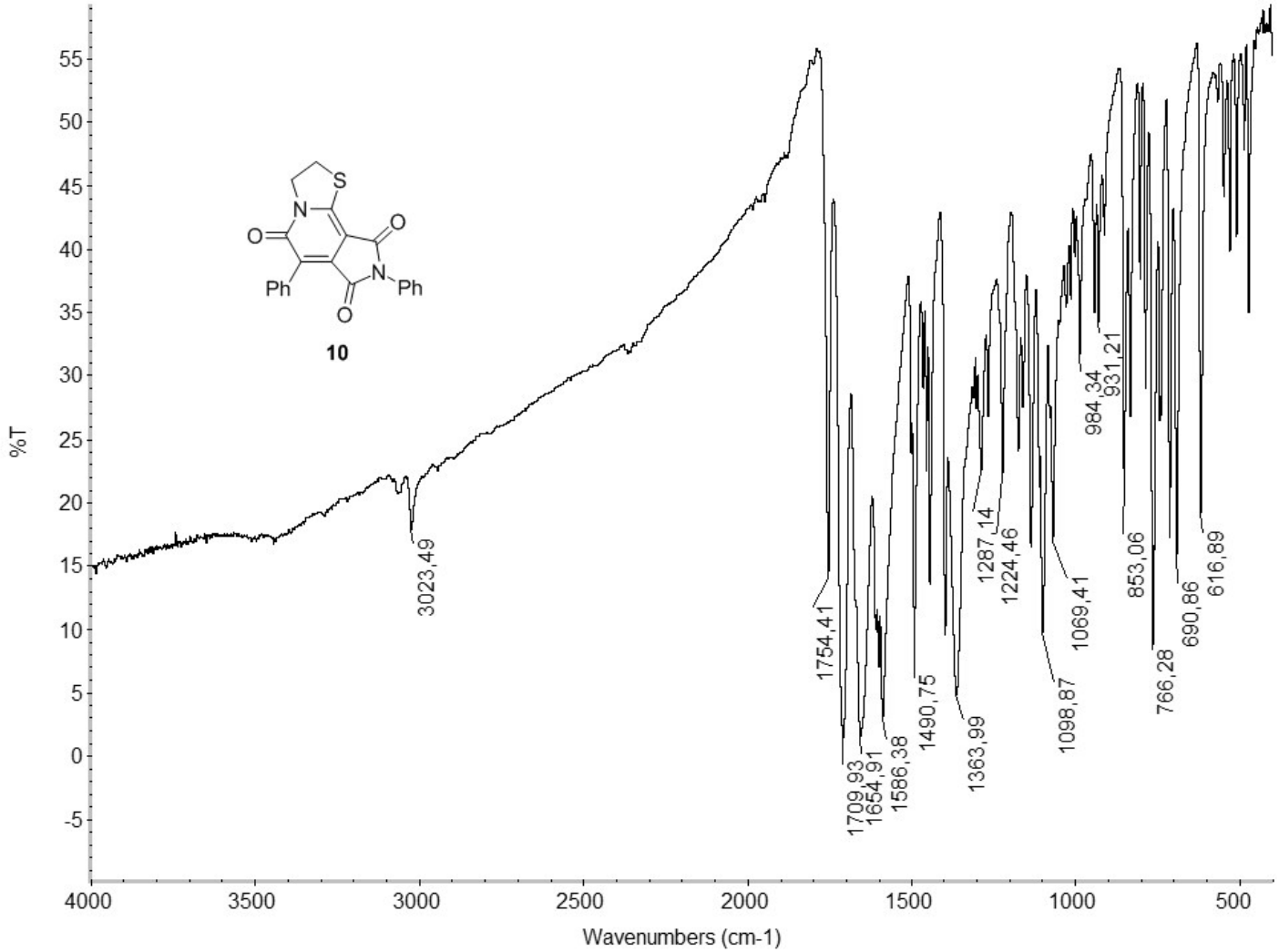
Compound **9**: NOE spectrum



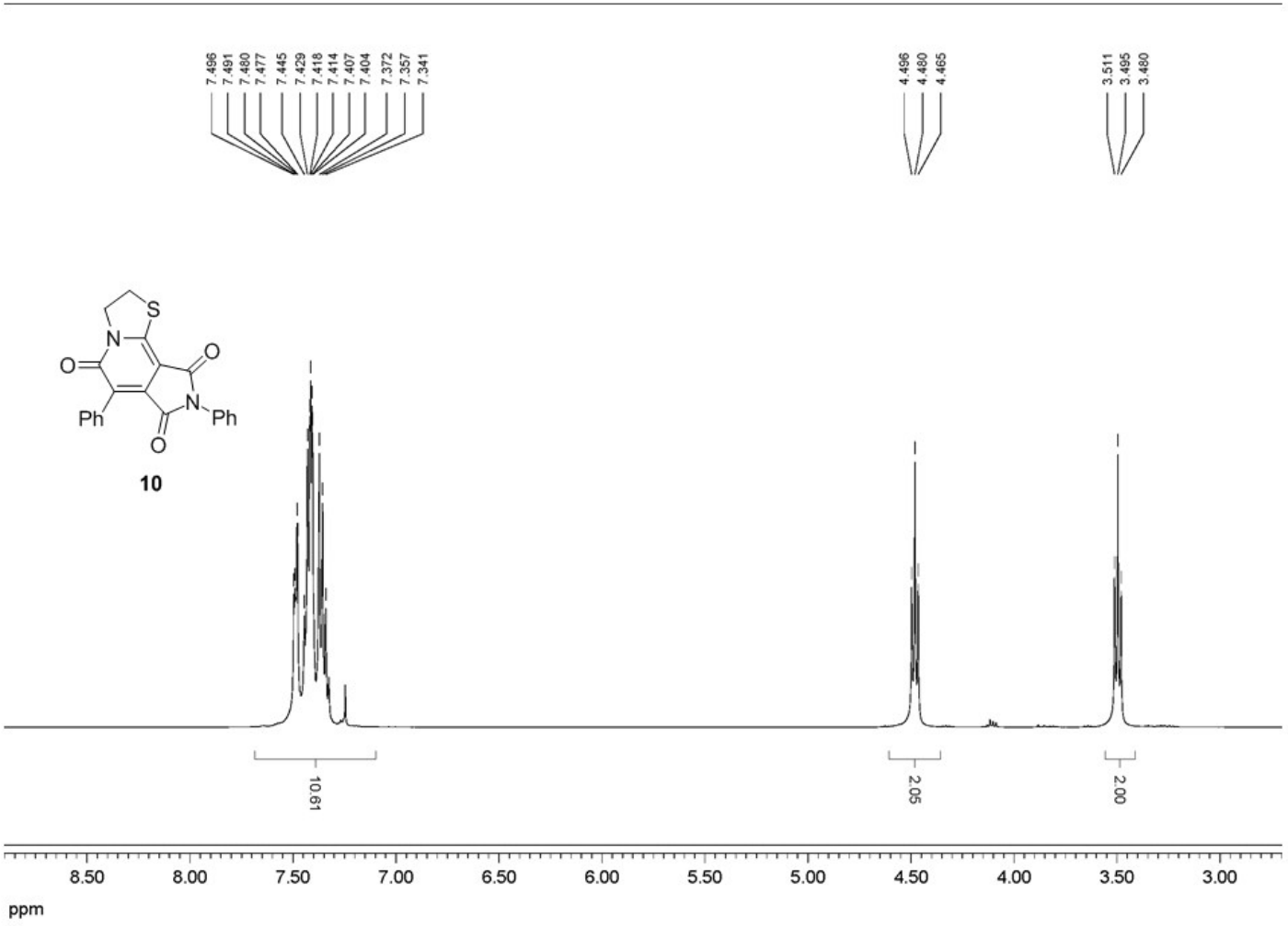
Compound **9**: NOE spectrum



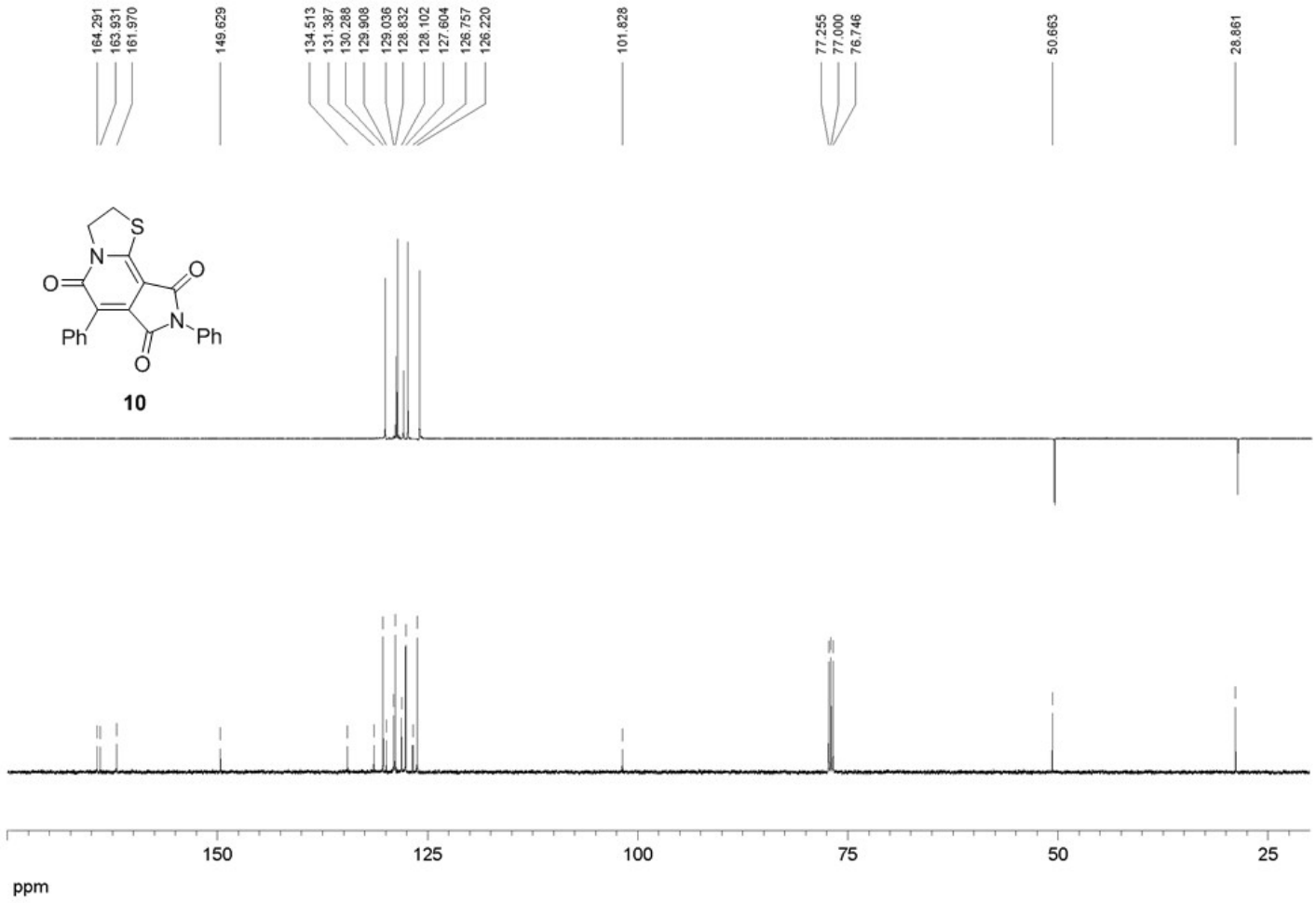
Compound **10**: FT-IR spectrum



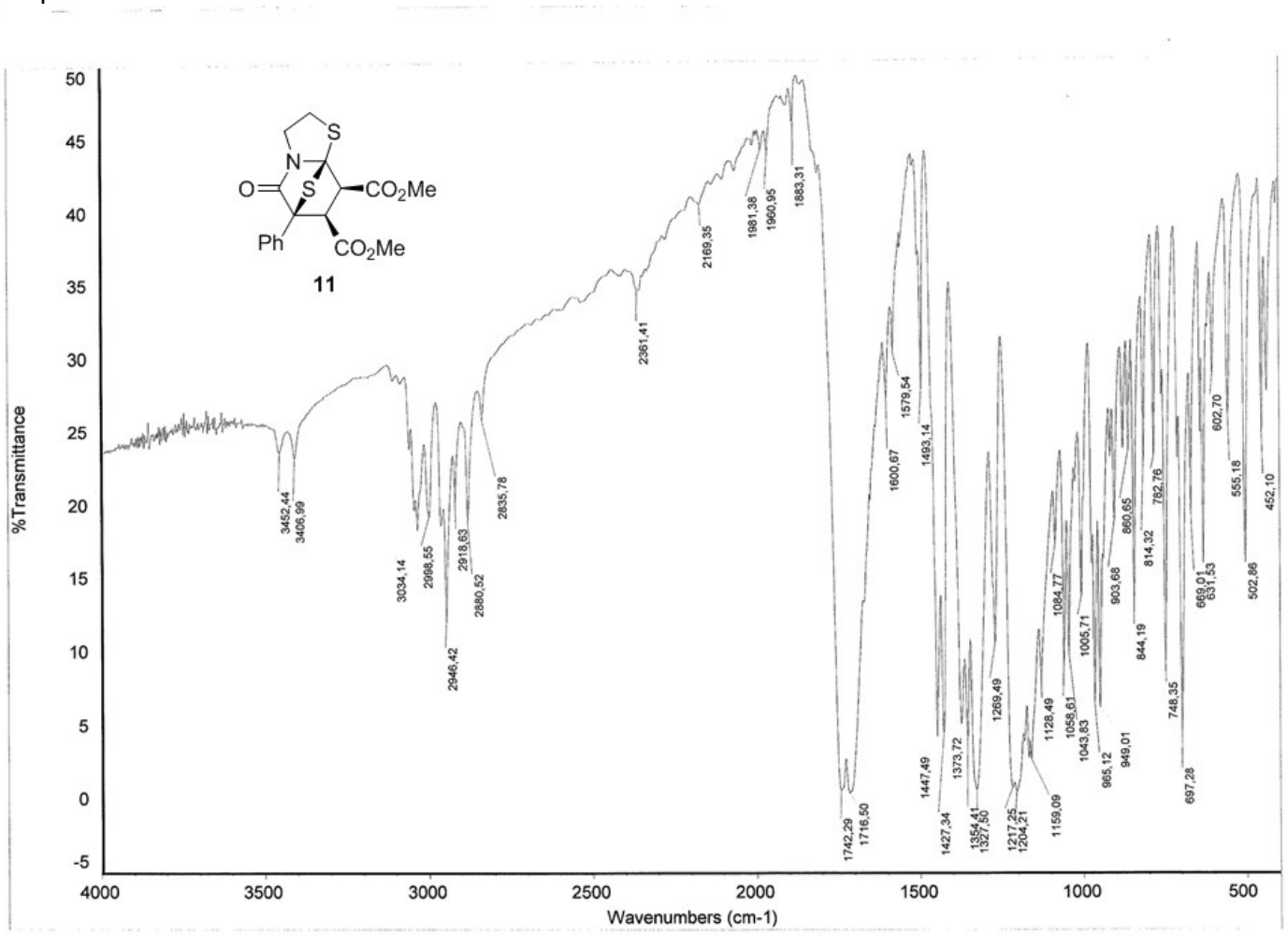
Compound **10**: ^{1}H NMR spectrum



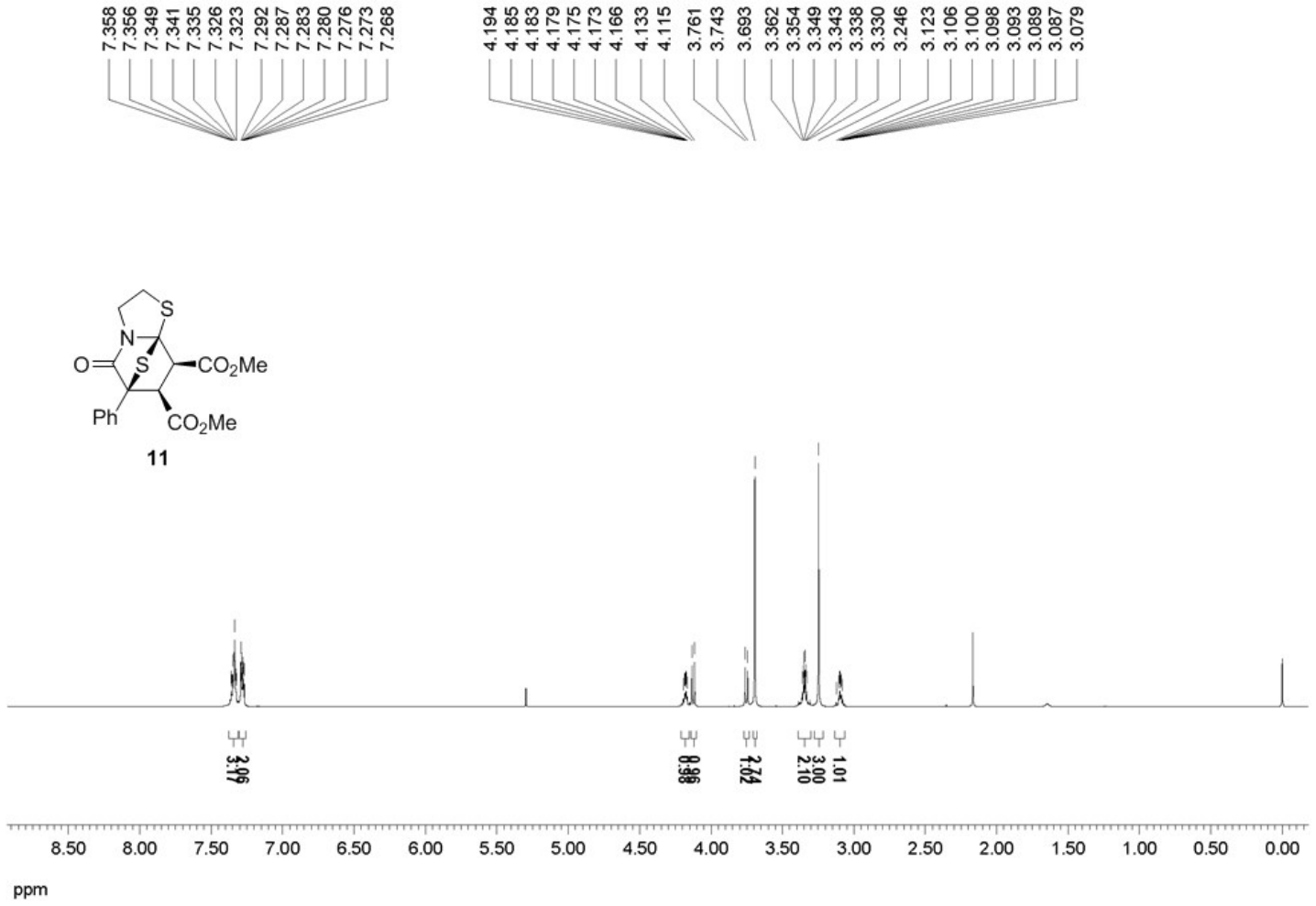
Compound **10**: ^{13}C NMR spectrum



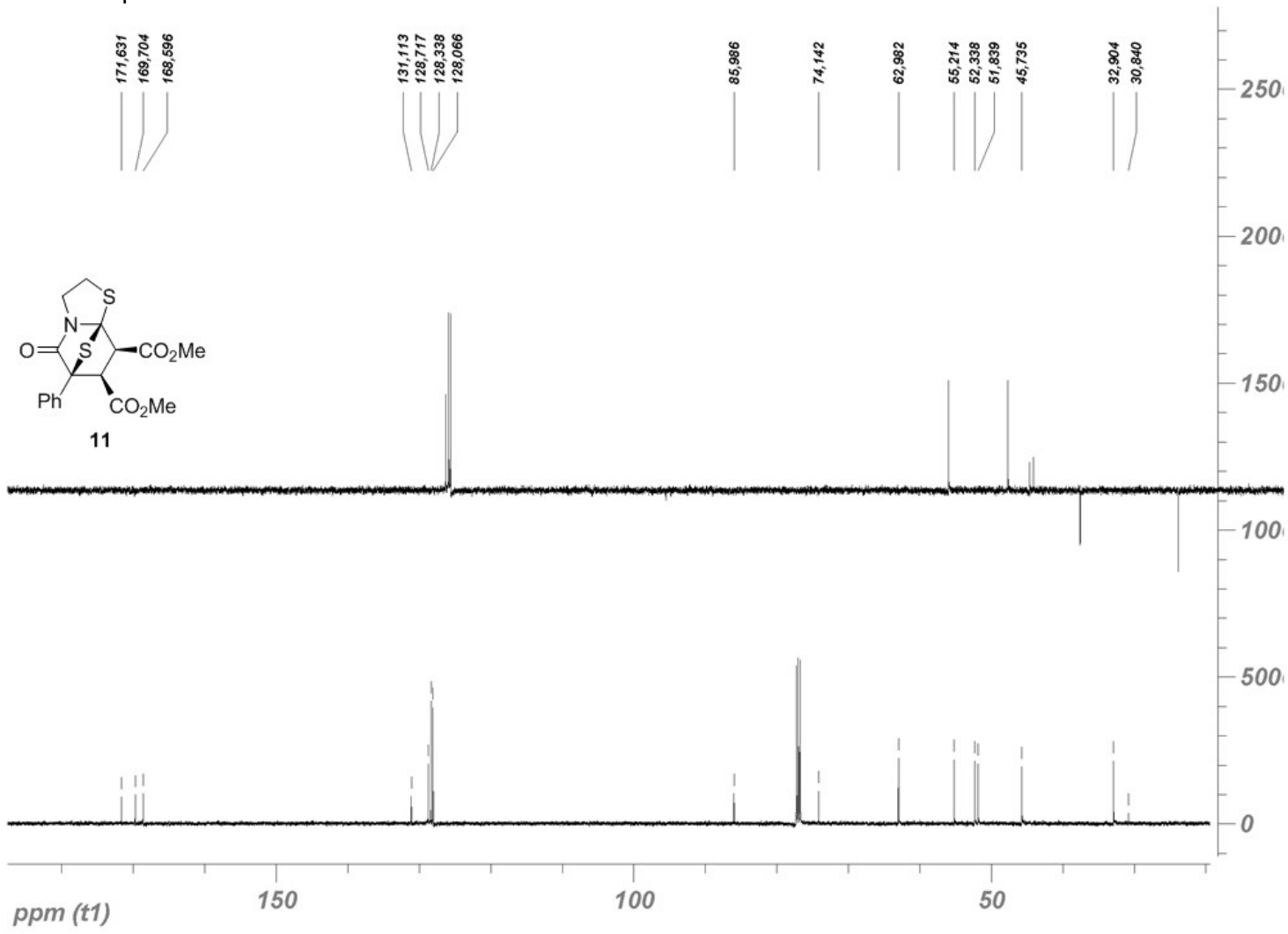
Compound **11**: FT-IR spectrum



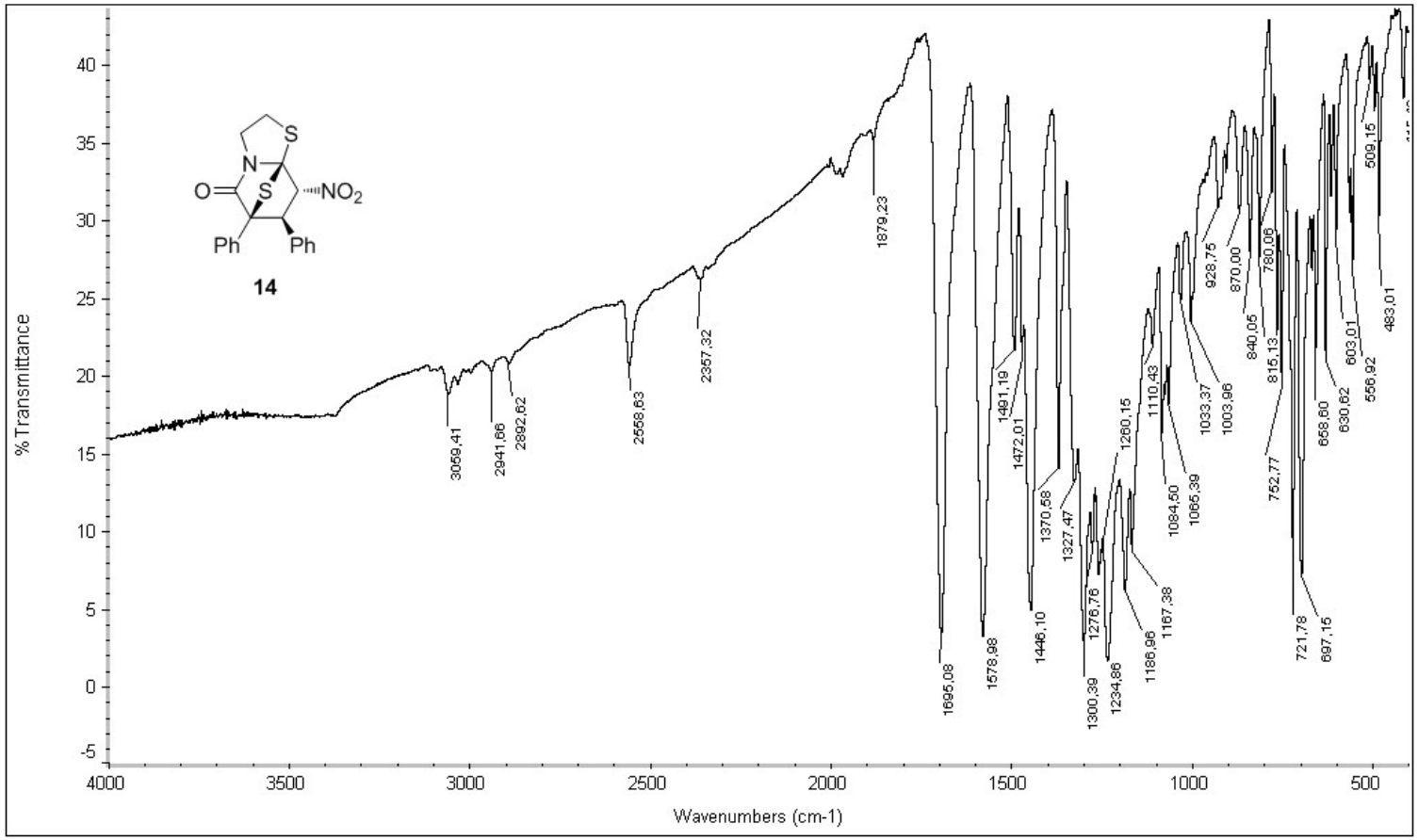
Compound **11**: ^{1}H NMR spectrum



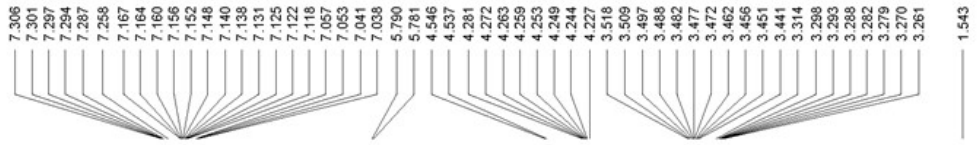
Compound **11**: ^{13}C NMR spectrum

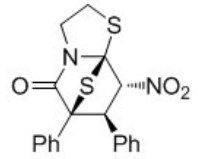


Compound **14**: FT-IR spectrum

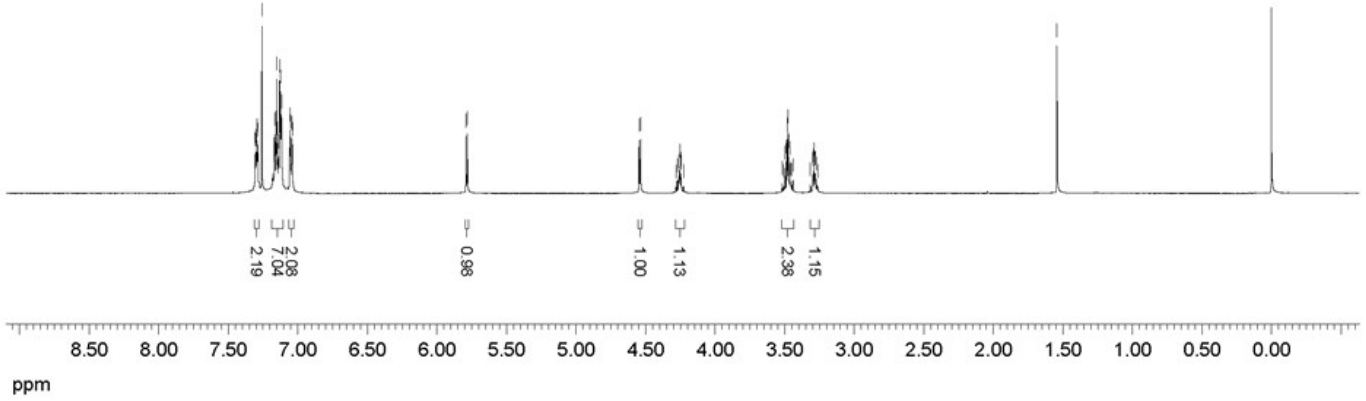


Compound **14**: ^{1}H NMR spectrum

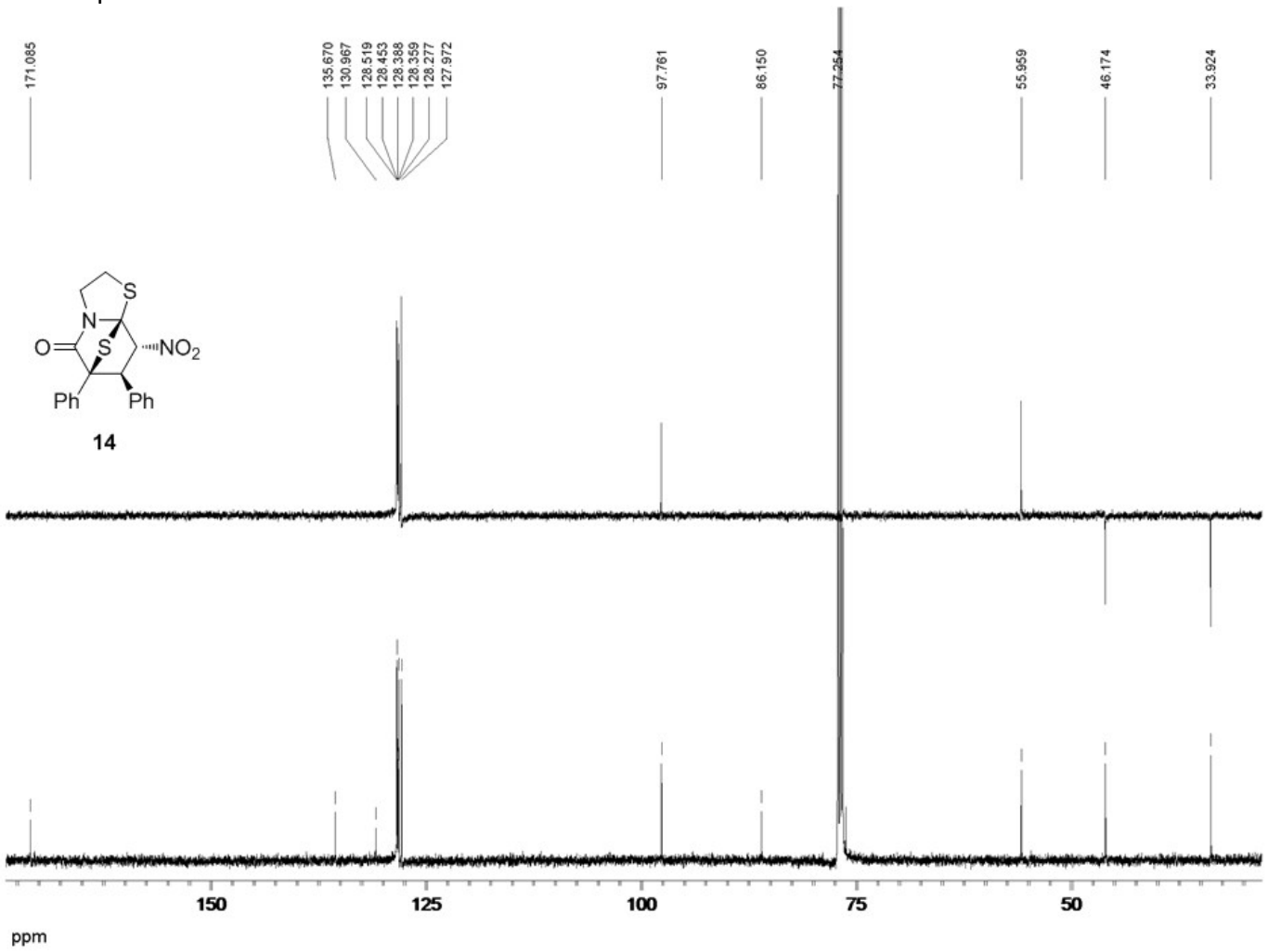




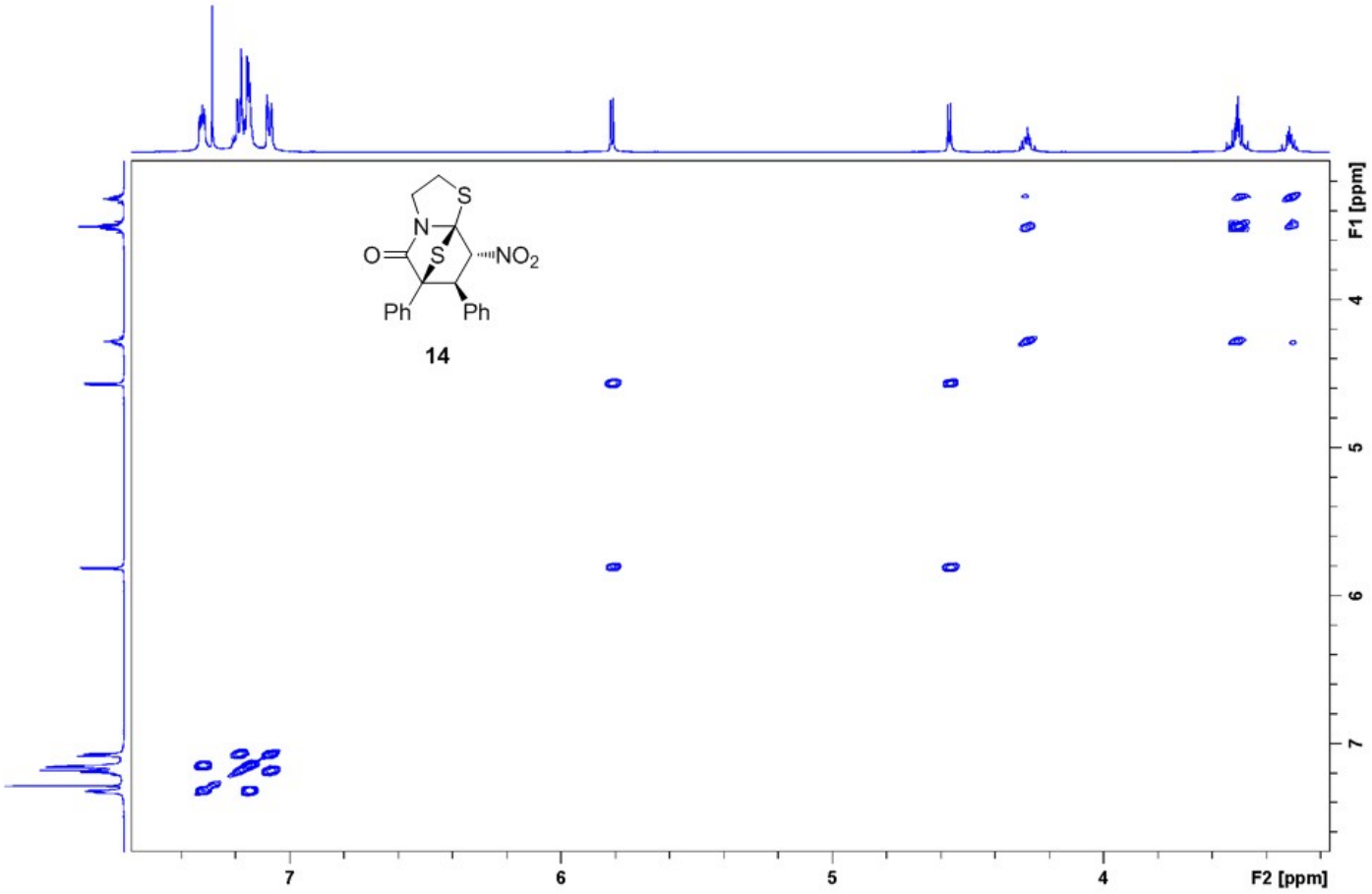
14



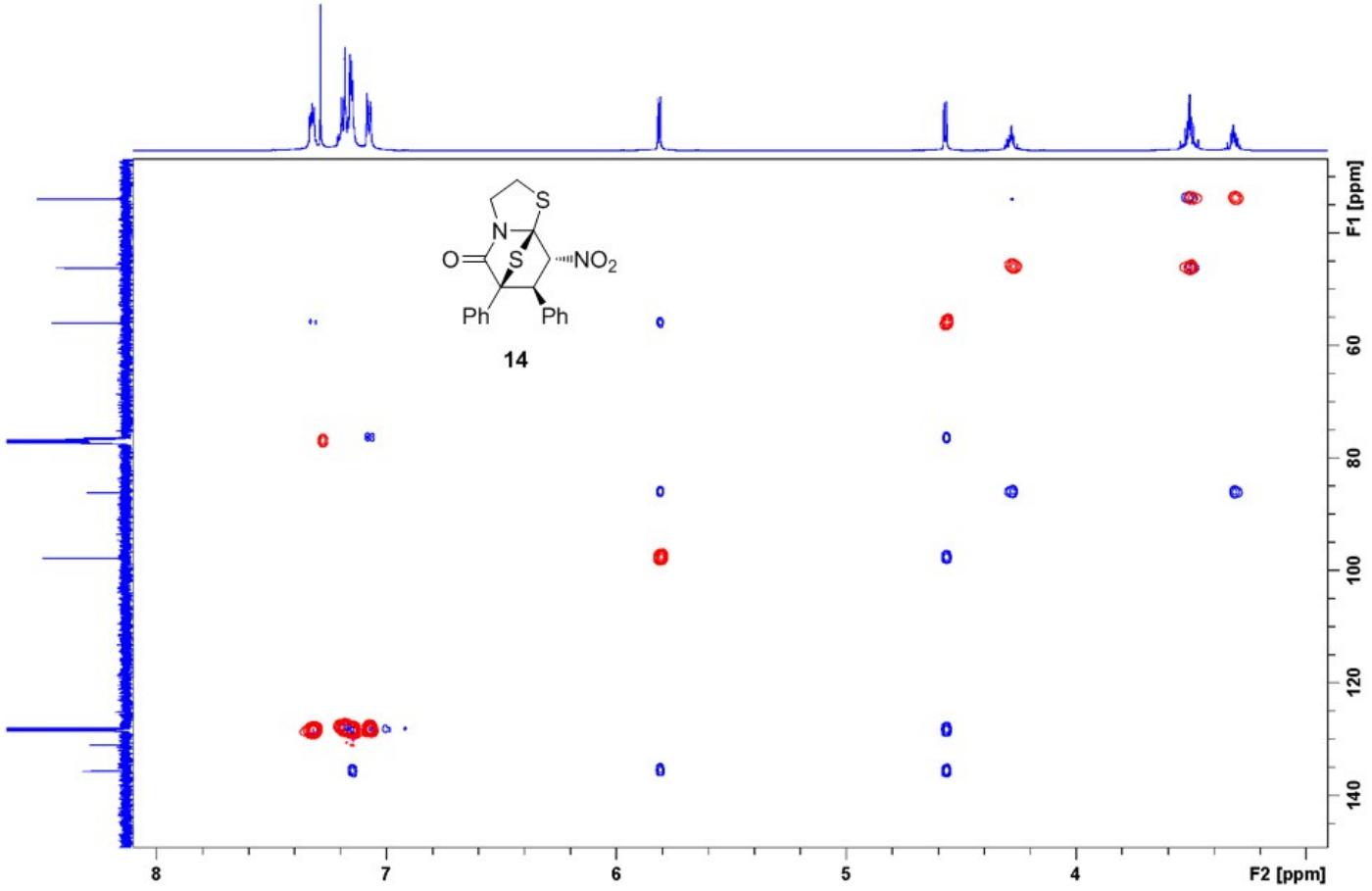
Compound **14**: ^{13}C NMR spectrum



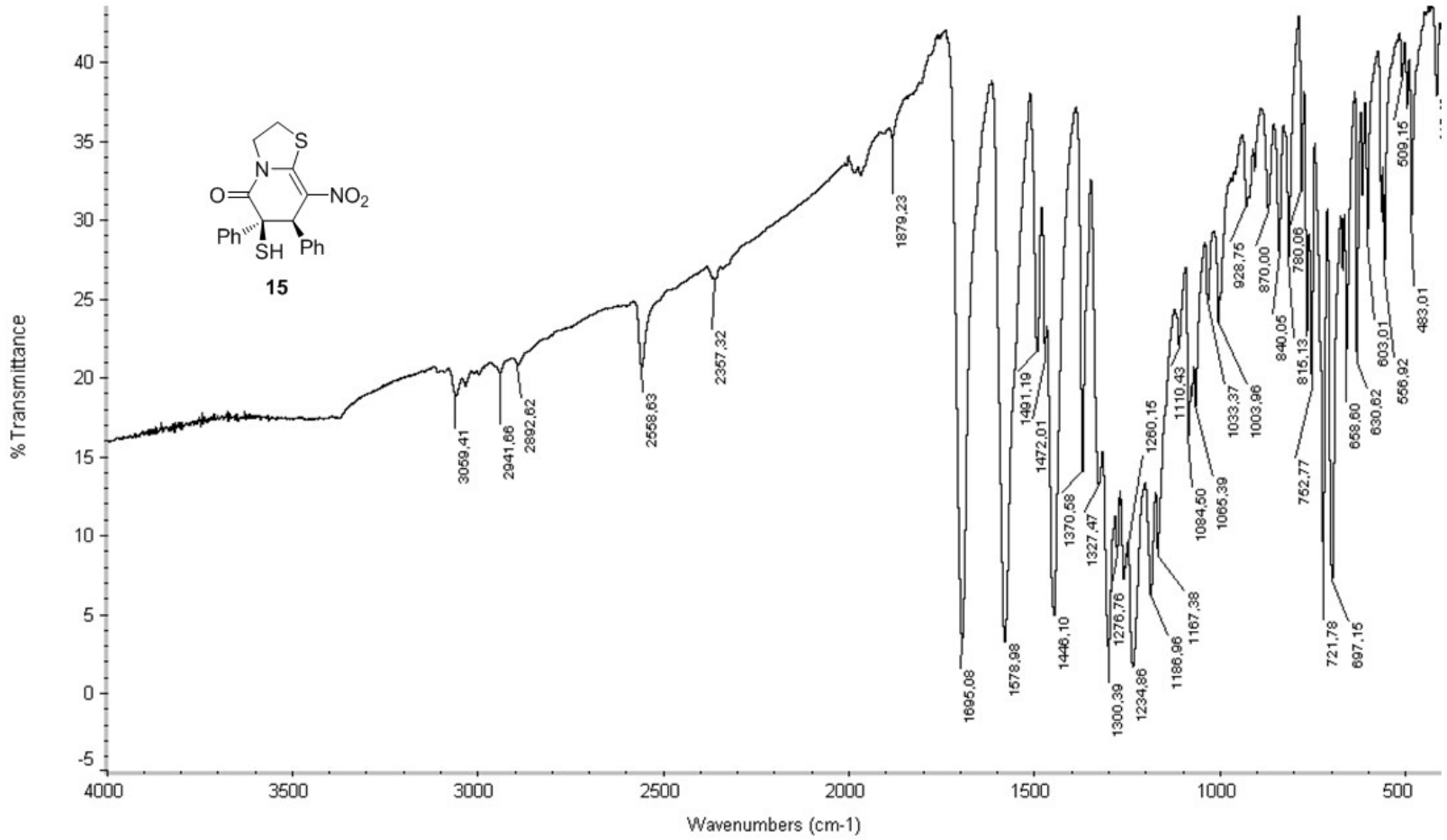
Compound **14**: COSY spectrum



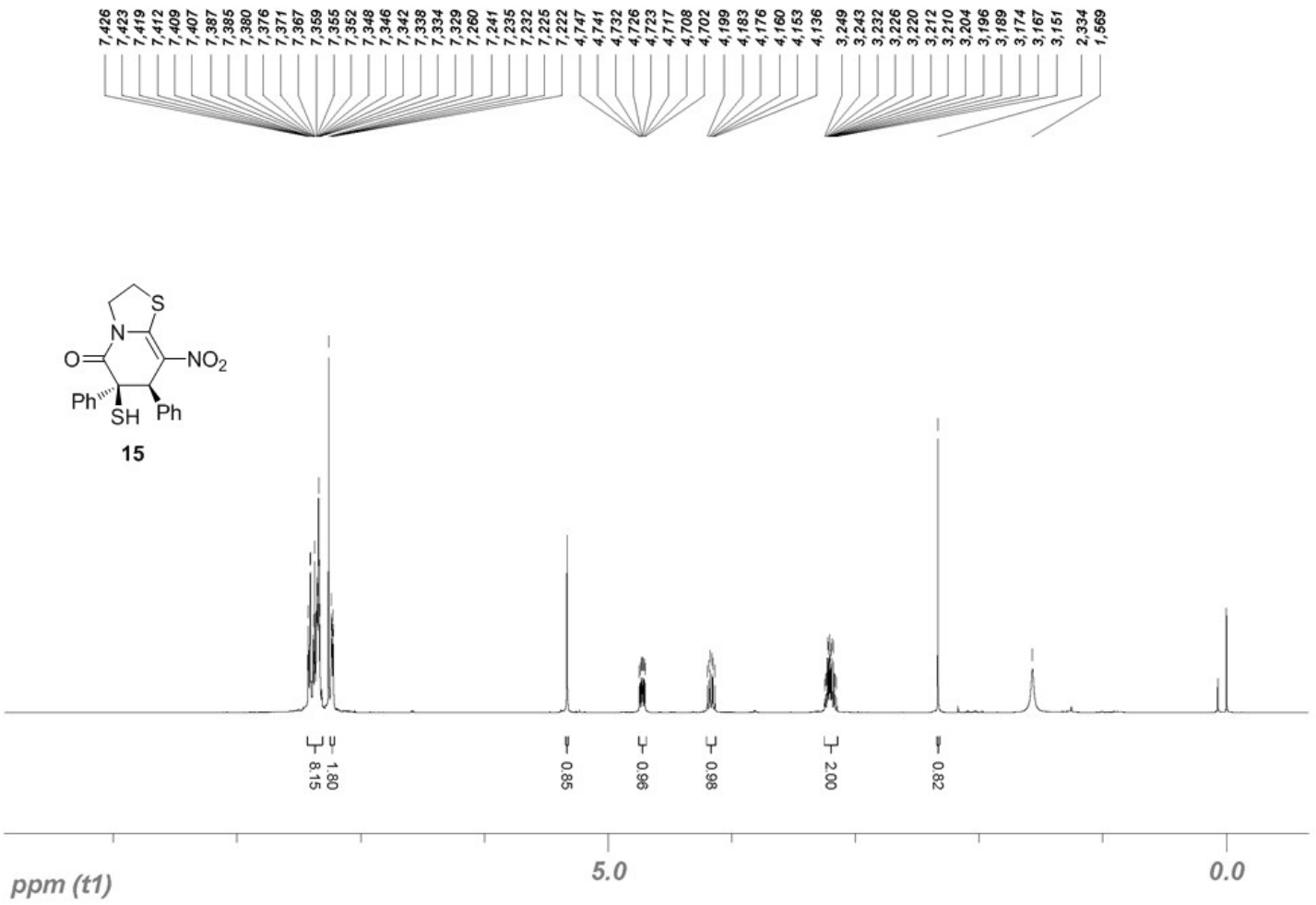
Compound **14**: HSQC and HMBC spectra



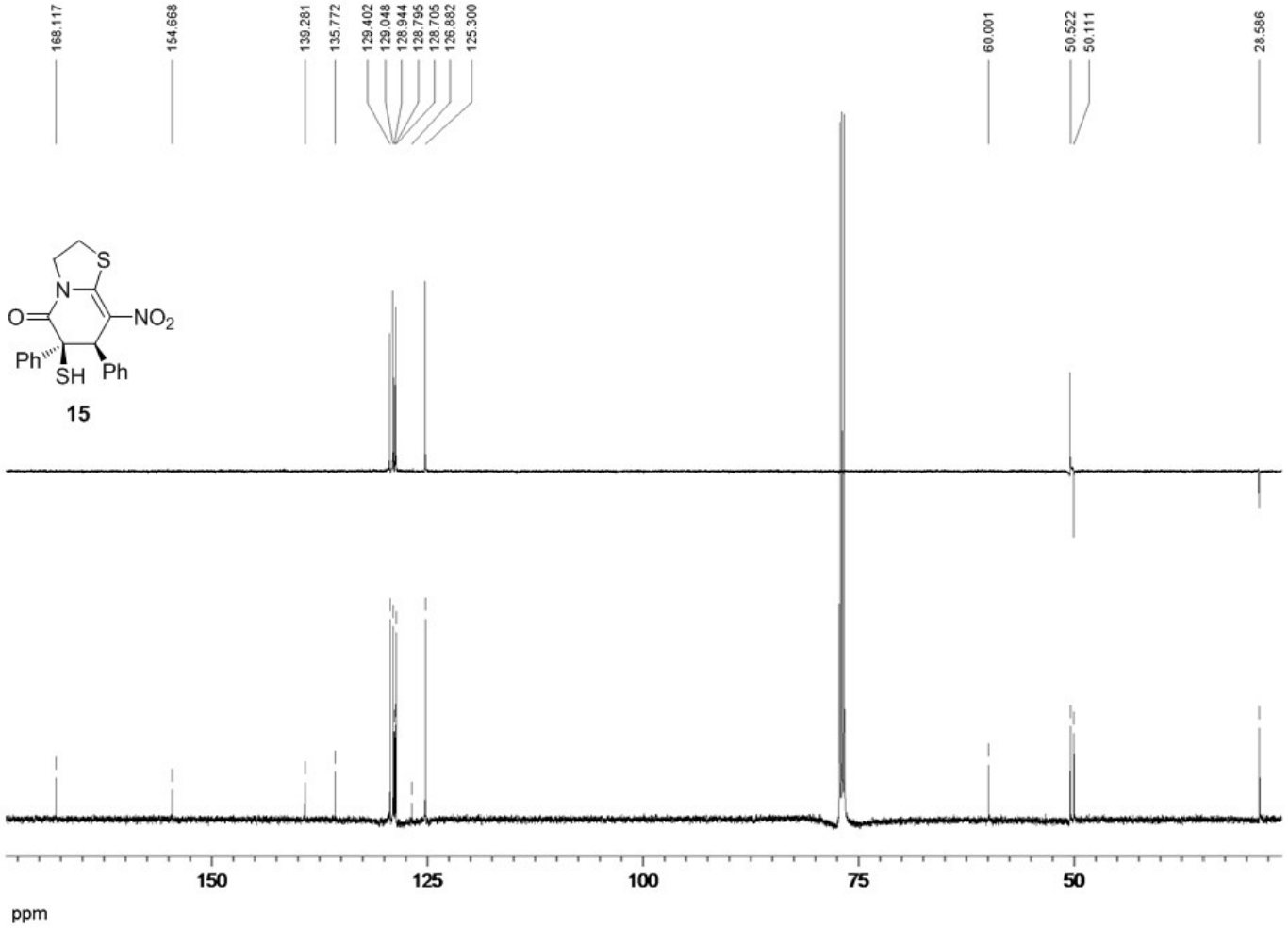
Compound **15**: FT-IR spectrum



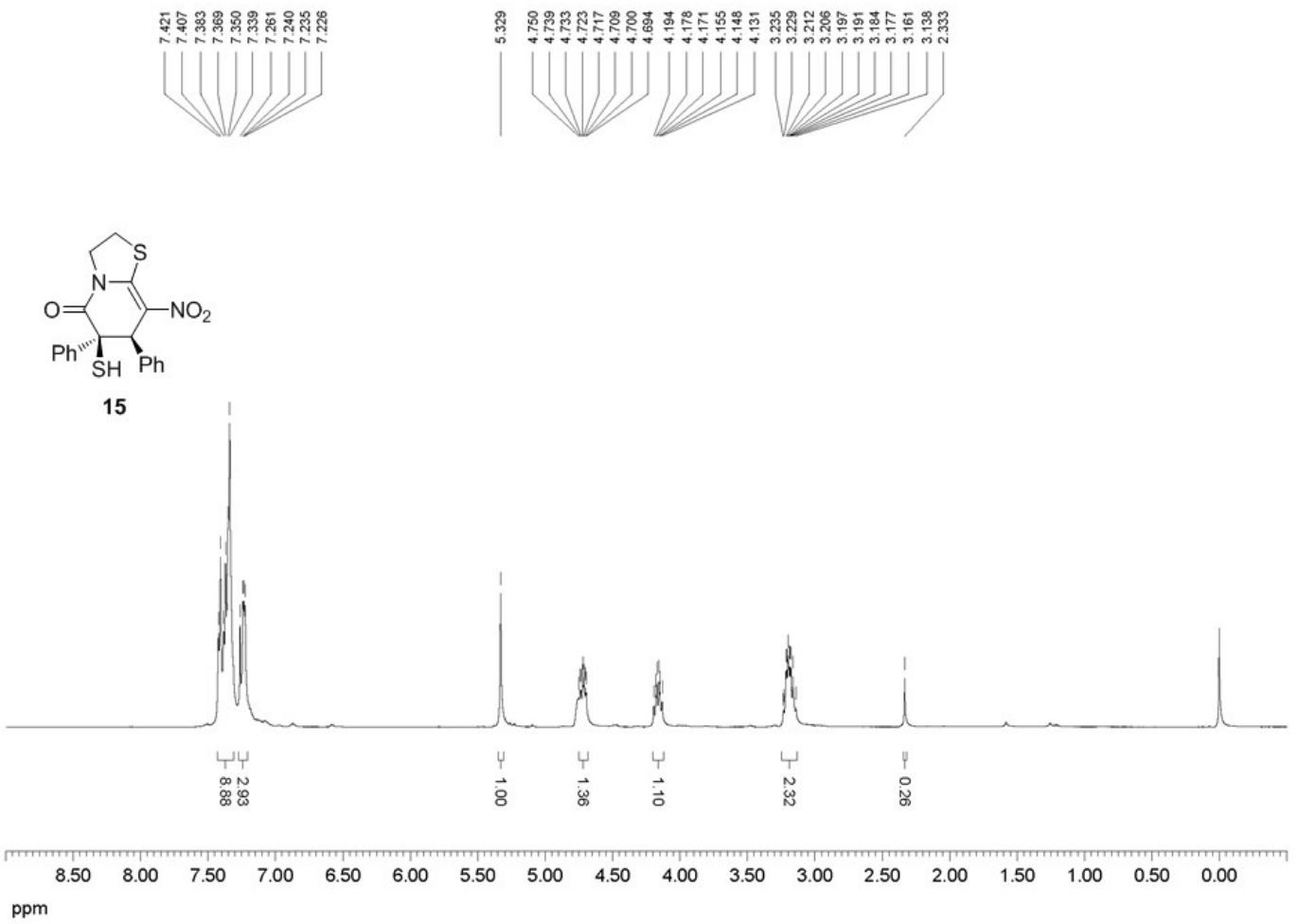
Compound **15**: ^{1}H NMR spectrum



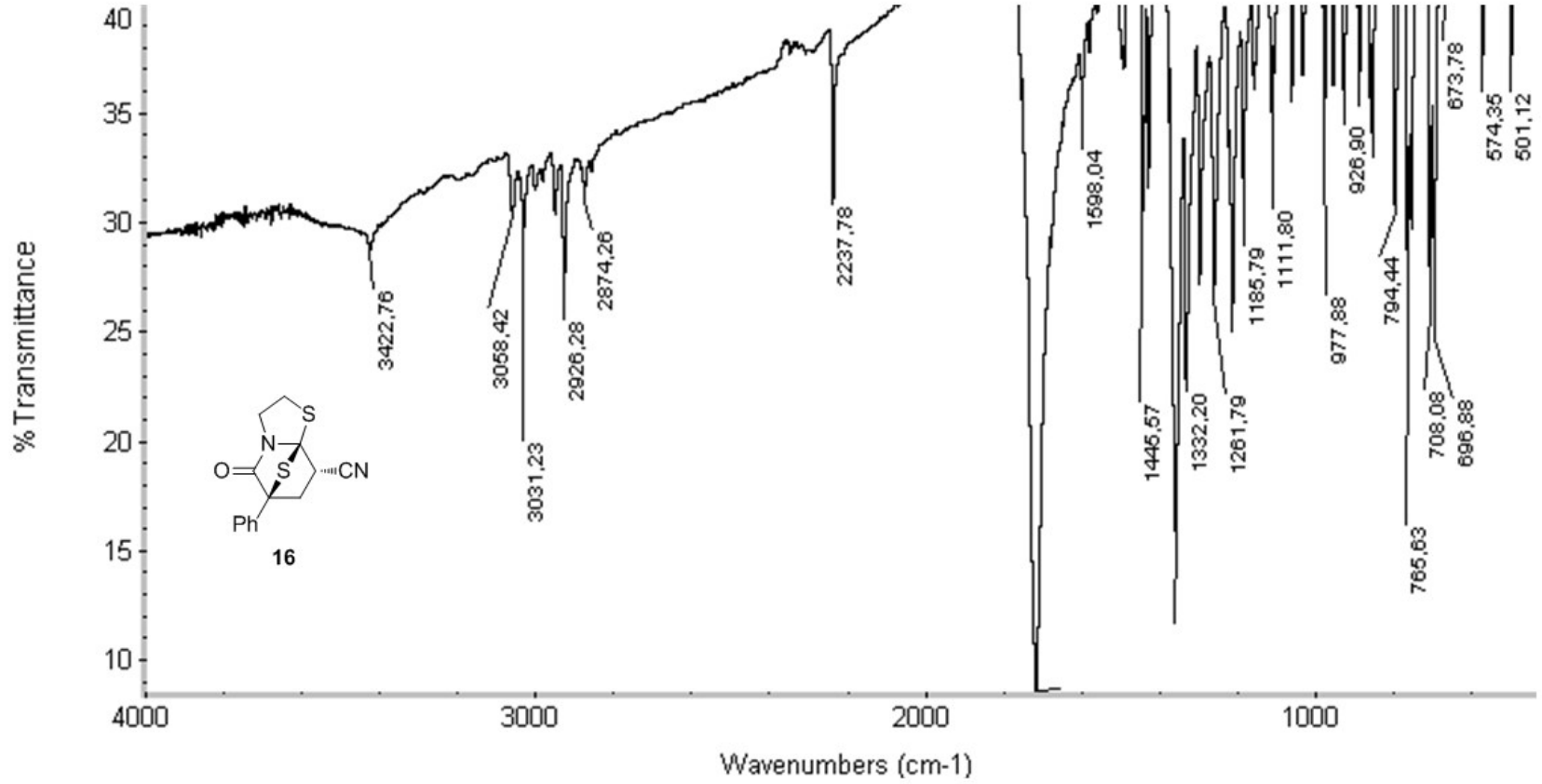
Compound **15**: ^{13}C NMR spectrum



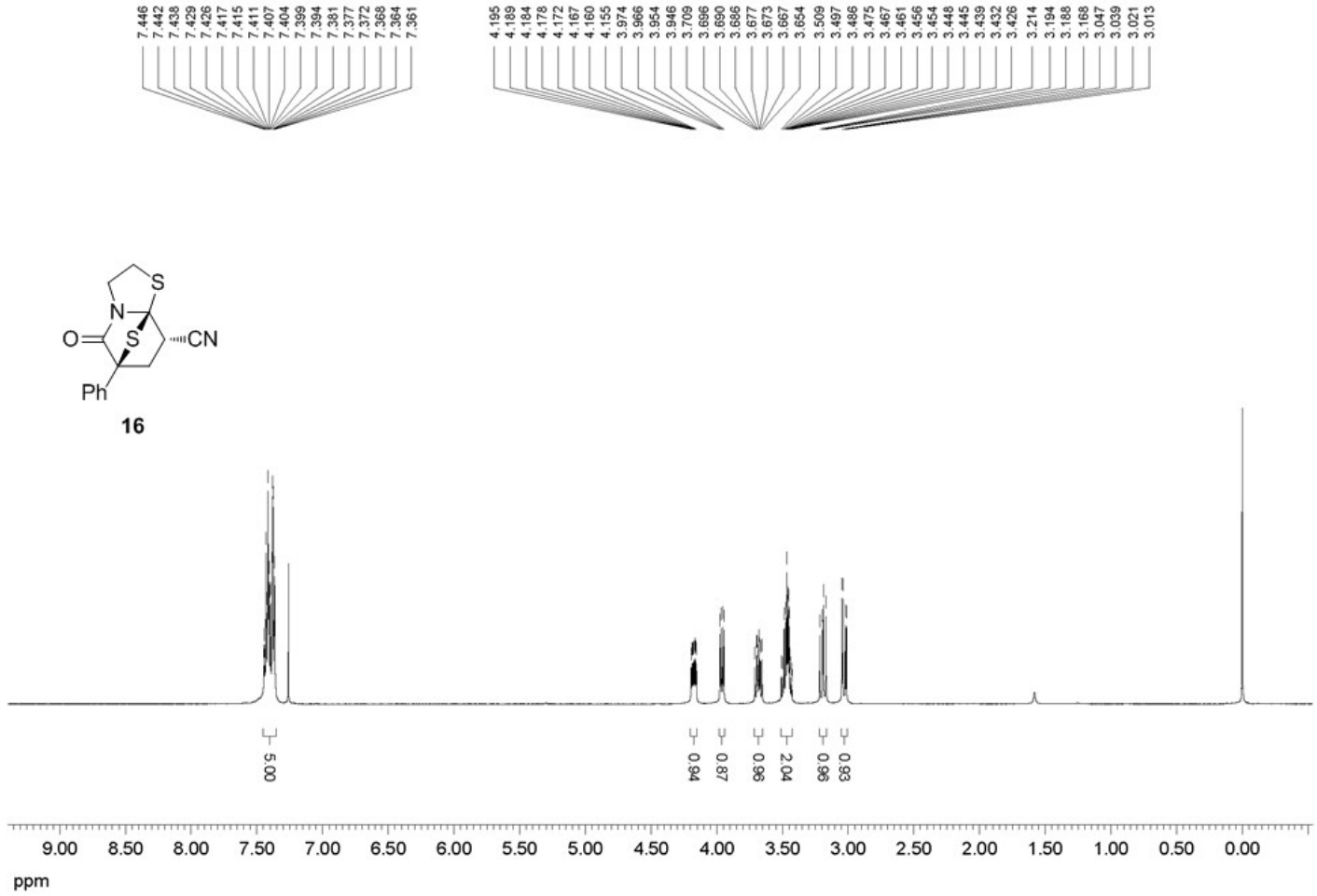
Compound **15**: ^{1}H NMR spectrum (D2O exange)



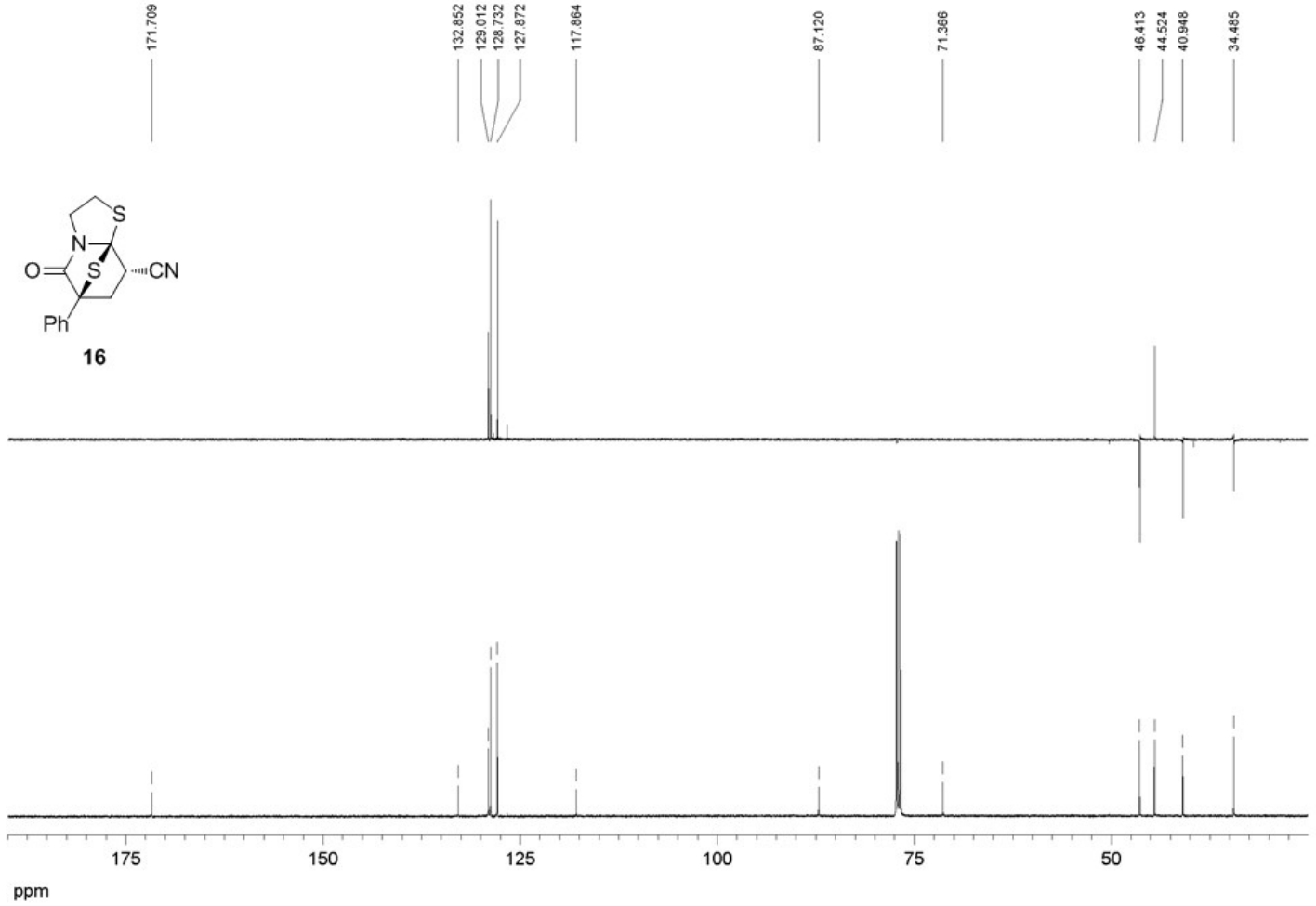
Compound **16**: FT-IR spectrum



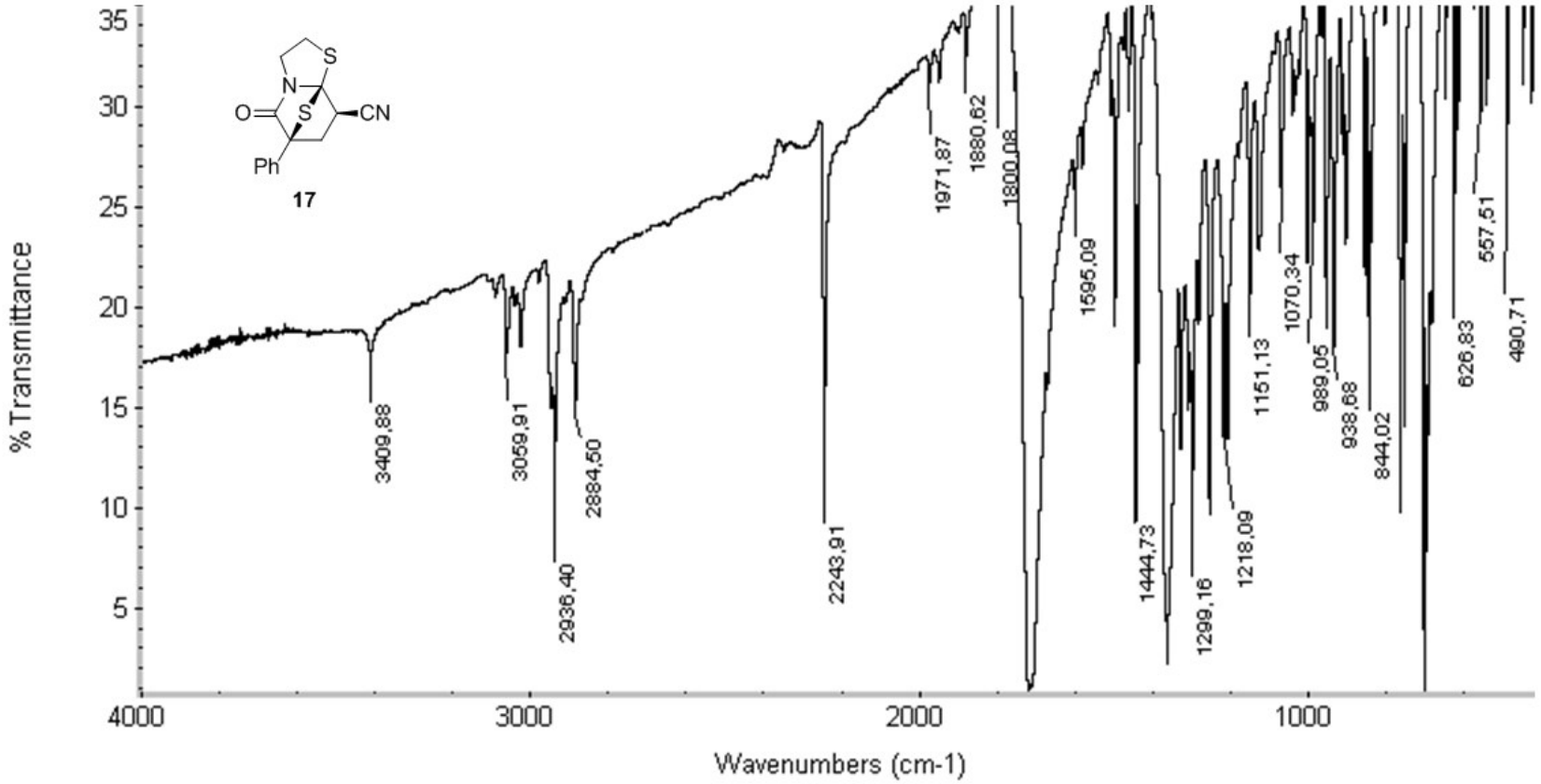
Compound **16**: ^{1}H NMR spectrum



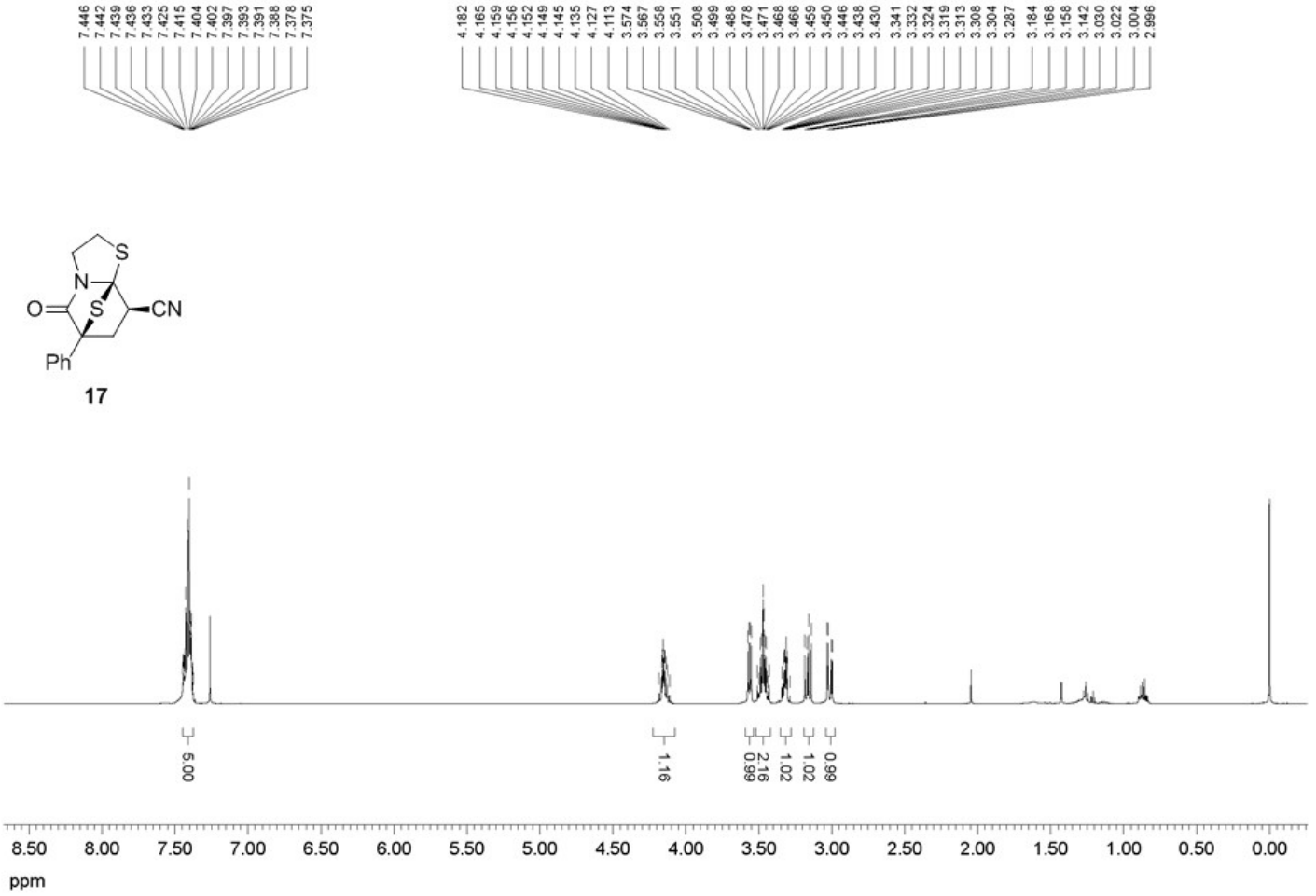
Compound **16**: ^{13}C NMR spectrum



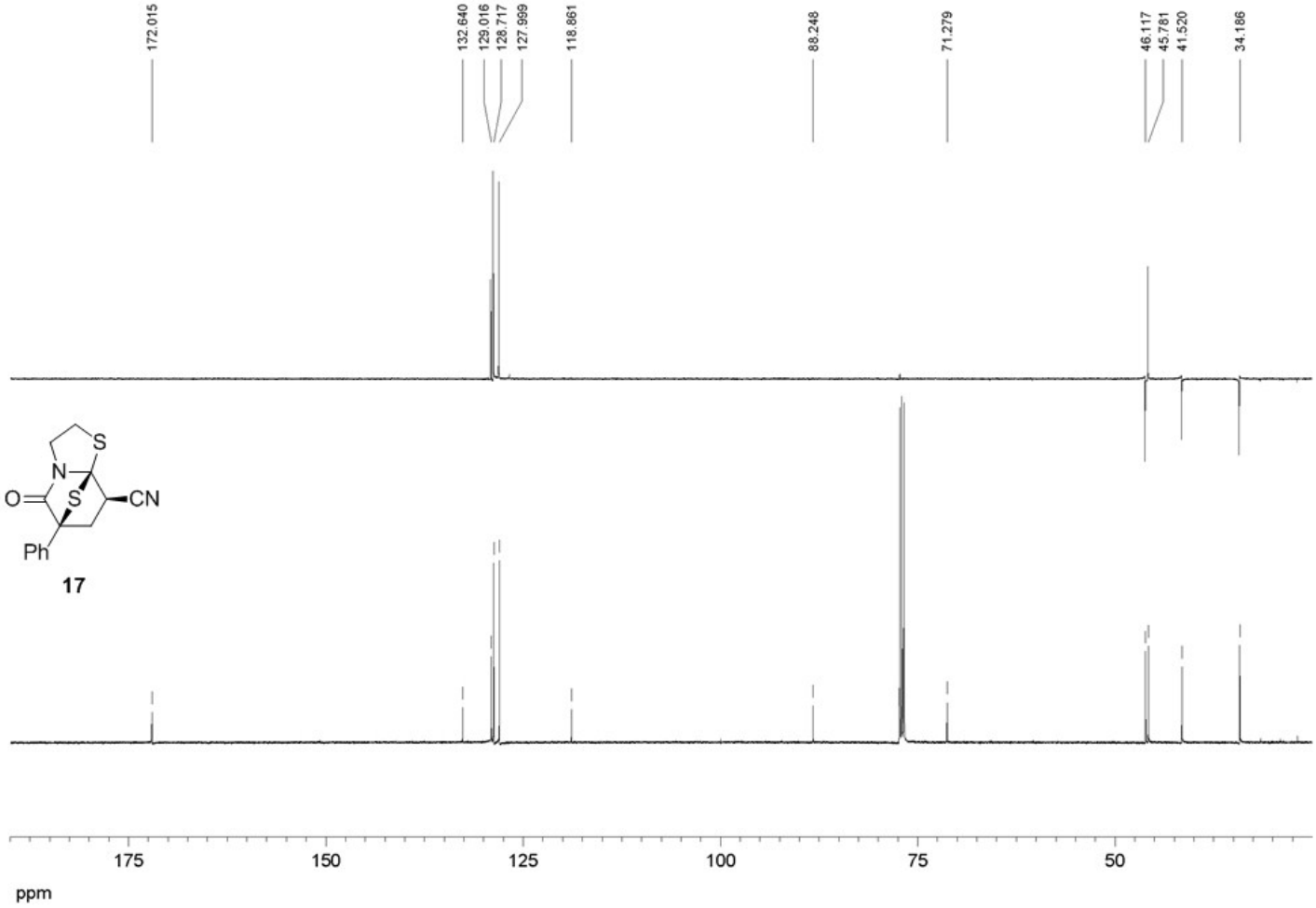
Compound **17**: FT-IR spectrum



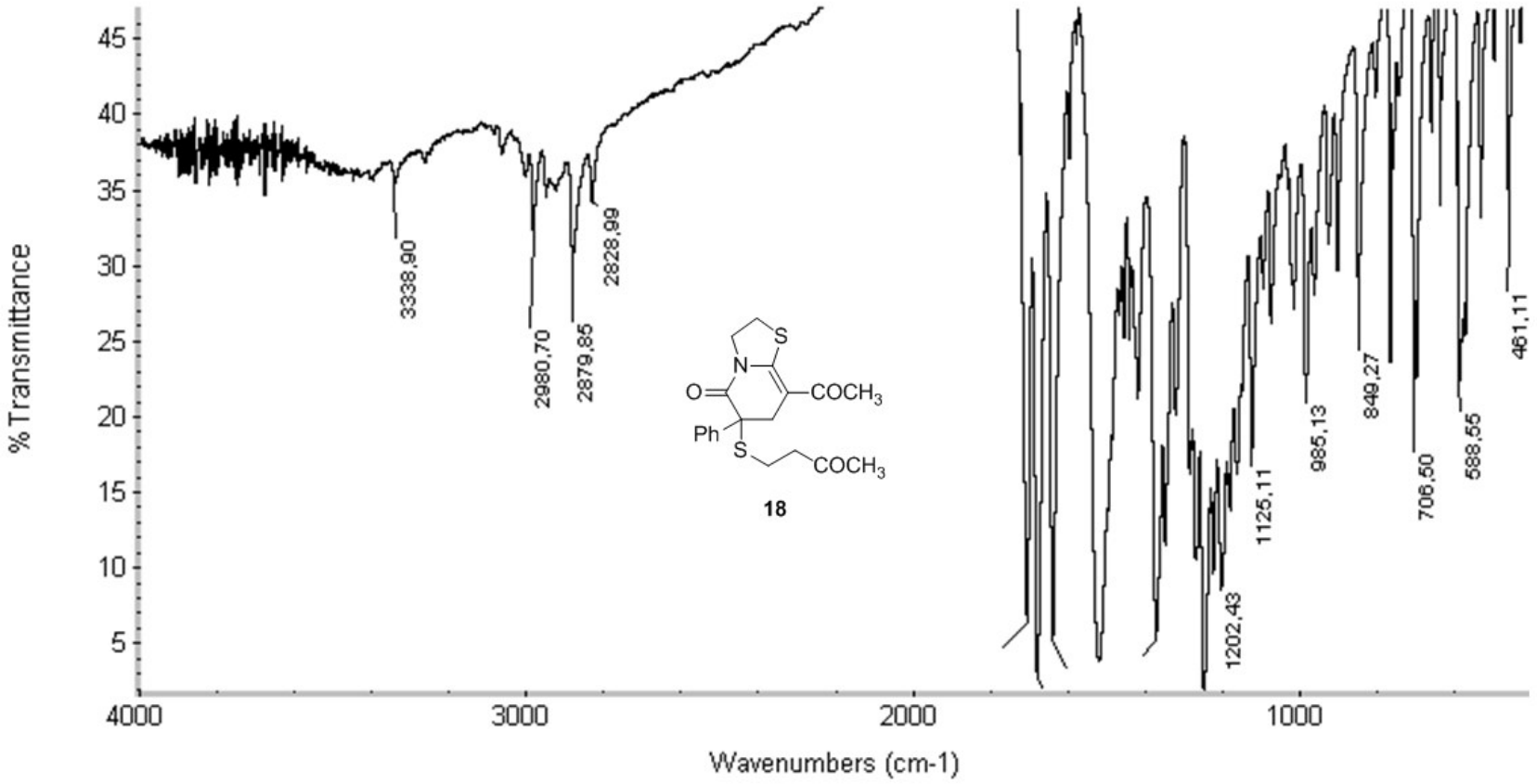
Compound **17**: ^{1}H NMR spectrum



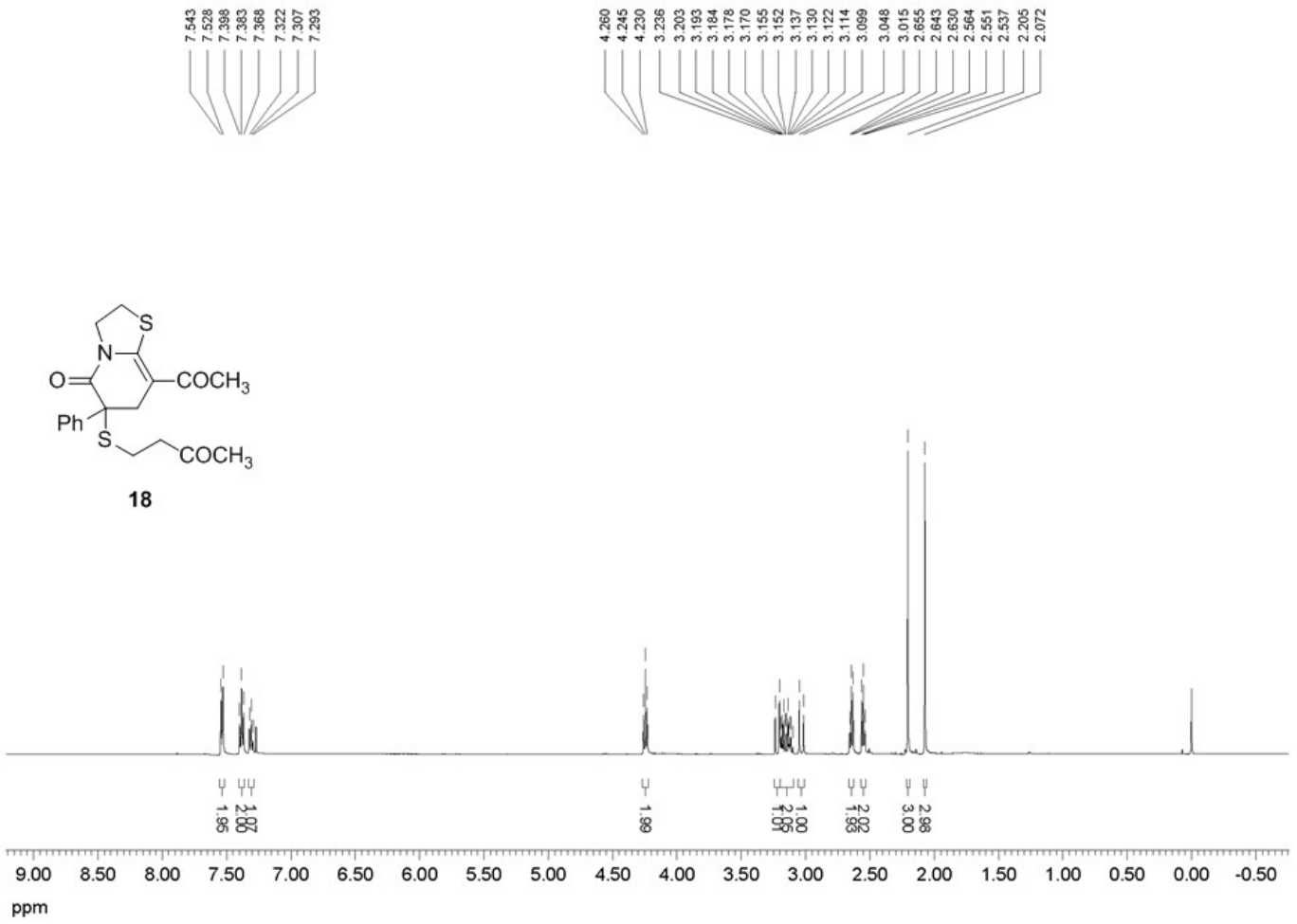
Compound **17**: ^{13}C NMR spectrum



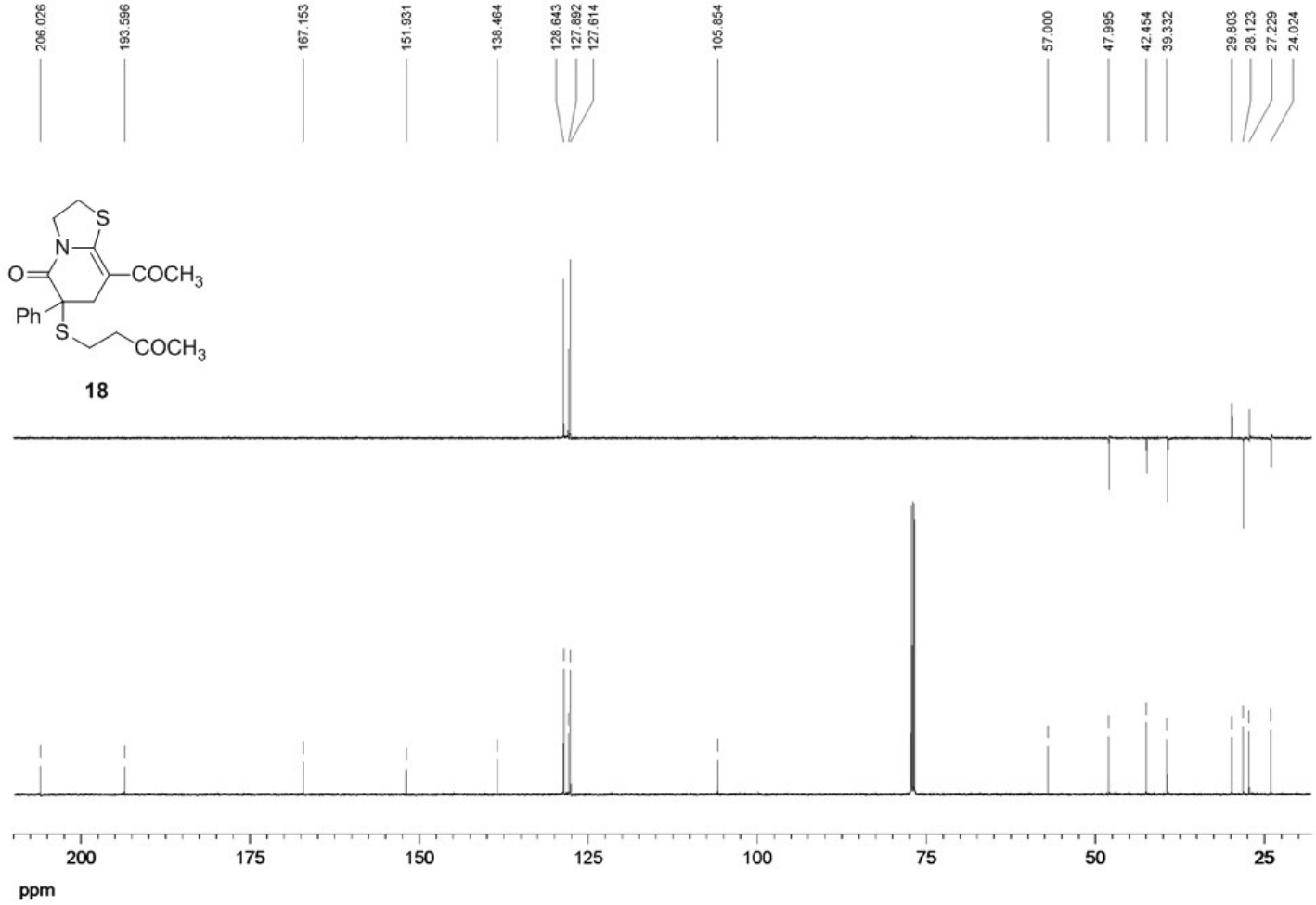
Compound **18**: FT-IR spectrum



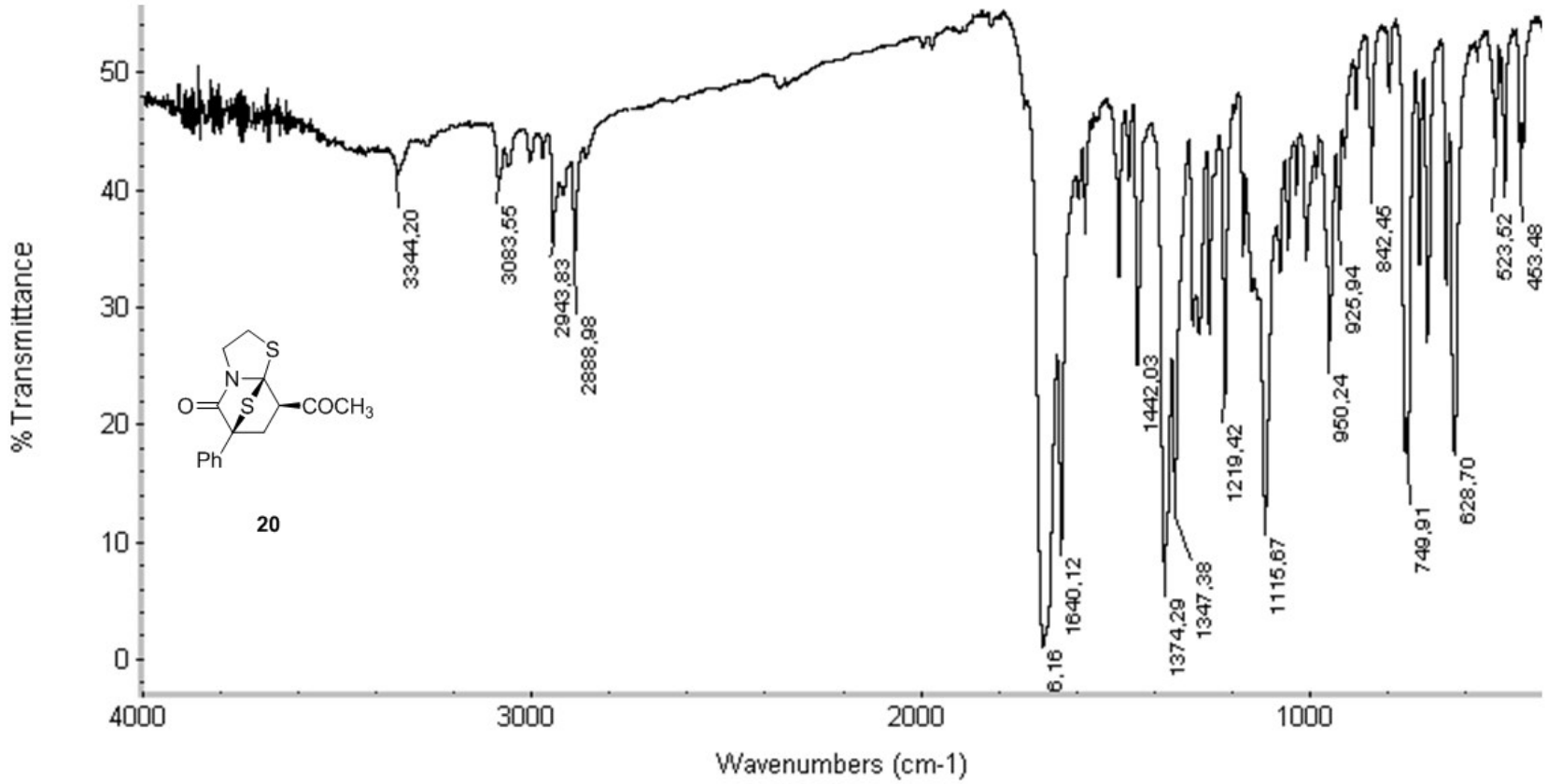
Compound **18**: ^{1}H NMR spectrum



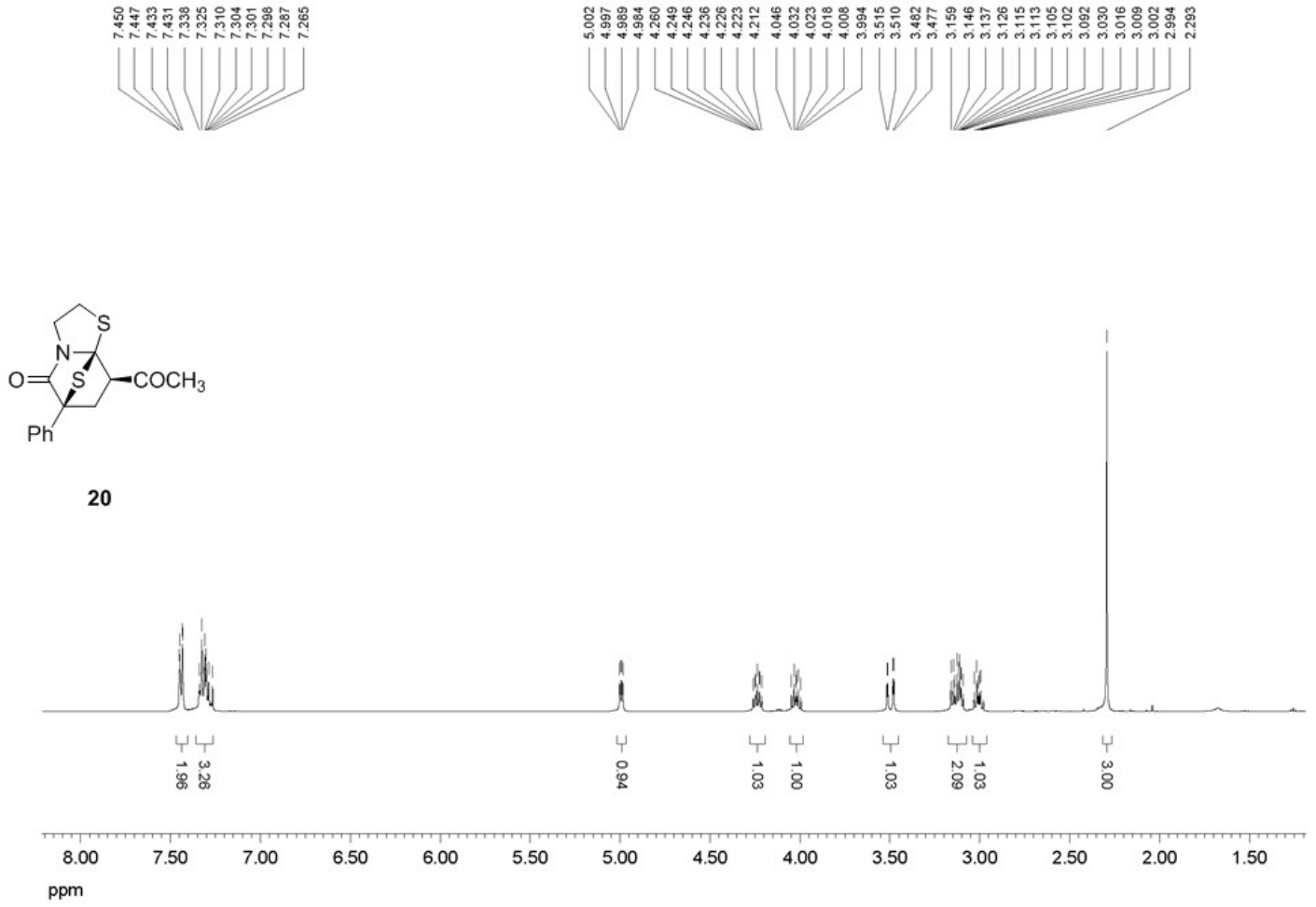
Compound **18**: ^{13}C NMR spectrum



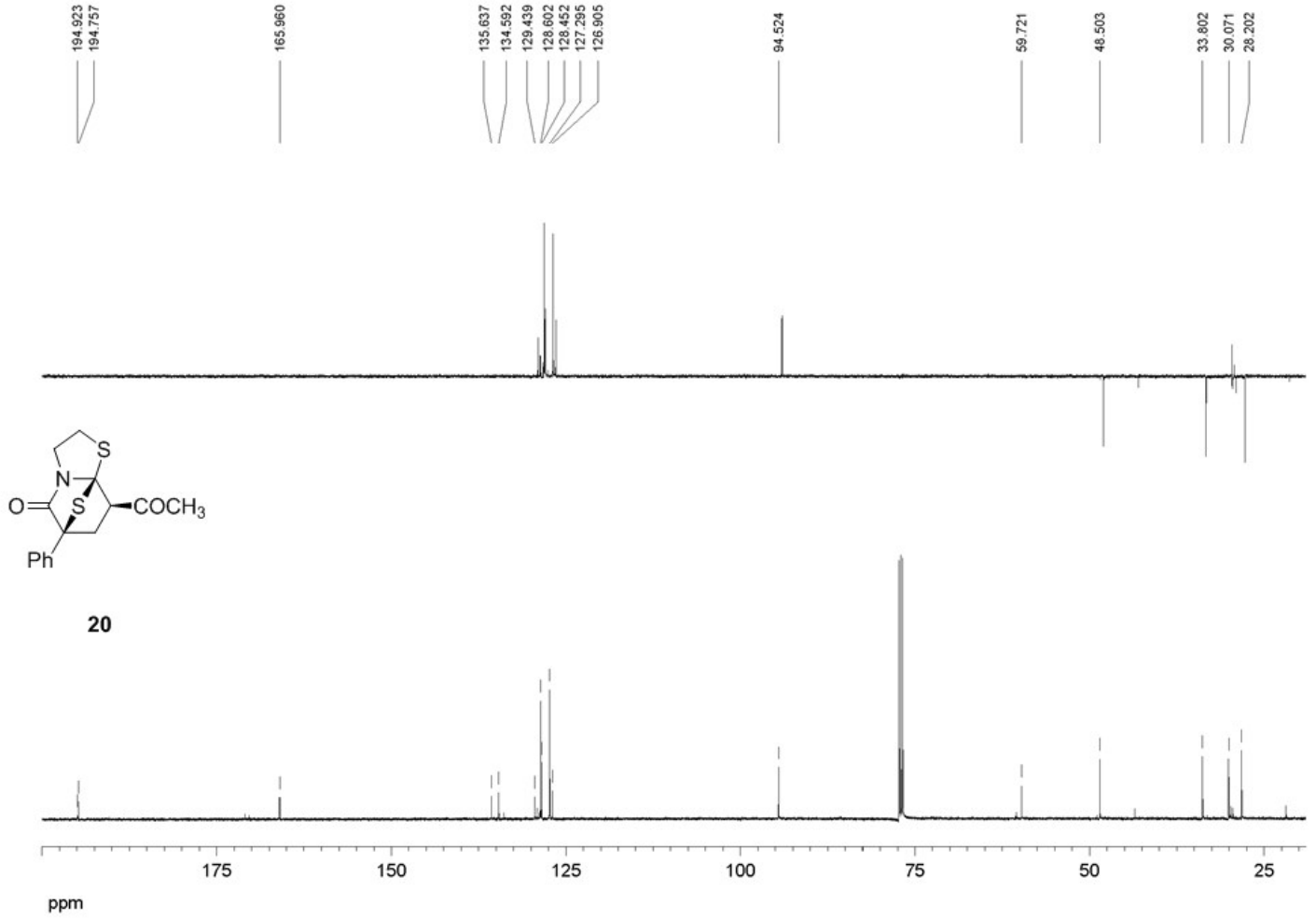
Compound **20**: FT-IR spectrum



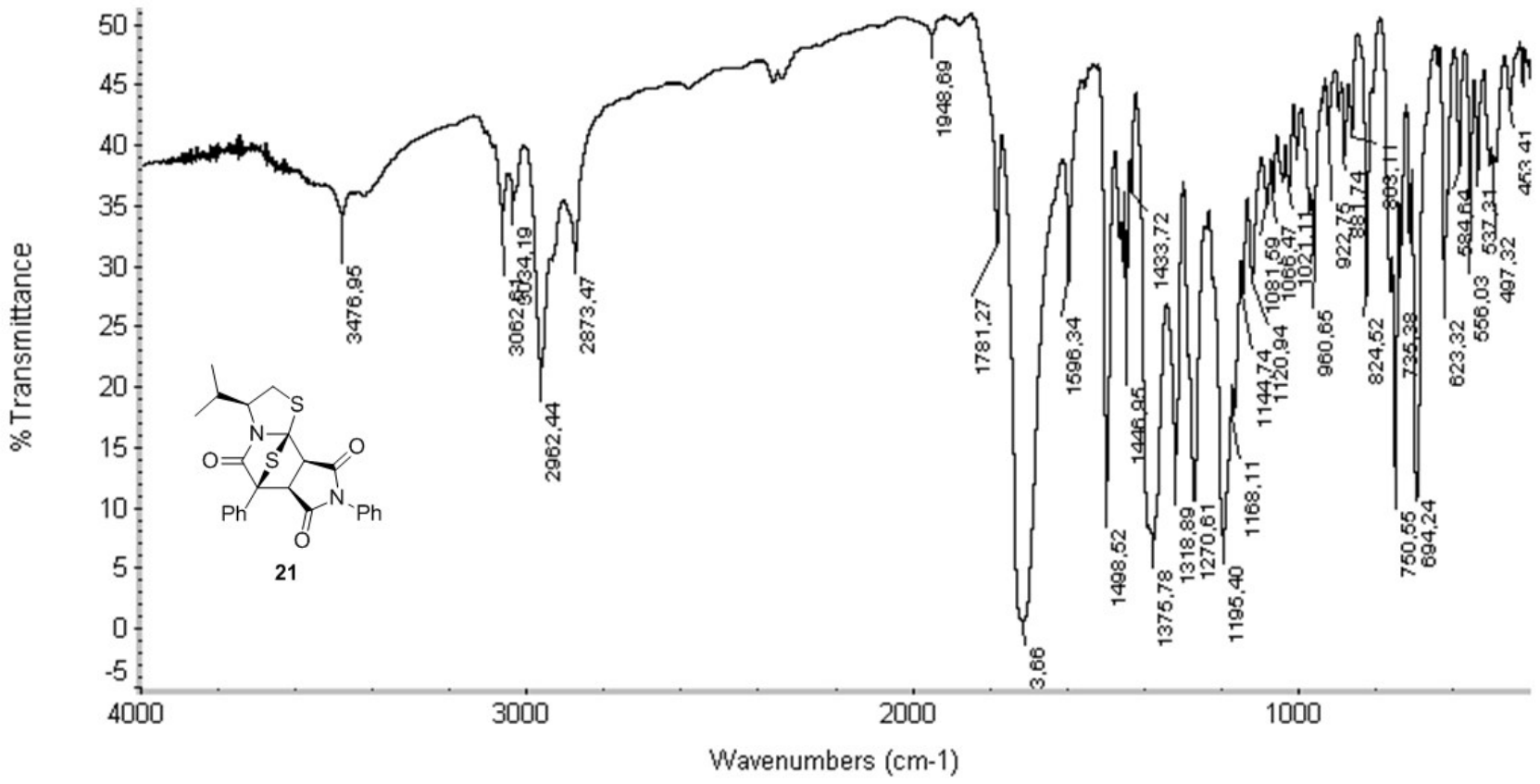
Compound **20**: ^{1}H NMR spectrum



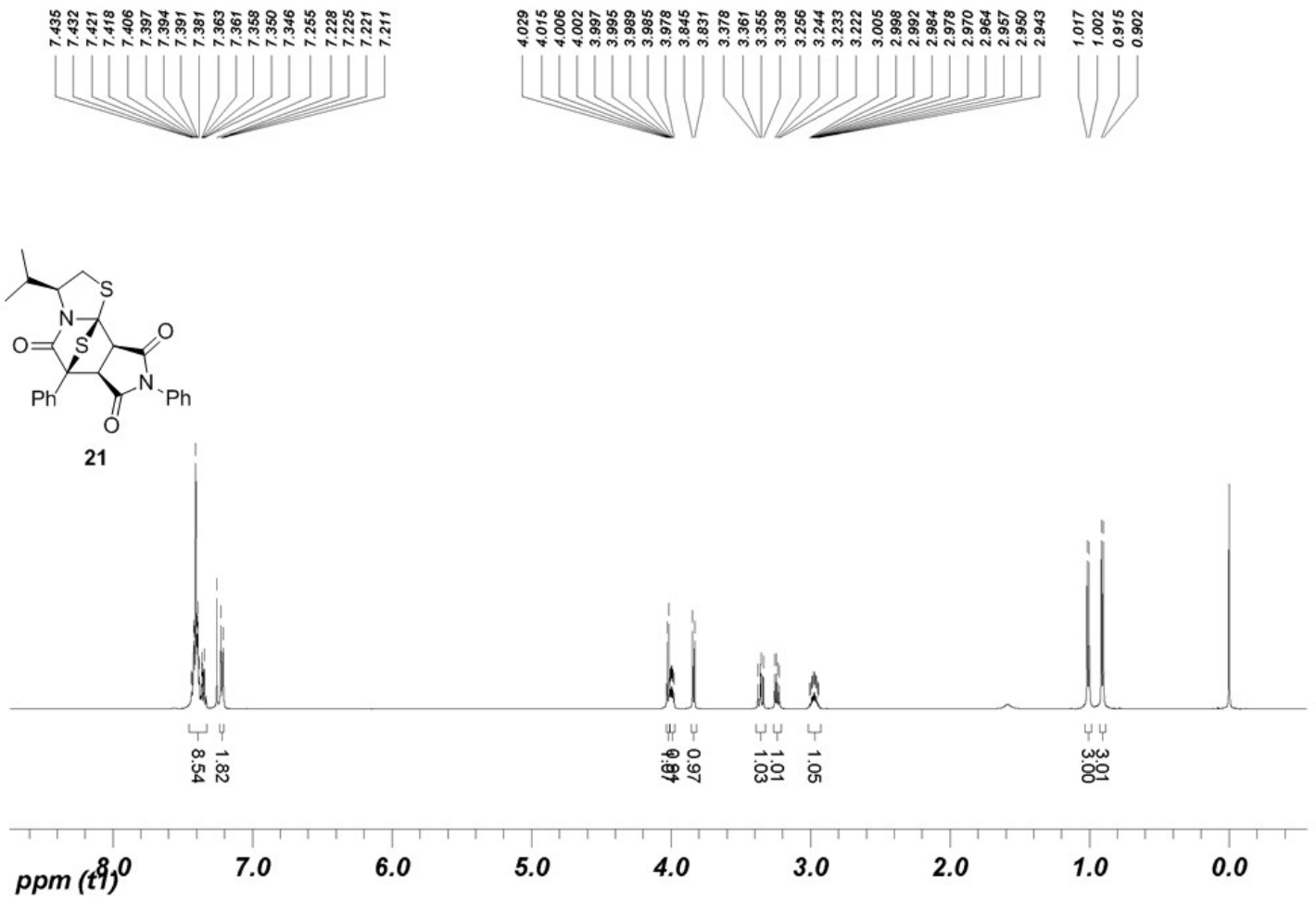
Compound **20**: ^{13}C NMR spectrum



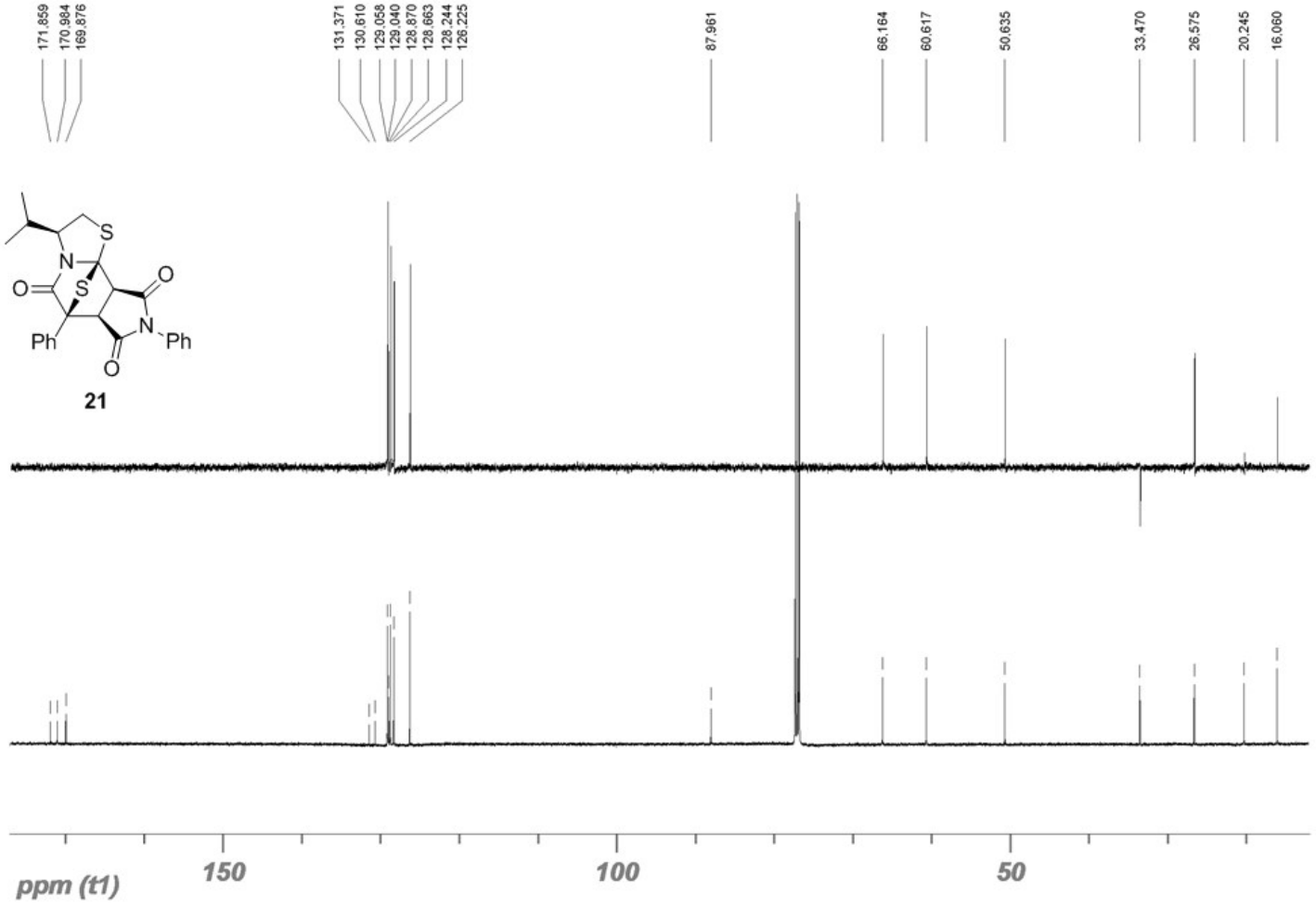
Compound **21**: FT-IR spectrum



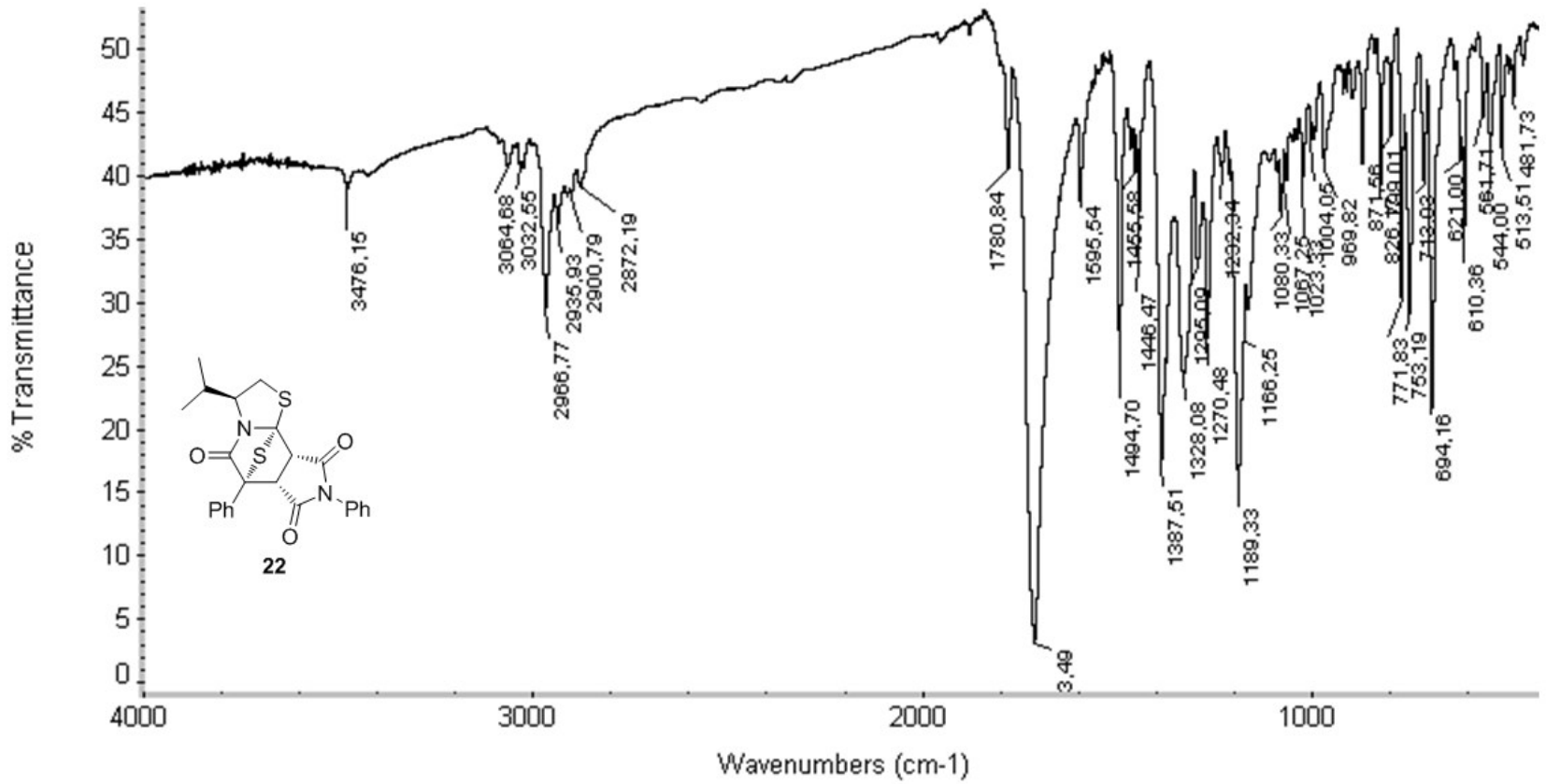
Compound **21**: ^{1}H NMR spectrum



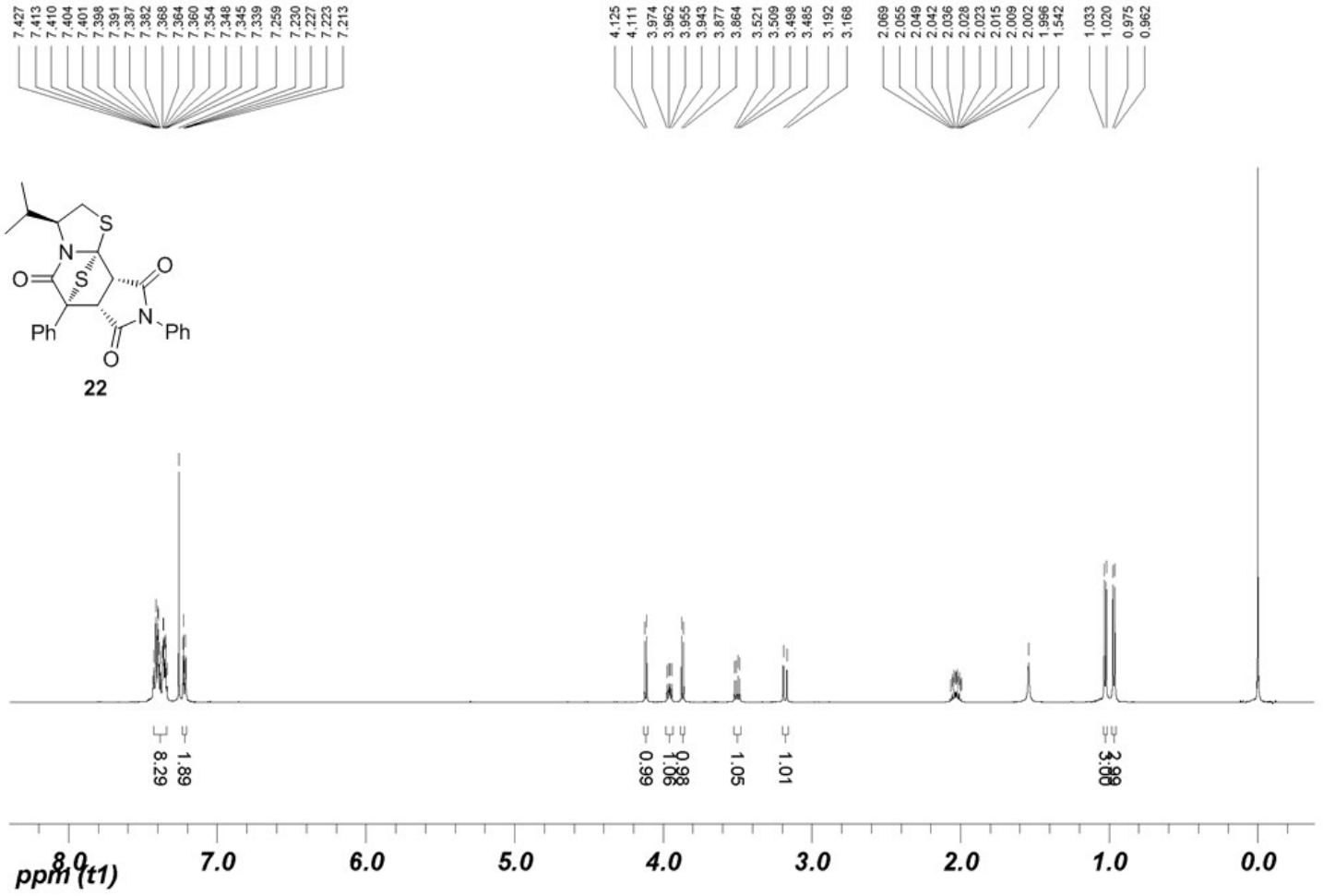
Compound **21**: ^{13}C NMR spectrum



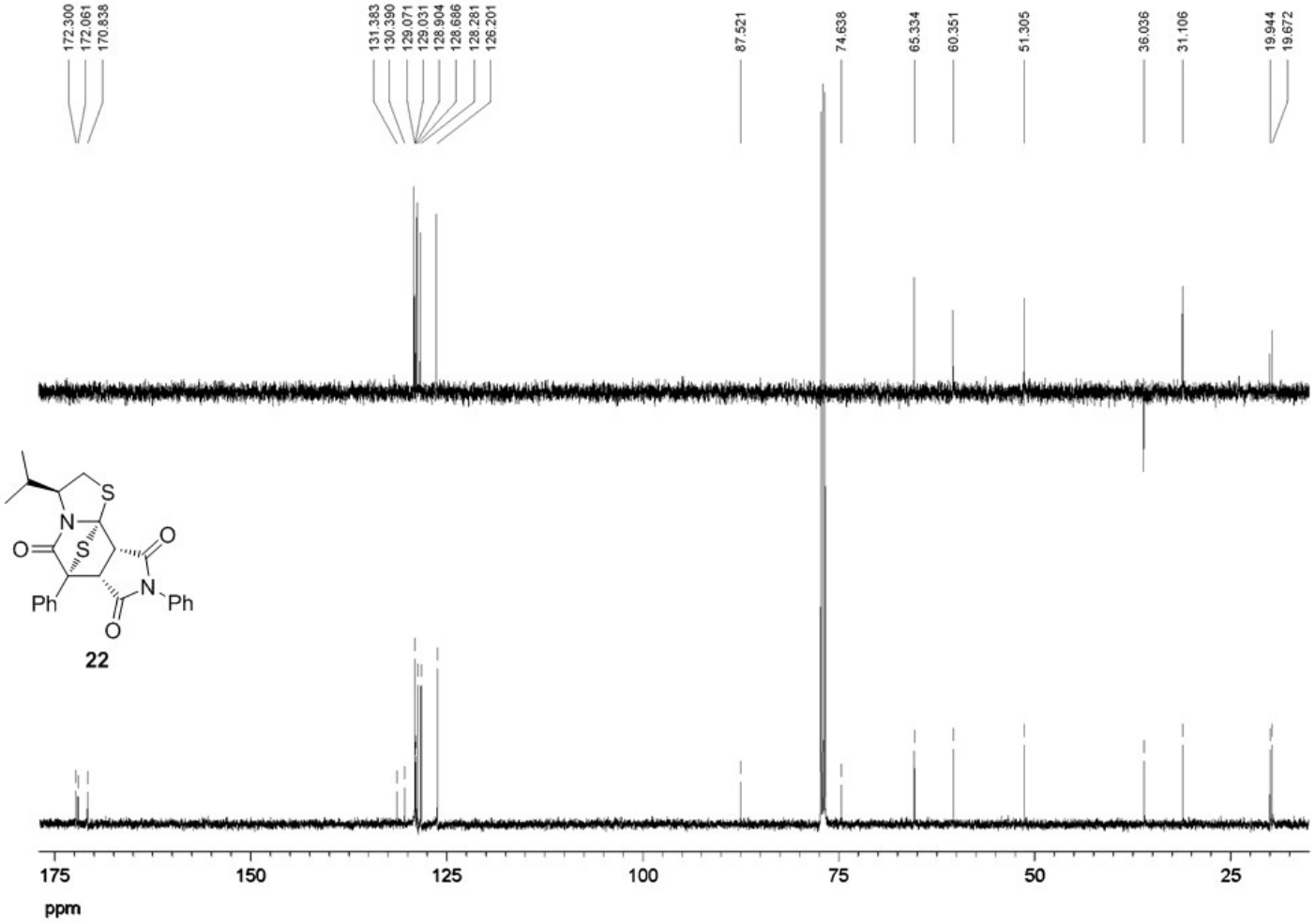
Compound **22**: FT-IR spectrum



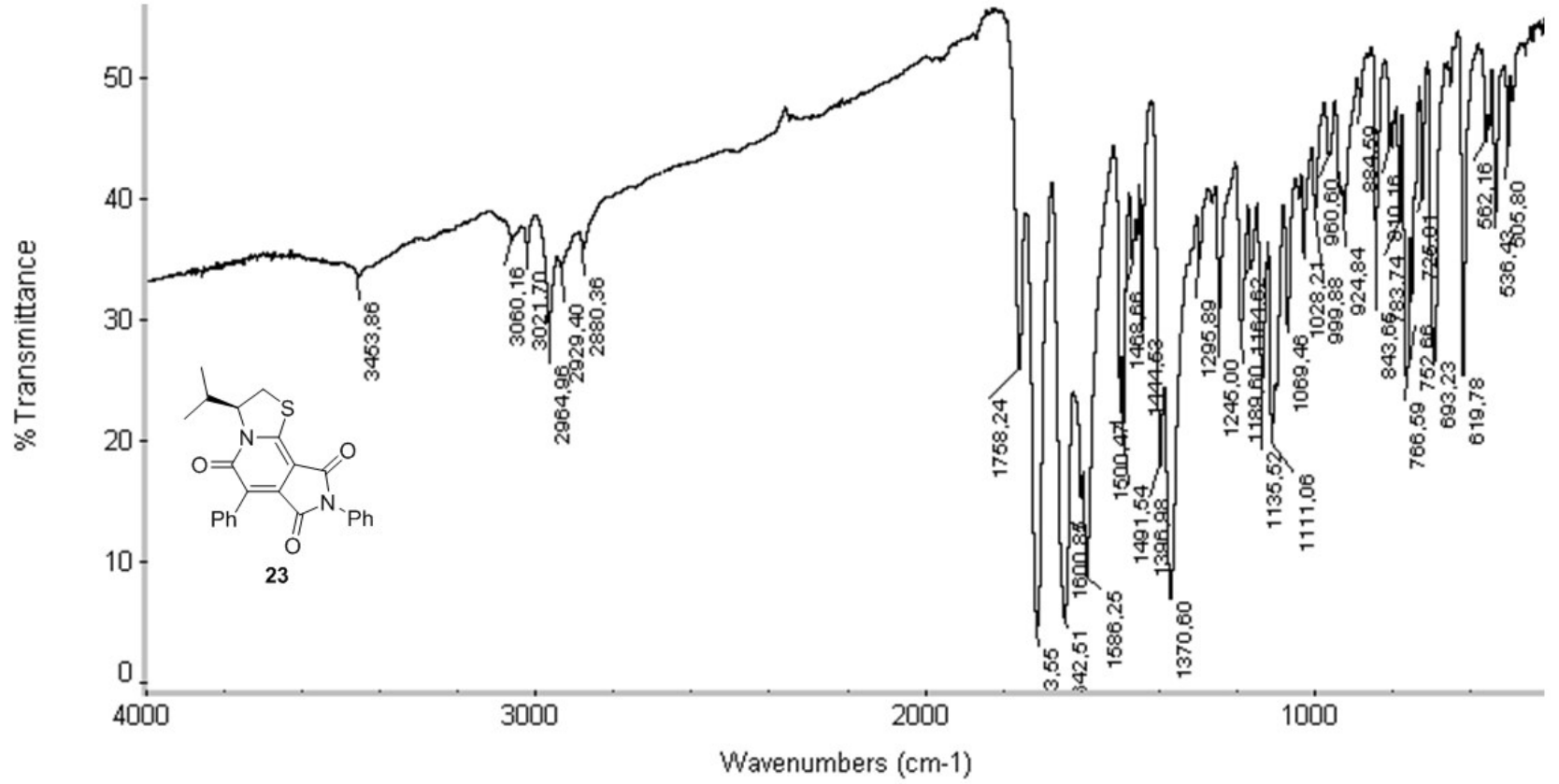
Compound **22**: ^{1}H NMR spectrum



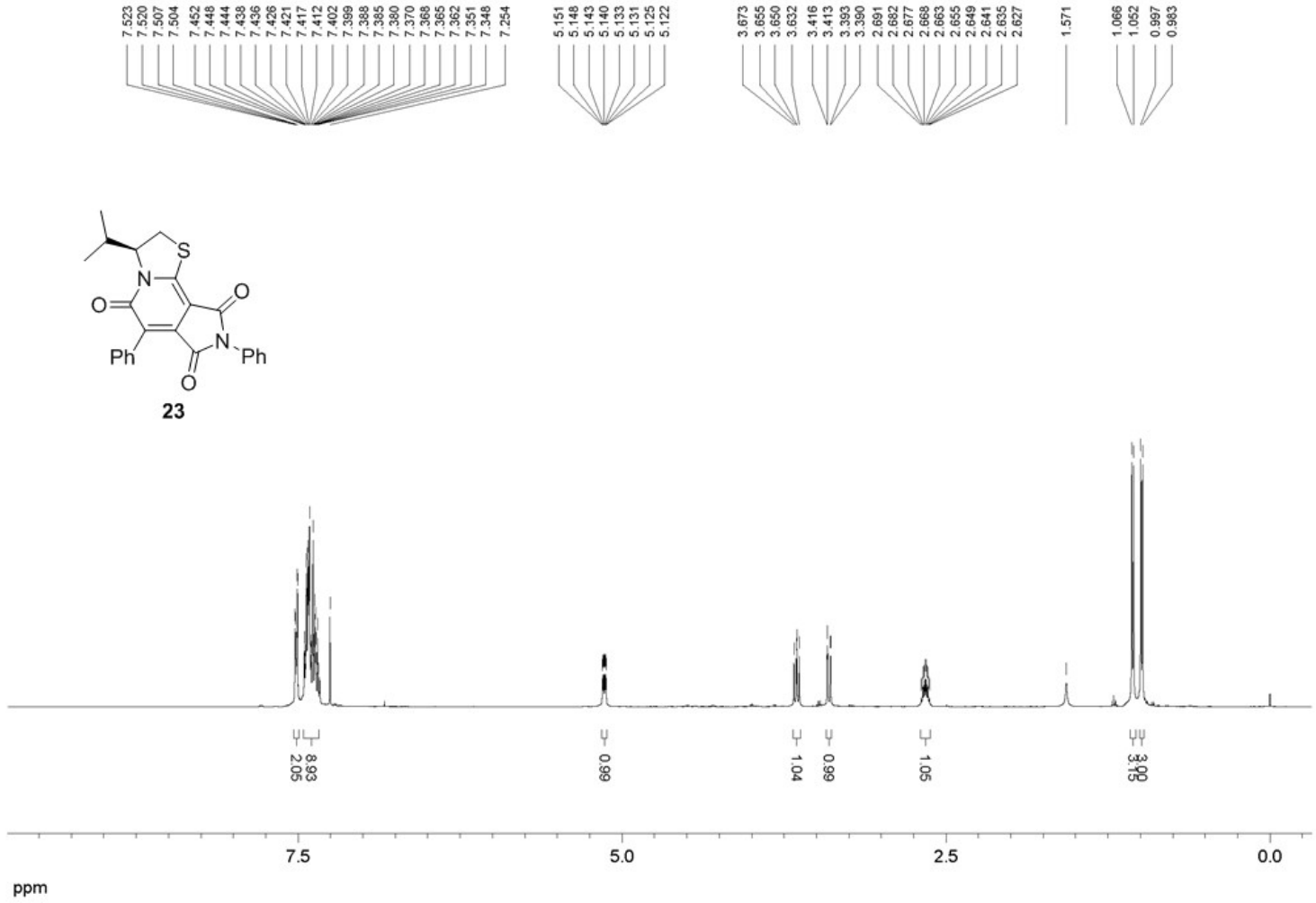
Compound **22**: ^{13}C NMR spectrum



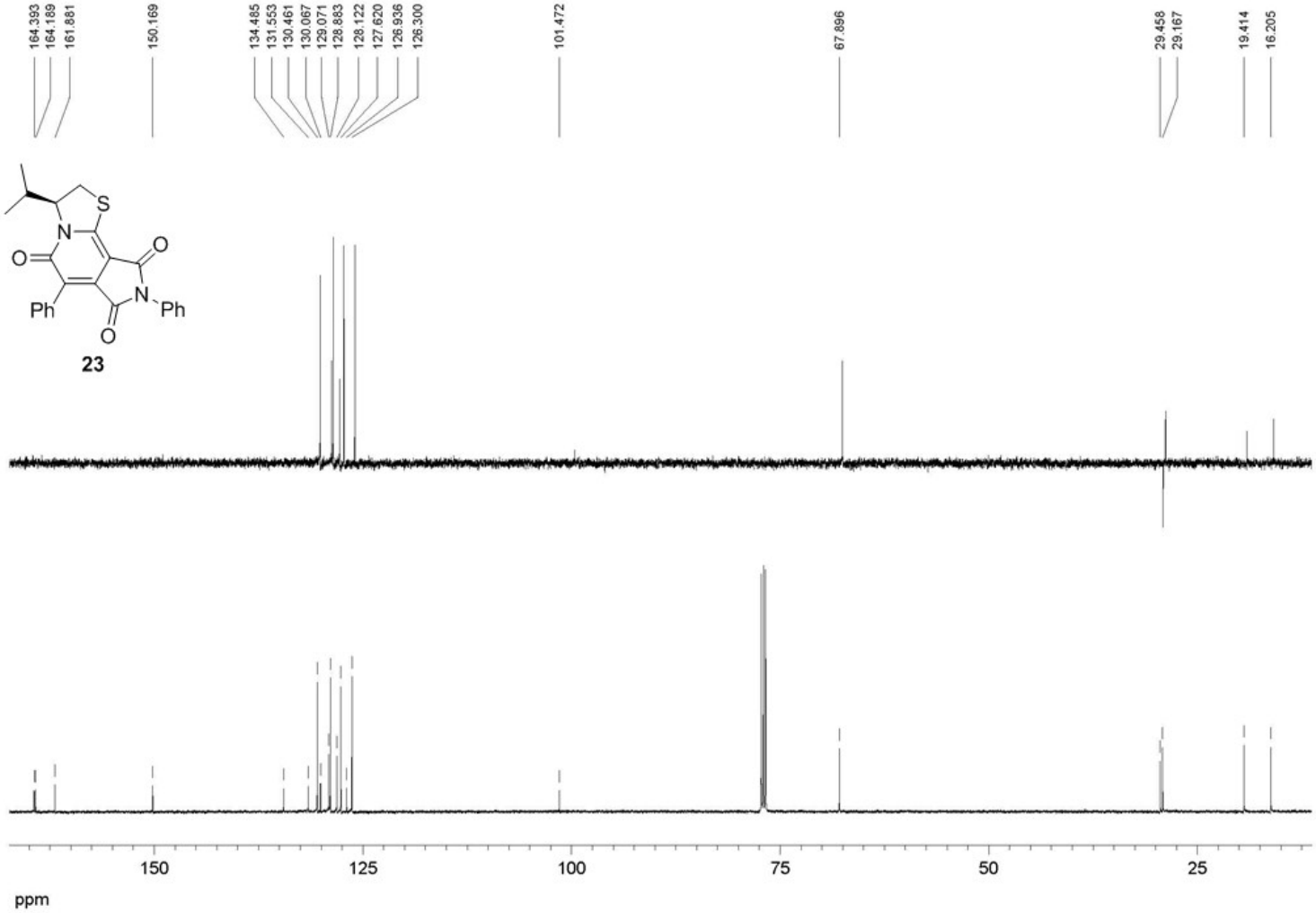
Compound **23**: FT-IR spectrum



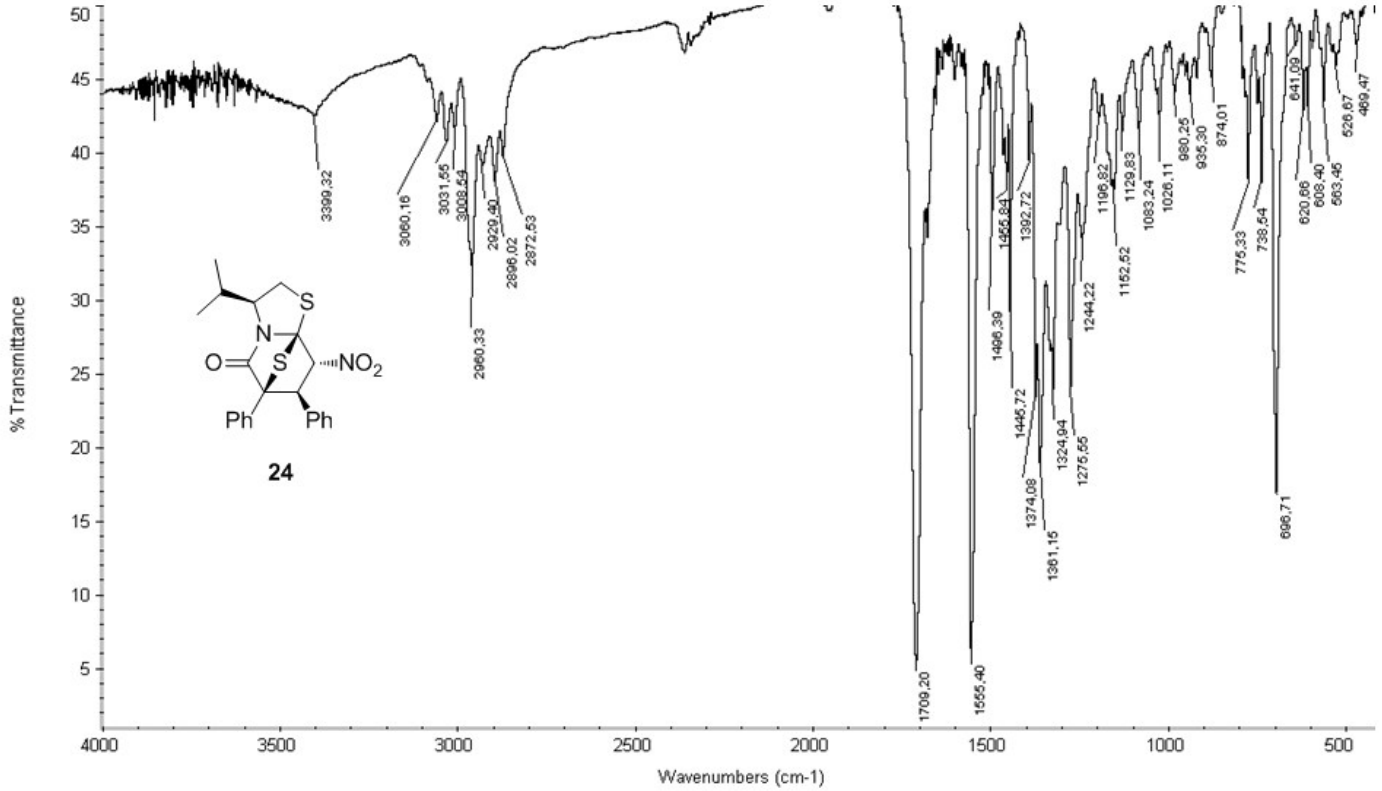
Compound **23**: ^{1}H NMR spectrum



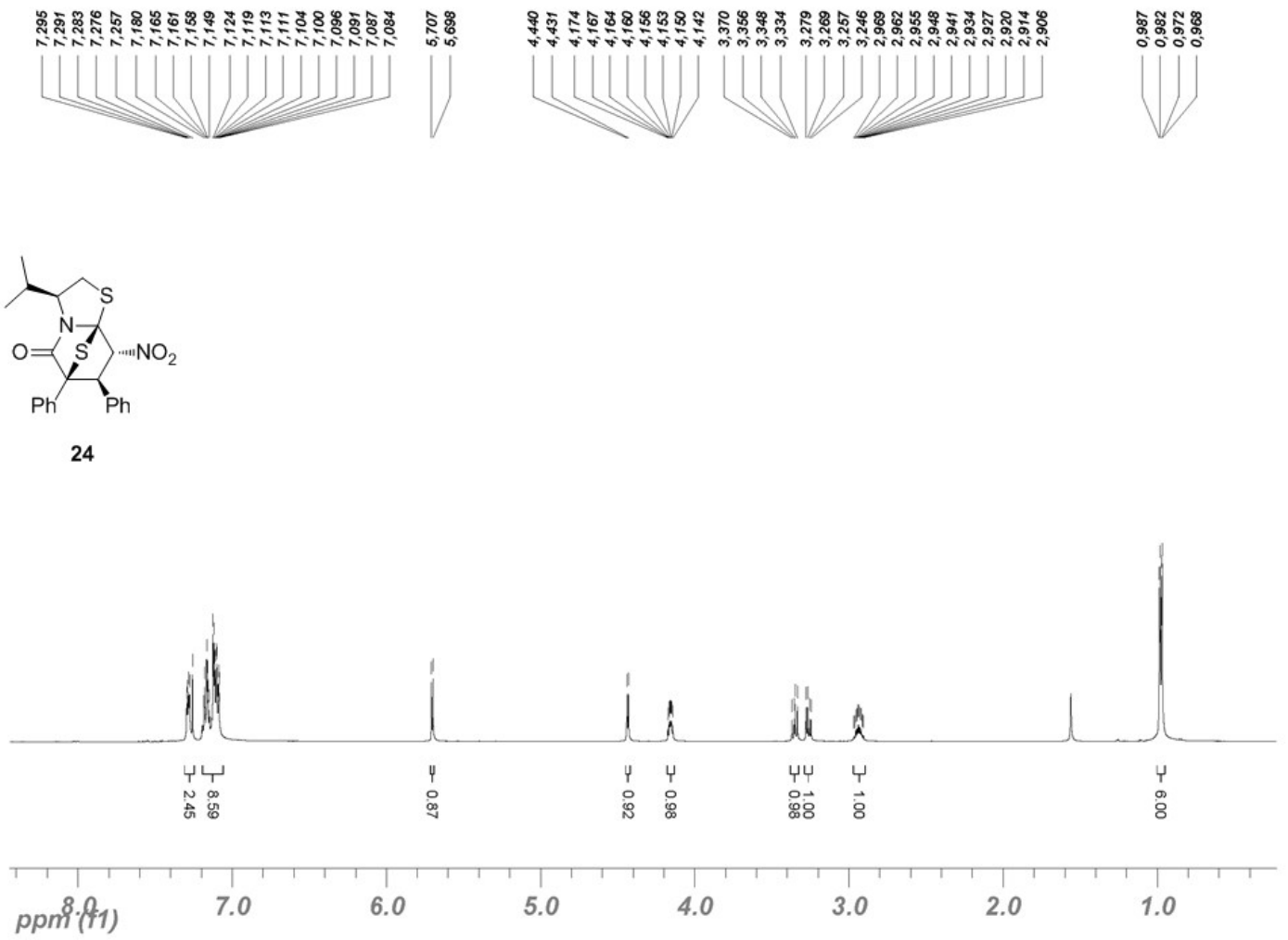
Compound **23**: ^{13}C NMR spectrum



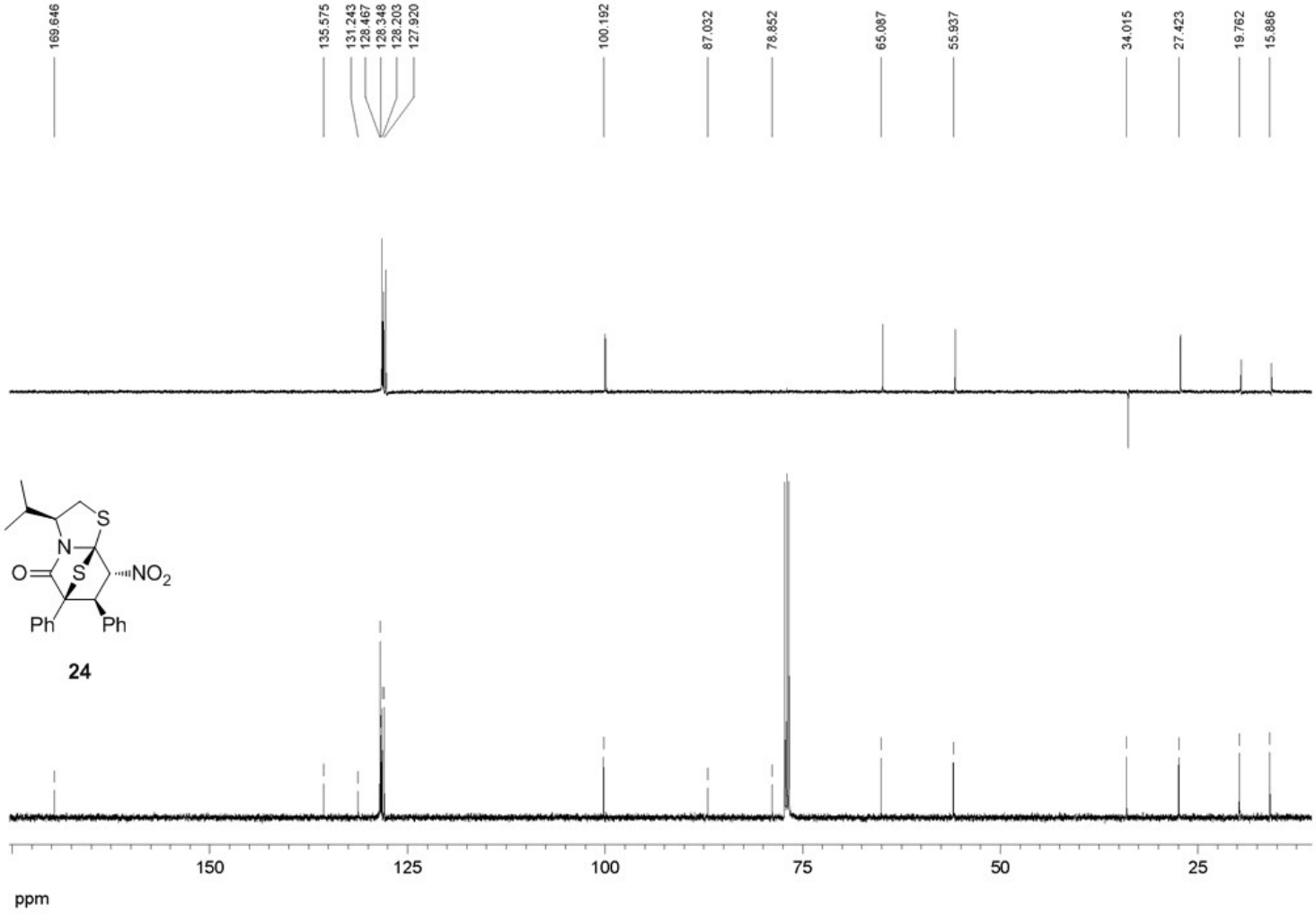
Compound **24**: FT-IR spectrum



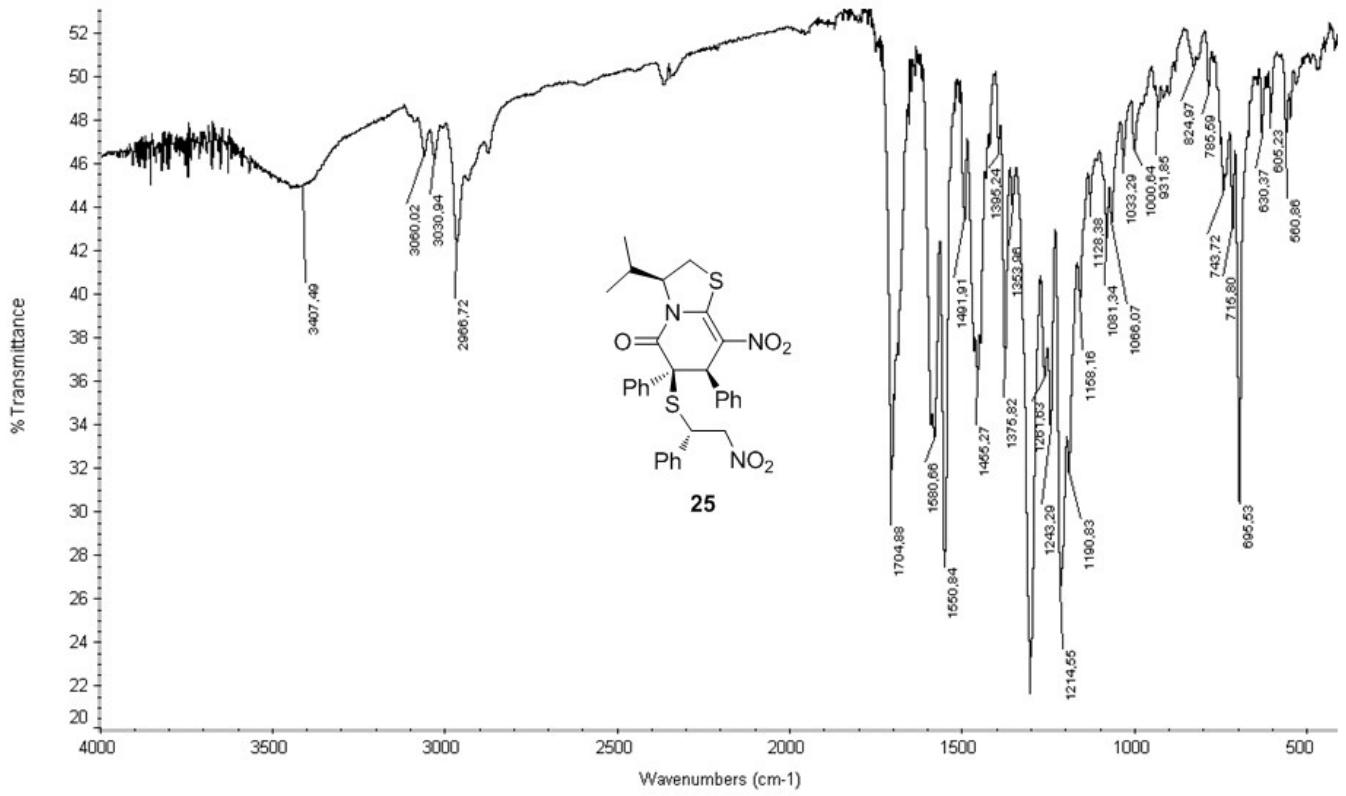
Compound **24**: ^{1}H NMR spectrum



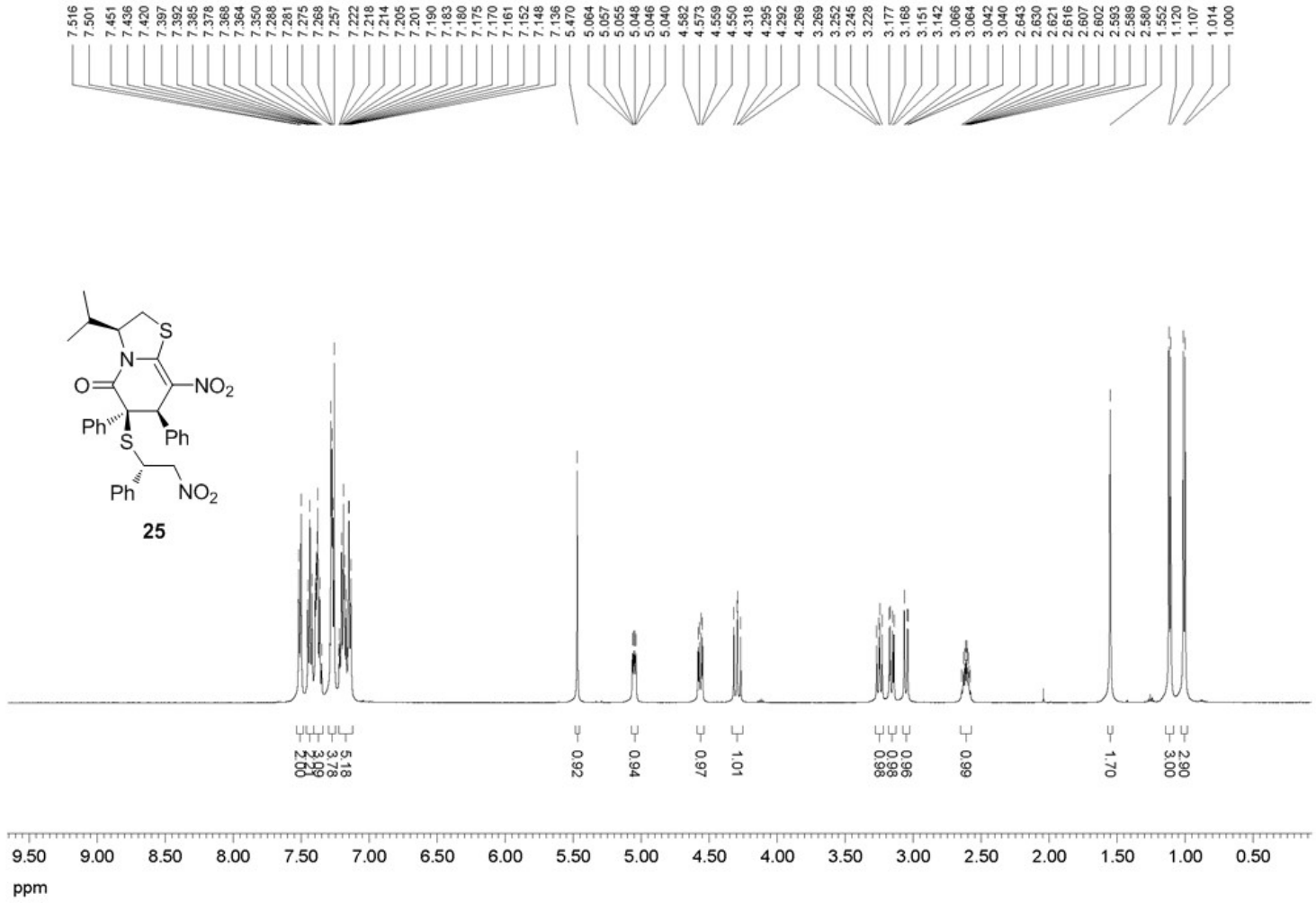
Compound **24**: ^{13}C NMR spectrum



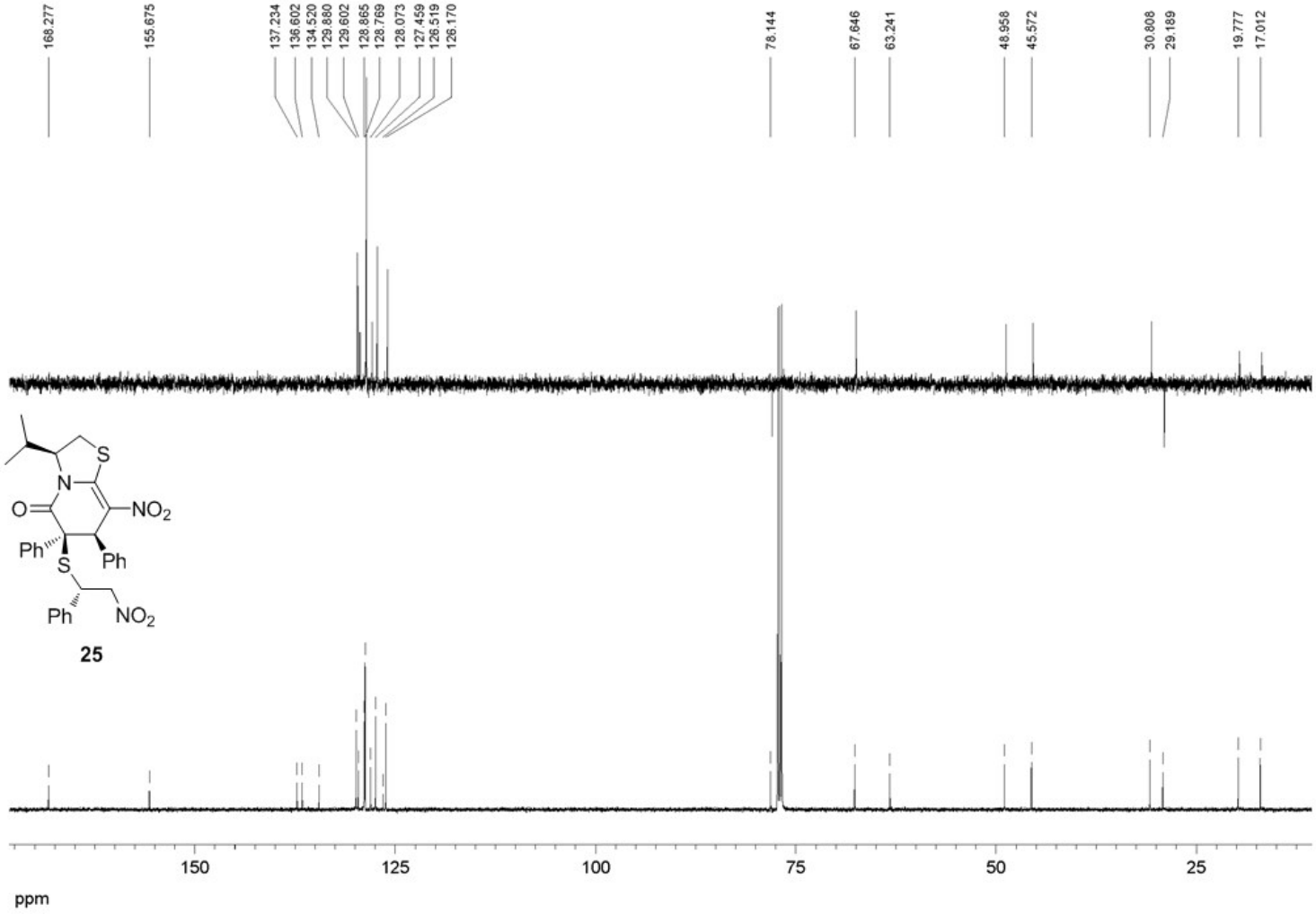
Compound **25**: FT-IR spectrum



Compound **25**: ^{1}H NMR spectrum



Compound **25**: ^{13}C NMR spectrum



Cartesian coordinates for structures 1, 3-9, 11, 12, 14-17, 20-22, 24 and 26-45 optimized at M06-2X/6-311++G(d,p).

Structure **1** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -514.087610853
Free Energy (Hartress): -1350.721740
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.519172	-0.007547	-0.007590
2	6	0	0.307659	1.131220	-0.015942
3	6	0	1.867564	-0.625298	-0.023630
4	6	0	2.876770	1.499178	-0.140878
5	6	0	4.016520	0.605328	0.339281
6	1	0	2.984795	1.776892	-1.192050
7	1	0	2.781488	2.394242	0.471228
8	1	0	4.132441	0.644260	1.421247
9	1	0	4.959739	0.834077	-0.151129
10	7	0	1.673818	0.677115	-0.002633
11	8	0	0.064793	2.342590	-0.030725
12	6	0	-1.971915	-0.043355	0.003746
13	6	0	-2.680429	-1.258987	0.033769
14	6	0	-2.719452	1.150753	-0.016341
15	6	0	-4.068792	-1.281190	0.042997
16	1	0	-2.149655	-2.206111	0.052374
17	6	0	-4.109149	1.116967	-0.006351
18	1	0	-2.197190	2.097713	-0.041077
19	6	0	-4.796855	-0.093540	0.022946
20	1	0	-4.583982	-2.235207	0.067685
21	1	0	-4.659628	2.051621	-0.023088
22	1	0	-5.880375	-0.112467	0.030053
23	16	0	3.528261	-1.122019	-0.106315
24	16	0	0.419290	-1.495901	-0.003876

Structure **1** in 2-propanol:

Electronic Energy (Hartrees): -514.087610853
Free Energy (Hartress): -1350.723179
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.517472	-0.003390	-0.013415
2	6	0	0.310570	1.124161	0.058262
3	6	0	1.866144	-0.624223	-0.062439
4	6	0	2.874669	1.506678	-0.026626
5	6	0	4.017496	0.578506	0.374698
6	1	0	2.976072	1.871719	-1.051179
7	1	0	2.781591	2.347816	0.658397
8	1	0	4.146214	0.540933	1.455204
9	1	0	4.955064	0.843086	-0.108919
10	7	0	1.671355	0.674934	0.049587
11	8	0	0.065329	2.342616	0.131344
12	6	0	-1.973581	-0.039795	0.002862
13	6	0	-2.673472	-1.232410	0.253940
14	6	0	-2.721775	1.126270	-0.238943
15	6	0	-4.061950	-1.260948	0.255240
16	1	0	-2.134992	-2.151586	0.464000
17	6	0	-4.111284	1.089857	-0.227591
18	1	0	-2.206705	2.056148	-0.440163
19	6	0	-4.792617	-0.099591	0.016822
20	1	0	-4.574474	-2.196355	0.451471
21	1	0	-4.665137	2.002817	-0.418711
22	1	0	-5.876218	-0.121850	0.021838
23	16	0	3.525973	-1.113191	-0.187359
24	16	0	0.416284	-1.489865	-0.111807

Structure **3** in dichloromethane:

Electronic Energy (Hartrees): -590.425412630
Free Energy (Hartress): -590.312185
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.985158	0.643862	-0.161479
2	6	0	2.985158	-0.643862	0.161476
3	1	0	3.818030	1.310886	-0.332583
4	1	0	3.818030	-1.310888	0.332577
5	7	0	0.761236	0.000000	0.000001
6	6	0	1.565677	1.110367	-0.281745
7	6	0	1.565677	-1.110366	0.281748
8	8	0	1.171108	2.208495	-0.569126
9	8	0	1.171108	-2.208495	0.569127
10	6	0	-0.662425	0.000000	0.000001
11	6	0	-1.348722	-0.948532	-0.753179
12	6	0	-1.348723	0.948532	0.753179
13	6	0	-2.739231	-0.949779	-0.742502
14	1	0	-0.796641	-1.674996	-1.337248
15	6	0	-2.739232	0.949778	0.742501
16	1	0	-0.796643	1.674996	1.337249
17	6	0	-3.435716	0.000000	-0.000001
18	1	0	-3.277697	-1.690894	-1.321494
19	1	0	-3.277699	1.690894	1.321492
20	1	0	-4.519479	-0.000001	-0.000002

Structure **4** in toluene:

Electronic Energy (Hartrees): -534.290367557
Free Energy (Hartress): -534.185672
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742203	-1.724011	-0.074108
2	6	0	0.581675	-1.764639	0.030199
3	1	0	-1.324283	-2.633253	-0.171262
4	1	0	1.109506	-2.710993	0.075151
5	6	0	1.443395	-0.550768	0.145076
6	6	0	-1.528839	-0.458901	-0.115992
7	8	0	1.217111	0.322460	-0.838265
8	8	0	-1.065965	0.451854	0.744393
9	8	0	2.265941	-0.401462	1.008799
10	8	0	-2.480767	-0.289469	-0.830982
11	6	0	1.916914	1.566034	-0.731067
12	1	0	2.994527	1.400075	-0.732131
13	1	0	1.622651	2.147184	-1.601742
14	1	0	1.629541	2.079980	0.187952
15	6	0	-1.679921	1.742082	0.674200
16	1	0	-1.538727	2.173645	-0.318283
17	1	0	-2.746391	1.670344	0.889957
18	1	0	-1.183510	2.347170	1.428954

Structure **5** in dichloromethane:

Electronic Energy (Hartrees): -514.087610853
Free Energy (Hartress): -513.989844
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.616123	0.457845	-0.000061
2	1	0	0.914037	1.502712	-0.000173

3	6	0	1.587389	-0.453420	0.000002
4	1	0	1.492817	-1.528425	0.000112
5	6	0	-0.820496	0.179982	0.000015
6	6	0	-1.703051	1.265551	-0.000032
7	6	0	-1.343030	-1.120609	0.000126
8	6	0	-3.077622	1.060336	0.000036
9	1	0	-1.304546	2.274352	-0.000123
10	6	0	-2.713809	-1.323566	0.000194
11	1	0	-0.677536	-1.975858	0.000157
12	6	0	-3.584582	-0.233981	0.000150
13	1	0	-3.750400	1.909509	-0.000001
14	1	0	-3.108093	-2.332683	0.000282
15	1	0	-4.655698	-0.398360	0.000202
16	7	0	2.980274	-0.033470	-0.000093
17	8	0	3.806454	-0.927525	-0.000074
18	8	0	3.251292	1.151302	-0.000223

Structure **6** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -170.811816015
Free Energy (Hartress): -170.786465
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.587743	-0.367406	0.000085
2	6	0	-0.592130	0.515944	0.000007
3	1	0	-1.403504	-1.435792	0.000117
4	1	0	-2.616187	-0.026186	0.000120
5	1	0	-0.757680	1.587151	-0.000026
6	6	0	0.778571	0.095568	-0.000039
7	7	0	1.883598	-0.227116	-0.000075

Structure **7** in 2-propanol:

Electronic Energy (Hartrees): -231.203332483
Free Energy (Hartress): -231.143096
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.005247	-0.099588	-0.000162
2	6	0	-0.798977	-0.660384	-0.000048
3	1	0	-2.118507	0.980351	-0.000188
4	1	0	-2.907992	-0.700514	-0.000228
5	1	0	-0.676034	-1.738896	-0.000026
6	6	0	0.446388	0.162542	0.000038
7	8	0	0.408754	1.379529	0.000102
8	6	0	1.739426	-0.596973	0.000065
9	1	0	1.776840	-1.246892	0.879676
10	1	0	1.776811	-1.247096	-0.879391
11	1	0	2.589314	0.083239	-0.000014

Structure **8** in dichloromethane:

Electronic Energy (Hartrees): -1941.35116568
Free Energy (Hartress): -1941.067517
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.688864	0.030866	-0.219585
2	6	0	0.459198	2.049875	-0.434557
3	6	0	0.555294	-0.240569	-1.256469
4	1	0	0.988230	-0.602217	-2.188262
5	6	0	-0.208170	1.082657	-1.442866

6	1	0	-0.164950	1.478555	-2.456137
7	16	0	2.261118	1.729314	-0.736298
8	7	0	0.222473	1.497121	0.895253
9	6	0	0.993448	0.392885	1.126293
10	8	0	1.093369	-0.198063	2.174247
11	6	0	2.797648	-0.974743	-0.101751
12	6	0	2.851366	-2.116131	-0.901129
13	6	0	3.818593	-0.747564	0.828452
14	6	0	3.911375	-3.011501	-0.778549
15	1	0	2.063948	-2.331088	-1.611822
16	6	0	4.873869	-1.641624	0.949879
17	1	0	3.786295	0.134828	1.458813
18	6	0	4.924087	-2.777299	0.143541
19	1	0	3.937382	-3.895710	-1.404918
20	1	0	5.657252	-1.453443	1.674903
21	1	0	5.746831	-3.476620	0.238238
22	16	0	-0.056723	3.780095	-0.382622
23	6	0	-0.260575	2.423209	1.917638
24	6	0	-1.023814	3.492896	1.151266
25	1	0	-0.910491	1.895307	2.616365
26	1	0	0.587165	2.853551	2.459142
27	1	0	-2.025137	3.161818	0.881164
28	1	0	-1.075038	4.430861	1.701117
29	7	0	-1.710638	-0.566648	-0.667510
30	6	0	-0.488612	-1.233571	-0.764114
31	6	0	-1.643084	0.772244	-1.056802
32	8	0	-0.317872	-2.391656	-0.491859
33	8	0	-2.574220	1.532390	-1.055858
34	6	0	-2.905931	-1.181498	-0.179860
35	6	0	-4.045449	-1.185839	-0.977297
36	6	0	-2.907811	-1.756129	1.086712
37	6	0	-5.209813	-1.769713	-0.490040
38	1	0	-4.016561	-0.735946	-1.962471
39	6	0	-4.074186	-2.347453	1.559594
40	1	0	-2.006736	-1.738791	1.689122
41	6	0	-5.224722	-2.351731	0.774585
42	1	0	-6.104032	-1.773131	-1.102218
43	1	0	-4.083592	-2.800520	2.543912
44	1	0	-6.133399	-2.808299	1.149680

Structure **9** in dichloromethane:

Electronic Energy (Hartrees): -1941.35020626
Free Energy (Hartress): -1941.068667
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.364417	0.690605	-0.040669
2	6	0	1.343127	-1.674708	0.108937
3	6	0	0.388750	0.177804	-1.153421
4	1	0	0.735796	0.511384	-2.132946
5	16	0	0.966418	-0.395730	1.413227
6	7	0	2.638986	-1.261085	-0.421037
7	6	0	2.758353	0.104474	-0.404627
8	8	0	3.771457	0.724216	-0.613001
9	6	0	1.358809	2.173059	0.191979
10	6	0	1.800152	3.011410	-0.835581
11	6	0	0.898075	2.734002	1.379821
12	6	0	1.779936	4.390282	-0.671521
13	1	0	2.158001	2.583423	-1.765222
14	6	0	0.877665	4.117217	1.543363
15	1	0	0.542150	2.101603	2.186435
16	6	0	1.317256	4.947391	0.519246
17	1	0	2.124544	5.031531	-1.474592
18	1	0	0.513580	4.540804	2.472075
19	1	0	1.299905	6.023757	0.645628
20	6	0	0.311222	-1.349748	-0.991531
21	7	0	-1.827200	-0.430113	-0.598051
22	6	0	-1.122327	-1.630738	-0.573303
23	6	0	-1.034482	0.667968	-0.935120
24	8	0	-1.590668	-2.697238	-0.276898
25	8	0	-1.433918	1.796780	-1.026457

26	6	0	-3.207533	-0.322998	-0.243670
27	6	0	-4.110637	0.208830	-1.157476
28	6	0	-3.619895	-0.752495	1.013433
29	6	0	-5.451148	0.313455	-0.801622
30	1	0	-3.765200	0.533943	-2.131627
31	6	0	-4.964222	-0.653325	1.355206
32	1	0	-2.894300	-1.157415	1.709191
33	6	0	-5.878824	-0.119909	0.450654
34	1	0	-6.161194	0.729753	-1.506348
35	1	0	-5.294794	-0.989160	2.330982
36	1	0	-6.925158	-0.041094	0.722087
37	16	0	1.519846	-3.382040	0.679886
38	6	0	3.756014	-2.163608	-0.146483
39	6	0	3.143697	-3.551942	-0.160163
40	1	0	3.741670	-4.270710	0.396977
41	1	0	2.984559	-3.910778	-1.176294
42	1	0	4.516267	-2.052625	-0.919347
43	1	0	4.192013	-1.932968	0.830645
44	1	0	0.544026	-1.910948	-1.897690

Structure **11** in toluene:

Electronic Energy (Hartrees): -1885.20842903
Free Energy (Hartress): -1884.936447
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.098331	-2.105866	0.535733
2	6	0	-0.686993	-0.762909	0.024199
3	6	0	1.664585	-0.674369	-0.056041
4	6	0	-0.239755	0.291631	1.112173
5	1	0	-0.477081	-0.110462	2.097957
6	6	0	1.307657	0.436495	0.954969
7	1	0	1.790444	0.201974	1.907725
8	16	0	0.429064	-0.446820	-1.412559
9	16	0	3.400801	-0.878497	-0.523366
10	7	0	1.255568	-1.934334	0.567412
11	8	0	-0.703655	-3.094353	0.870418
12	6	0	-2.164172	-0.763290	-0.250304
13	6	0	-3.041489	-1.192194	0.749111
14	6	0	-2.684627	-0.276254	-1.448489
15	6	0	-4.414736	-1.142965	0.544443
16	1	0	-2.650064	-1.569964	1.686079
17	6	0	-4.060050	-0.230670	-1.652879
18	1	0	-2.017901	0.080010	-2.226418
19	6	0	-4.927889	-0.663988	-0.657161
20	1	0	-5.084644	-1.480378	1.326498
21	1	0	-4.450106	0.146622	-2.591186
22	1	0	-5.999410	-0.627967	-0.815736
23	6	0	2.262822	-2.979670	0.667560
24	1	0	1.771122	-3.948835	0.569851
25	1	0	2.771684	-2.928290	1.633166
26	6	0	3.231669	-2.700635	-0.473973
27	6	0	1.754156	1.847662	0.616786
28	6	0	-1.045128	1.573661	1.000964
29	8	0	1.524565	2.786765	1.331876
30	8	0	-1.766230	1.980435	1.870278
31	8	0	-0.890839	2.164992	-0.182839
32	8	0	2.455519	1.917222	-0.508684
33	6	0	2.894912	3.224860	-0.895286
34	1	0	3.397508	3.095167	-1.850428
35	1	0	2.036753	3.889316	-1.000842
36	1	0	3.583628	3.628862	-0.152887
37	6	0	-1.636787	3.371053	-0.372516
38	1	0	-2.705716	3.170226	-0.288217
39	1	0	-1.341749	4.115458	0.368281
40	1	0	-1.393477	3.713898	-1.375493
41	1	0	2.835451	-3.053212	-1.426450
42	1	0	4.216814	-3.132814	-0.303109

Structure **12** in toluene:

Electronic Energy (Hartrees): -1885.20698361
Free Energy (Hartress): -1884.932201
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.270497	-0.624871	1.214259
2	6	0	-1.021485	-0.586244	-0.150177
3	6	0	1.230314	-1.235502	-0.453729
4	6	0	-0.381676	0.502331	-1.079047
5	1	0	-0.922838	0.476121	-2.022867
6	6	0	1.102550	0.050624	-1.296779
7	1	0	1.228994	-0.201235	-2.351174
8	16	0	-0.339574	-2.142078	-0.895129
9	16	0	2.739853	-2.225928	-0.580283
10	7	0	1.046474	-0.893760	0.944506
11	6	0	-2.516679	-0.485496	-0.049472
12	6	0	-3.078569	0.506738	0.758560
13	6	0	-3.357609	-1.319484	-0.784588
14	6	0	-4.457707	0.658661	0.824996
15	1	0	-2.436971	1.149411	1.350205
16	6	0	-4.738754	-1.168636	-0.713204
17	1	0	-2.940284	-2.090637	-1.423486
18	6	0	-5.291686	-0.179068	0.090815
19	1	0	-4.881220	1.430205	1.457142
20	1	0	-5.379590	-1.826033	-1.289100
21	1	0	-6.367594	-0.060606	0.145953
22	6	0	2.090833	1.175340	-1.036013
23	6	0	-0.556352	1.906553	-0.531648
24	8	0	-1.216329	2.762050	-1.049986
25	8	0	2.053809	2.199022	-1.668518
26	8	0	0.101181	2.061447	0.624101
27	8	0	2.984158	0.927586	-0.084855
28	6	0	3.895519	1.997272	0.195837
29	1	0	4.533158	1.641025	1.001749
30	1	0	4.491949	2.231924	-0.685947
31	1	0	3.345128	2.884542	0.511565
32	6	0	0.028534	3.363572	1.215141
33	1	0	0.449860	4.106011	0.535893
34	1	0	-1.007397	3.621358	1.438979
35	1	0	0.609197	3.305831	2.132711
36	8	0	-0.750163	-0.505422	2.312423
37	6	0	1.927511	-1.562598	1.894200
38	6	0	3.224604	-1.833525	1.143010
39	1	0	1.468213	-2.498167	2.231306
40	1	0	2.096297	-0.917930	2.757646
41	1	0	3.751353	-2.694412	1.551566
42	1	0	3.877622	-0.964466	1.134624

Structure **14** in dichloromethane:

Electronic Energy (Hartrees): -1865.00727424
Free Energy (Hartress): -1864.735786
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.883012	-1.609351	0.708441
2	6	0	-0.201278	-0.810653	-0.068866
3	6	0	1.946225	0.012798	-0.590961
4	6	0	-0.139941	0.657044	0.534305
5	6	0	1.203947	1.224492	0.030033
6	16	0	0.622969	-0.629529	-1.719249
7	16	0	3.597720	0.312628	-1.249887
8	7	0	2.073436	-1.029237	0.406880
9	8	0	0.708011	-2.537423	1.463141
10	6	0	-1.567379	-1.428318	-0.060049
11	6	0	-2.153734	-1.751283	1.167778
12	6	0	-2.293399	-1.625816	-1.232619
13	6	0	-3.440941	-2.272165	1.214300
14	1	0	-1.602767	-1.593059	2.087352

15	6	0	-3.583230	-2.149102	-1.184789
16	1	0	-1.865160	-1.366854	-2.195807
17	6	0	-4.159067	-2.474332	0.037634
18	1	0	-3.884555	-2.520382	2.171798
19	1	0	-4.134044	-2.298835	-2.106131
20	1	0	-5.163443	-2.880219	0.076030
21	6	0	3.416349	-1.510654	0.690645
22	1	0	3.362638	-2.562932	0.972477
23	1	0	3.863369	-0.935099	1.504624
24	6	0	4.179436	-1.307462	-0.612868
25	1	0	3.944114	-2.083050	-1.341023
26	1	0	5.256032	-1.245815	-0.463565
27	1	0	1.097696	2.028204	-0.692746
28	1	0	-0.097061	0.553565	1.621522
29	6	0	-1.346822	1.497841	0.186148
30	6	0	-2.352530	1.649172	1.143747
31	6	0	-1.521028	2.079834	-1.072016
32	6	0	-3.511789	2.360977	0.852899
33	1	0	-2.224434	1.202809	2.124769
34	6	0	-2.679972	2.793988	-1.363101
35	1	0	-0.761315	1.973926	-1.838270
36	6	0	-3.678451	2.935743	-0.403839
37	1	0	-4.280672	2.470063	1.609414
38	1	0	-2.800714	3.241584	-2.343178
39	1	0	-4.578809	3.494067	-0.633603
40	7	0	2.039080	1.823169	1.137881
41	8	0	2.149583	1.211436	2.177277
42	8	0	2.586660	2.875788	0.894363

Structure **15** in dichloromethane:

Electronic Energy (Hartrees): -1865.00332606
Free Energy (Hartress): -1864.736123
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.327677	-0.858692	0.373859
2	6	0	-2.338685	0.000829	-0.158573
3	6	0	0.108548	0.417498	-0.503548
4	6	0	-1.323701	0.872069	-0.401780
5	16	0	0.194508	-0.388781	2.165301
6	7	0	-2.082506	-1.341092	0.036445
7	6	0	-0.818174	-1.865962	0.248898
8	8	0	-0.670887	-3.050847	0.436627
9	6	0	1.653826	-1.506560	-0.003970
10	6	0	2.808429	-1.381336	0.761754
11	6	0	1.724660	-2.174960	-1.230670
12	6	0	4.016149	-1.911259	0.308842
13	1	0	2.780053	-0.853628	1.706957
14	6	0	2.926467	-2.703885	-1.682177
15	1	0	0.834431	-2.279969	-1.843543
16	6	0	4.080165	-2.571640	-0.911649
17	1	0	4.907935	-1.799074	0.914888
18	1	0	2.962201	-3.220616	-2.634415
19	1	0	5.020317	-2.981119	-1.263348
20	16	0	-4.055947	0.333258	-0.123128
21	6	0	-3.258777	-2.170471	0.344157
22	6	0	-4.437511	-1.449152	-0.274841
23	1	0	-3.120450	-3.161969	-0.080950
24	1	0	-4.551988	-1.689735	-1.331169
25	1	0	-5.365612	-1.652601	0.255312
26	8	0	-2.724701	2.673455	-0.507118
27	8	0	-0.878660	2.740329	-1.614927
28	1	0	0.295307	0.096863	-1.536088
29	6	0	1.135450	1.486618	-0.158953
30	6	0	0.912061	2.426718	0.848206
31	6	0	2.348240	1.505361	-0.846275
32	6	0	1.890387	3.362414	1.167766
33	1	0	-0.034005	2.443729	1.382167
34	6	0	3.328841	2.439039	-0.526641
35	1	0	2.525123	0.783149	-1.637429
36	6	0	3.103398	3.368940	0.484062

37	1	0	1.702301	4.090992	1.948180
38	1	0	4.265941	2.441544	-1.071629
39	1	0	3.864451	4.100344	0.731227
40	7	0	-1.661040	2.178052	-0.864595
41	1	0	0.323463	-1.655964	2.603490
42	1	0	-3.352325	-2.249198	1.431161

Structure **16** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -1521.73505266
Free Energy (Hartress): -1521.542424
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.745745	0.237759	-0.117239
2	6	0	1.546608	-0.053445	-0.611974
3	6	0	-0.153568	1.666251	-0.201906
4	1	0	-0.671441	2.235188	-0.972398
5	6	0	1.337747	1.486554	-0.607952
6	1	0	1.526927	1.891787	-1.602644
7	16	0	0.062694	-0.628232	-1.558915
8	7	0	1.306557	-0.513669	0.748196
9	6	0	-0.025651	-0.483263	1.054331
10	8	0	-0.534518	-0.927077	2.055484
11	6	0	-2.241440	0.120005	-0.074266
12	6	0	-3.057614	1.245058	0.039132
13	6	0	-2.832692	-1.147356	-0.116328
14	6	0	-4.443173	1.106053	0.099492
15	1	0	-2.626419	2.237637	0.088863
16	6	0	-4.213134	-1.284268	-0.059032
17	1	0	-2.208077	-2.031716	-0.191018
18	6	0	-5.023925	-0.155315	0.048258
19	1	0	-5.065218	1.989674	0.186151
20	1	0	-4.656970	-2.272566	-0.096236
21	1	0	-6.101881	-0.261973	0.092713
22	16	0	3.158929	-0.699755	-1.112865
23	6	0	2.285166	-1.441853	1.307613
24	6	0	3.597644	-1.083624	0.630287
25	1	0	2.349665	-1.305652	2.387364
26	1	0	1.994814	-2.472983	1.083895
27	1	0	4.061898	-0.208855	1.083413
28	1	0	4.298674	-1.916390	0.627488
29	1	0	-0.261912	2.182565	0.754173
30	6	0	2.272074	2.120155	0.320815
31	7	0	3.018632	2.599588	1.051155

Structure **17** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -1521.73270545
Free Energy (Hartress): -1521.539833
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.689085	0.059267	-0.135521
2	6	0	-1.647947	0.134133	0.150022
3	6	0	0.150933	0.963397	-1.283662
4	1	0	0.371081	0.522167	-2.256545
5	16	0	-0.304997	0.608408	1.332831
6	7	0	-1.276231	-1.200691	-0.294013
7	6	0	0.077671	-1.348924	-0.365442
8	8	0	0.673398	-2.376321	-0.587139
9	6	0	2.181901	0.063289	0.019221
10	6	0	2.968723	-0.222180	-1.101460
11	6	0	2.806484	0.325883	1.237129
12	6	0	4.354671	-0.238997	-1.001682
13	1	0	2.497236	-0.435922	-2.054348
14	6	0	4.196036	0.311029	1.335386

15	1	0	2.219987	0.544963	2.123493
16	6	0	4.973048	0.029694	0.217526
17	1	0	4.952134	-0.463550	-1.878102
18	1	0	4.667419	0.519401	2.289047
19	1	0	6.054346	0.018558	0.294060
20	6	0	-1.385555	1.067950	-1.067077
21	16	0	-3.328630	0.021009	0.804821
22	6	0	-2.259714	-2.259718	-0.091534
23	6	0	-3.601670	-1.546940	-0.112694
24	1	0	-4.379030	-2.109592	0.400850
25	1	0	-3.920052	-1.317135	-1.128918
26	1	0	-2.187300	-2.993159	-0.895047
27	1	0	-2.089210	-2.751129	0.870904
28	1	0	-1.948757	0.695068	-1.925454
29	1	0	0.631897	1.938886	-1.221083
30	6	0	-1.826395	2.434000	-0.798070
31	7	0	-2.178417	3.506414	-0.582706

Structure **20** in 2-propanol:

Electronic Energy (Hartrees): -1582.12549892
Free Energy (Hartress): -1581.896006
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.795748	-0.054953	-0.106999
2	6	0	-1.548917	-0.185638	0.146580
3	6	0	0.194773	1.045158	-1.026504
4	1	0	0.451529	0.848198	-2.069022
5	16	0	-0.225933	0.071981	1.437029
6	7	0	-1.092837	-1.378804	-0.573776
7	6	0	0.275098	-1.411476	-0.624426
8	8	0	0.940301	-2.357634	-0.987837
9	6	0	2.286285	0.011876	0.057147
10	6	0	3.089547	-0.084038	-1.084097
11	6	0	2.893769	0.170273	1.301449
12	6	0	4.473556	-0.020615	-0.978000
13	1	0	2.630824	-0.214177	-2.058717
14	6	0	4.281384	0.235383	1.406717
15	1	0	2.293557	0.244456	2.202475
16	6	0	5.074099	0.140031	0.268998
17	1	0	5.083953	-0.097024	-1.870853
18	1	0	4.738685	0.360106	2.381852
19	1	0	6.154047	0.189602	0.351306
20	6	0	-1.342404	1.007309	-0.796649
21	6	0	-1.872752	2.324649	-0.262781
22	8	0	-2.449452	2.401519	0.800007
23	16	0	-3.225304	-0.537361	0.737977
24	6	0	-1.885747	-2.588570	-0.349602
25	6	0	-3.315734	-2.104630	-0.213775
26	1	0	-3.933258	-2.809817	0.339835
27	1	0	-3.764971	-1.905926	-1.186293
28	1	0	-1.770528	-3.266854	-1.194901
29	1	0	-1.549301	-3.088924	0.564899
30	1	0	-1.868981	0.812365	-1.736996
31	1	0	0.628511	2.004356	-0.738879
32	6	0	-1.637502	3.535858	-1.124239
33	1	0	-0.828286	4.120935	-0.676309
34	1	0	-1.354542	3.270189	-2.143213
35	1	0	-2.535589	4.155446	-1.129131

Structure **21** in dichloromethane:

Electronic Energy (Hartrees): -2059.26625150
Free Energy (Hartress): -2058.905174
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.579997	1.047645	0.053799
2	6	0	1.026359	-1.260149	0.189542
3	6	0	-0.235140	0.368269	-1.100615
4	1	0	0.059891	0.786335	-2.064973
5	16	0	0.334749	-0.109383	1.473371
6	7	0	2.251664	-0.589968	-0.250164
7	6	0	2.080437	0.764215	-0.284385
8	8	0	2.894766	1.617694	-0.544795
9	6	0	0.276654	2.498368	0.296179
10	6	0	0.468905	3.406975	-0.748253
11	6	0	-0.200711	2.960136	1.519980
12	6	0	0.187332	4.754517	-0.567215
13	1	0	0.837111	3.056788	-1.705918
14	6	0	-0.483670	4.312354	1.701469
15	1	0	-0.363315	2.272295	2.343000
16	6	0	-0.290986	5.211440	0.659842
17	1	0	0.338915	5.450182	-1.384460
18	1	0	-0.856790	4.657469	2.658836
19	1	0	-0.513556	6.263074	0.799907
20	6	0	0.012973	-1.141768	-0.964700
21	7	0	-2.286056	-0.726104	-0.650105
22	6	0	-1.336114	-1.740859	-0.617478
23	6	0	-1.737025	0.531776	-0.920692
24	8	0	-1.555853	-2.893613	-0.352172
25	8	0	-2.369603	1.549729	-0.987955
26	6	0	-3.666554	-0.927271	-0.340716
27	6	0	-4.638937	-0.522033	-1.248454
28	6	0	-4.010811	-1.517929	0.870785
29	6	0	-5.980099	-0.710945	-0.932502
30	1	0	-4.344859	-0.064589	-2.185614
31	6	0	-5.354338	-1.712496	1.171483
32	1	0	-3.233820	-1.819413	1.563374
33	6	0	-6.338307	-1.307944	0.273306
34	1	0	-6.744557	-0.393338	-1.631848
35	1	0	-5.630759	-2.176373	2.111017
36	1	0	-7.384644	-1.457446	0.513245
37	16	0	1.478188	-2.913639	0.747466
38	6	0	3.461504	-1.443004	-0.247826
39	6	0	3.218047	-2.383867	0.930229
40	1	0	3.358702	-1.875918	1.886426
41	1	0	3.840354	-3.276031	0.885760
42	1	0	3.449748	-2.043585	-1.166294
43	1	0	0.410189	-1.618786	-1.862075
44	6	0	4.784952	-0.667108	-0.198661
45	1	0	4.674220	0.162552	0.504511
46	6	0	5.914580	-1.577585	0.290017
47	1	0	6.868167	-1.049920	0.212659
48	1	0	5.784498	-1.881939	1.330622
49	1	0	5.982368	-2.479533	-0.327405
50	6	0	5.135016	-0.129970	-1.587870
51	1	0	5.402398	-0.961337	-2.248490
52	1	0	4.307375	0.419147	-2.036752
53	1	0	5.993270	0.544134	-1.531242

Structure **22** in dichloromethane:

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Electronic Energy (Hartrees): -2059.27142820
Free Energy (Hartress): -2058.906913
No imaginary frequencies.
Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.241272	-0.939755	0.398391
2	6	0	-0.470740	1.277490	0.069647
3	6	0	-2.008979	1.184931	-0.162302
4	6	0	-0.273170	-1.040287	-0.793858
5	6	0	0.176413	0.404752	-1.058569
6	16	0	-0.320141	0.195832	1.569203
7	16	0	-1.907942	-2.469010	1.056401
8	7	0	-2.368115	-0.129149	-0.040140
9	6	0	-3.723017	-0.565077	0.331278
10	1	0	-4.208829	0.290395	0.810123

11	6	0	-3.521579	-1.664993	1.386330
12	1	0	-3.508179	-1.245099	2.391115
13	1	0	-4.288806	-2.437179	1.333027
14	8	0	-2.755908	2.105143	-0.390668
15	6	0	0.041591	2.684660	0.181113
16	6	0	0.659227	3.160332	1.334404
17	6	0	-0.105926	3.537058	-0.916891
18	6	0	1.128780	4.470758	1.392278
19	1	0	0.786888	2.515139	2.197400
20	6	0	0.362751	4.842716	-0.858745
21	1	0	-0.586761	3.176206	-1.819702
22	6	0	0.981962	5.313799	0.297582
23	1	0	1.609762	4.827361	2.295760
24	1	0	0.245166	5.494762	-1.716622
25	1	0	1.348644	6.332892	0.341885
26	6	0	-4.563641	-0.950368	-0.894531
27	1	0	-4.492458	-0.091860	-1.572276
28	6	0	-4.048269	-2.186439	-1.625975
29	1	0	-2.999272	-2.079569	-1.913697
30	1	0	-4.138566	-3.082609	-1.004892
31	1	0	-4.632224	-2.351151	-2.535129
32	6	0	-6.029830	-1.117865	-0.497877
33	1	0	-6.410214	-0.227175	0.009670
34	1	0	-6.643851	-1.289744	-1.384900
35	1	0	-6.168428	-1.974888	0.168229
36	1	0	-0.107627	0.786943	-2.040638
37	1	0	-0.768467	-1.518565	-1.639739
38	6	0	1.693920	0.362925	-0.956475
39	6	0	0.994762	-1.798310	-0.449378
40	7	0	2.074158	-0.937301	-0.608758
41	8	0	2.458653	1.270984	-1.133693
42	8	0	1.063904	-2.945602	-0.094677
43	6	0	3.425525	-1.308409	-0.327467
44	6	0	3.748824	-1.776462	0.941765
45	6	0	4.391107	-1.184536	-1.320084
46	6	0	5.064465	-2.133549	1.215741
47	1	0	2.977381	-1.857952	1.699065
48	6	0	5.705996	-1.534829	-1.032570
49	1	0	4.111281	-0.820520	-2.301548
50	6	0	6.042510	-2.010469	0.231912
51	1	0	5.325985	-2.501344	2.200954
52	1	0	6.466054	-1.437658	-1.798968
53	1	0	7.067900	-2.285017	0.451490

Structure **24** in dichloromethane:

Electronic Energy (Hartrees): -1982.92407340
Free Energy (Hartress): -1982.572907
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.528643	0.647537	-0.105635
2	6	0	-1.311021	-0.694405	-0.706699
3	6	0	0.823051	-0.773739	0.537876
4	6	0	-0.325854	-1.662405	0.026359
5	1	0	-0.011330	-2.463583	-0.636078
6	16	0	-0.136888	0.223707	-1.785385
7	7	0	-1.761087	0.308438	0.231933
8	6	0	-0.756796	1.131933	0.626263
9	8	0	-0.838145	2.024841	1.439627
10	6	0	1.688349	1.597299	-0.066926
11	6	0	2.388056	1.949928	-1.219506
12	6	0	2.125974	2.080877	1.170471
13	6	0	3.500750	2.783834	-1.143438
14	1	0	2.076845	1.575589	-2.189421
15	6	0	3.235490	2.914375	1.244547
16	1	0	1.597234	1.805430	2.074885
17	6	0	3.926872	3.268071	0.087984
18	1	0	4.033979	3.048798	-2.049072
19	1	0	3.563625	3.284756	2.209083
20	1	0	4.793649	3.916397	0.147244
21	16	0	-2.789570	-1.401914	-1.451038

22	6	0	-3.170931	0.341195	0.630480
23	6	0	-3.783962	-0.935450	0.025955
24	1	0	-3.214880	0.262555	1.721286
25	1	0	-3.771392	-1.761769	0.736014
26	1	0	-4.808481	-0.779470	-0.309780
27	8	0	-1.475805	-3.475226	0.908973
28	6	0	-3.851866	1.655291	0.208987
29	1	0	-3.217907	2.454257	0.605147
30	6	0	-3.951512	1.828096	-1.304675
31	1	0	-2.976352	1.731524	-1.789722
32	1	0	-4.627947	1.091127	-1.748532
33	1	0	-4.345917	2.820846	-1.536137
34	6	0	-5.222806	1.768495	0.873909
35	1	0	-5.148768	1.668706	1.960216
36	1	0	-5.668343	2.741641	0.655122
37	1	0	-5.911950	1.001835	0.506753
38	8	0	-1.271447	-1.752115	2.172683
39	1	0	0.732547	-0.656736	1.620464
40	6	0	2.210160	-1.293750	0.233699
41	6	0	2.557951	-1.848582	-1.000495
42	6	0	3.199654	-1.154942	1.210587
43	6	0	3.868506	-2.245550	-1.251172
44	1	0	1.814971	-1.971590	-1.779840
45	6	0	4.509514	-1.550088	0.960414
46	1	0	2.940503	-0.729284	2.174579
47	6	0	4.848613	-2.093977	-0.274802
48	1	0	4.122082	-2.674724	-2.213903
49	1	0	5.263109	-1.433579	1.731081
50	1	0	5.868562	-2.402943	-0.473504
51	7	0	-1.070106	-2.357400	1.141140

Structure **26** in dichloromethane:

Electronic Energy (Hartrees): -1982.92307680
Free Energy (Hartress): -1982.575546
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550773	-0.801246	0.128272
2	6	0	-1.687949	0.824543	-0.624160
3	6	0	0.818079	0.569244	-0.574480
4	6	0	-0.445243	1.383201	-0.652798
5	16	0	0.332389	-0.504744	1.948512
6	7	0	-1.851737	-0.532697	-0.455563
7	6	0	-0.803935	-1.416164	-0.241932
8	8	0	-0.995797	-2.609214	-0.236331
9	6	0	1.678748	-1.768205	-0.214135
10	6	0	2.680065	-2.128135	0.681114
11	6	0	1.744204	-2.243241	-1.528340
12	6	0	3.731198	-2.948620	0.271565
13	1	0	2.659041	-1.759901	1.698989
14	6	0	2.788221	-3.061816	-1.936792
15	1	0	0.973212	-1.967691	-2.241718
16	6	0	3.789791	-3.417193	-1.034492
17	1	0	4.506224	-3.214846	0.981195
18	1	0	2.820355	-3.422332	-2.958569
19	1	0	4.607766	-4.054571	-1.350442
20	16	0	-3.215671	1.628576	-0.885716
21	6	0	-3.243491	-1.034471	-0.380733
22	6	0	-4.087224	0.031758	-1.074515
23	1	0	-3.280591	-1.958118	-0.958751
24	1	0	-4.193547	-0.172645	-2.138593
25	1	0	-5.075533	0.131523	-0.627471
26	8	0	-1.282545	3.490469	-0.940982
27	6	0	-3.634817	-1.351426	1.073278
28	1	0	-2.852188	-2.015730	1.455630
29	6	0	-3.700442	-0.118299	1.972825
30	1	0	-2.764142	0.445650	1.969366
31	1	0	-4.509814	0.553099	1.670945
32	1	0	-3.896143	-0.427435	3.002786
33	6	0	-4.954395	-2.122316	1.100181
34	1	0	-4.905748	-3.022485	0.481641

35	1	0	-5.189594	-2.426655	2.122579
36	1	0	-5.784615	-1.505329	0.743333
37	8	0	0.711005	3.071047	-1.639228
38	1	0	1.124454	0.322669	-1.597981
39	6	0	1.986735	1.286964	0.088983
40	6	0	1.796611	2.186939	1.138282
41	6	0	3.284456	1.010235	-0.339941
42	6	0	2.888014	2.789269	1.756502
43	1	0	0.792040	2.430191	1.472734
44	6	0	4.377109	1.609135	0.279613
45	1	0	3.440301	0.320034	-1.163344
46	6	0	4.181603	2.498701	1.332030
47	1	0	2.725768	3.490859	2.566797
48	1	0	5.380163	1.383719	-0.064620
49	1	0	5.031249	2.969943	1.812997
50	7	0	-0.331176	2.730703	-1.098591
51	1	0	-0.085718	-1.758855	2.207213

Structure **27** in dichloromethane:

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Electronic Energy (Hartrees): -1865.00897656
Free Energy (Hartress): -1864.736476
No imaginary frequencies.

Standard orientation:
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.239780	-0.474026	-1.516609
2	6	0	0.277501	-0.826229	-0.099122
3	6	0	-2.023104	-0.270811	-0.004265
4	6	0	0.177683	0.484785	0.781232
5	6	0	-1.336068	0.813748	0.839827
6	16	0	-1.157374	-1.819037	0.529535
7	16	0	-3.827284	-0.285250	-0.113289
8	7	0	-1.526381	-0.050856	-1.358659
9	8	0	0.363250	-0.532720	-2.561922
10	6	0	1.622162	-1.493720	-0.027000
11	6	0	2.685801	-1.013967	-0.798907
12	6	0	1.850743	-2.547267	0.860159
13	6	0	3.946365	-1.592654	-0.690768
14	1	0	2.529184	-0.192473	-1.486161
15	6	0	3.112703	-3.123843	0.966285
16	1	0	1.046081	-2.925911	1.481980
17	6	0	4.163728	-2.649341	0.188734
18	1	0	4.760369	-1.214042	-1.298372
19	1	0	3.269710	-3.943417	1.657902
20	1	0	5.146835	-3.099186	0.269078
21	6	0	-2.524781	0.129592	-2.405581
22	1	0	-2.130923	-0.280177	-3.336553
23	1	0	-2.745928	1.191118	-2.540166
24	6	0	-3.749062	-0.626994	-1.911361
25	1	0	-3.647670	-1.700214	-2.072506
26	1	0	-4.672648	-0.269315	-2.364194
27	1	0	0.510038	0.186092	1.776222
28	1	0	-1.581983	1.811304	0.469548
29	7	0	-1.812938	0.838570	2.274845
30	8	0	-1.155801	1.493918	3.050911
31	8	0	-2.828804	0.244532	2.555370
32	6	0	1.069645	1.606434	0.301851
33	6	0	2.285986	1.821407	0.952504
34	6	0	0.747603	2.393324	-0.807228
35	6	0	3.168487	2.798788	0.503004
36	1	0	2.541677	1.215804	1.816384
37	6	0	1.631062	3.368090	-1.259992
38	1	0	-0.195631	2.254649	-1.326742
39	6	0	2.844050	3.572086	-0.607821
40	1	0	4.107945	2.955533	1.020672
41	1	0	1.369023	3.969485	-2.123085
42	1	0	3.530164	4.333113	-0.961782

Structure **28** in dichloromethane:

Electronic Energy (Hartrees): -1865.00803088
Free Energy (Hartress): -1864.73679
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.501372	1.144727	1.191088
2	6	0	1.211936	0.368776	0.034677
3	6	0	-0.939276	1.044301	-0.647096
4	6	0	0.335912	-0.928513	-0.120941
5	6	0	-1.012967	-0.508979	-0.742014
6	16	0	0.713417	1.411719	-1.405244
7	16	0	-2.353783	1.983979	-1.250248
8	7	0	-0.753621	1.417592	0.751411
9	8	0	0.969653	1.428610	2.267876
10	6	0	2.679671	0.115069	0.224071
11	6	0	3.129731	-0.444214	1.424257
12	6	0	3.590920	0.352491	-0.803958
13	6	0	4.476310	-0.740027	1.594064
14	1	0	2.426649	-0.649682	2.222196
15	6	0	4.940202	0.054696	-0.630693
16	1	0	3.256044	0.764811	-1.750303
17	6	0	5.385242	-0.489012	0.568524
18	1	0	4.816859	-1.169143	2.529409
19	1	0	5.638773	0.245916	-1.436789
20	1	0	6.435224	-0.721874	0.704074
21	6	0	-1.697328	2.380752	1.303770
22	1	0	-1.184622	2.991418	2.048181
23	1	0	-2.536966	1.860247	1.770595
24	6	0	-2.161463	3.202457	0.106667
25	1	0	-1.420674	3.948932	-0.179522
26	1	0	-3.125996	3.678658	0.275052
27	1	0	-1.003666	-0.772138	-1.800345
28	1	0	0.241458	-1.430301	0.840826
29	7	0	1.082653	-1.923333	-0.977166
30	8	0	1.084419	-1.772895	-2.178040
31	8	0	1.679778	-2.798836	-0.389576
32	6	0	-2.237178	-1.108829	-0.090690
33	6	0	-3.261001	-1.589980	-0.908544
34	6	0	-2.402493	-1.156065	1.296250
35	6	0	-4.429978	-2.105085	-0.357028
36	1	0	-3.139520	-1.558770	-1.986676
37	6	0	-3.572235	-1.668826	1.848803
38	1	0	-1.622332	-0.794141	1.957491
39	6	0	-4.589220	-2.143342	1.024685
40	1	0	-5.213458	-2.476671	-1.007533
41	1	0	-3.686857	-1.700162	2.926350
42	1	0	-5.498034	-2.545485	1.457707

Structure **29** in dichloromethane:

Electronic Energy (Hartrees): -1865.00782214
Free Energy (Hartress): -1864.736272
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.119734	1.678107	0.348811
2	6	0	1.173881	0.227367	-0.225218
3	6	0	-1.032114	1.061045	-0.323766
4	6	0	0.276383	-0.713122	0.645936
5	6	0	-1.165165	-0.147541	0.645339
6	16	0	0.060764	0.420373	-1.690273
7	16	0	-2.555004	1.903766	-0.788675
8	7	0	-0.185270	2.050753	0.326737
9	8	0	2.059803	2.346890	0.705232
10	6	0	2.549216	-0.324765	-0.472978
11	6	0	3.511102	-0.241247	0.539067
12	6	0	2.867688	-0.976150	-1.664762
13	6	0	4.769969	-0.802386	0.354610
14	1	0	3.285077	0.273132	1.465950

15	6	0	4.129772	-1.533381	-1.847329
16	1	0	2.133697	-1.056961	-2.459988
17	6	0	5.082915	-1.448055	-0.838052
18	1	0	5.507964	-0.728849	1.145052
19	1	0	4.364244	-2.034123	-2.779472
20	1	0	6.066201	-1.881929	-0.979958
21	6	0	-0.723747	3.399610	0.444830
22	1	0	0.095759	4.115624	0.368408
23	1	0	-1.227519	3.524251	1.405884
24	6	0	-1.708833	3.528629	-0.711148
25	1	0	-1.198330	3.717446	-1.655315
26	1	0	-2.461643	4.295347	-0.536057
27	1	0	0.345543	-1.725573	0.257113
28	1	0	-1.390912	0.277384	1.626237
29	6	0	-2.258338	-1.127020	0.278675
30	6	0	-3.491373	-1.001911	0.925487
31	6	0	-2.110173	-2.109770	-0.703817
32	6	0	-4.556833	-1.832459	0.594350
33	1	0	-3.615386	-0.245975	1.694180
34	6	0	-3.175237	-2.943581	-1.032342
35	1	0	-1.168029	-2.233038	-1.224641
36	6	0	-4.400760	-2.806451	-0.387545
37	1	0	-5.505521	-1.721162	1.106840
38	1	0	-3.043943	-3.702673	-1.795048
39	1	0	-5.228281	-3.457158	-0.646053
40	7	0	0.829825	-0.807183	2.047604
41	8	0	0.869655	0.210868	2.705582
42	8	0	1.231606	-1.886315	2.417781

Structure **30** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -1521.73278087
Free Energy (Hartress): -1521.540263
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.446265	-0.001469	-0.063144
2	6	0	-1.858369	0.455277	0.122933
3	6	0	0.105202	1.087640	-1.147372
4	1	0	0.293873	0.677513	-2.143044
5	16	0	-0.516742	0.567525	1.410420
6	7	0	-1.697842	-0.889004	-0.425880
7	6	0	-0.386004	-1.257740	-0.454674
8	8	0	0.045863	-2.354465	-0.716657
9	6	0	1.911391	-0.262434	0.126285
10	6	0	2.653291	-0.706091	-0.973068
11	6	0	2.553807	-0.051976	1.344151
12	6	0	4.017492	-0.937136	-0.849648
13	1	0	2.161601	-0.871888	-1.925784
14	6	0	3.922032	-0.285250	1.466191
15	1	0	1.998203	0.296602	2.208771
16	6	0	4.655526	-0.727587	0.371570
17	1	0	4.583718	-1.280179	-1.708112
18	1	0	4.410354	-0.117745	2.419331
19	1	0	5.720273	-0.907815	0.466854
20	6	0	-1.394980	1.449854	-0.948380
21	16	0	-3.564067	0.580331	0.713700
22	6	0	-2.823341	-1.802486	-0.251171
23	6	0	-4.051141	-0.908249	-0.245455
24	1	0	-4.897189	-1.376386	0.254233
25	1	0	-4.334257	-0.608987	-1.253845
26	1	0	-2.856228	-2.514307	-1.076207
27	1	0	-2.724203	-2.341772	0.696110
28	1	0	-1.963059	1.301507	-1.866975
29	1	0	-1.520177	2.474138	-0.600964
30	6	0	0.974713	2.249156	-0.978600
31	7	0	1.654672	3.164757	-0.837084

Structure **31** in N,N-dimethylacetamide:

Electronic Energy (Hartrees): -1521.73302335
Free Energy (Hartress): -1521.540172
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.516649	0.071313	-0.229949
2	6	0	1.807298	-0.071064	-0.631853
3	6	0	-0.066759	1.460994	-0.796074
4	1	0	-0.624105	1.668199	-1.710634
5	6	0	1.455033	1.341276	-1.113232
6	1	0	1.627050	1.447662	-2.182488
7	16	0	0.423821	-1.100865	-1.320825
8	7	0	1.575926	-0.109507	0.809174
9	6	0	0.251096	-0.126967	1.110887
10	8	0	-0.239144	-0.253540	2.208893
11	6	0	-1.990306	-0.204343	-0.149178
12	6	0	-2.947911	0.734424	-0.532053
13	6	0	-2.412302	-1.450331	0.329099
14	6	0	-4.305452	0.431439	-0.440116
15	1	0	-2.658250	1.710344	-0.903572
16	6	0	-3.764259	-1.751626	0.415559
17	1	0	-1.676756	-2.187056	0.634404
18	6	0	-4.716588	-0.809361	0.030548
19	1	0	-5.037971	1.171464	-0.741397
20	1	0	-4.076669	-2.722138	0.783724
21	1	0	-5.772874	-1.043850	0.097962
22	16	0	3.493833	-0.668054	-0.900232
23	6	0	2.663485	-0.606182	1.644923
24	6	0	3.926973	-0.318443	0.849805
25	1	0	2.669823	-0.079665	2.599684
26	1	0	2.541301	-1.679459	1.818782
27	1	0	4.231443	0.723501	0.942919
28	1	0	4.750916	-0.970293	1.134017
29	1	0	2.051169	2.076213	-0.570963
30	6	0	-0.353585	2.534246	0.156947
31	7	0	-0.572333	3.367200	0.918178

Structure **32** in 2-propanol:

Electronic Energy (Hartrees): -1582.12583718
Free Energy (Hartress): -1581.894813
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.904442	0.114864	-0.180605
2	6	0	1.344912	-0.418641	-0.646355
3	6	0	-0.189479	1.466681	-0.443835
4	1	0	-0.675907	1.981011	-1.271553
5	6	0	1.272048	1.130232	-0.833343
6	1	0	1.459863	1.347553	-1.884425
7	16	0	-0.191854	-0.983233	-1.505782
8	7	0	1.065401	-0.713354	0.753138
9	6	0	-0.222161	-0.475305	1.079092
10	8	0	-0.730623	-0.639587	2.173074
11	6	0	-2.403385	0.117609	-0.113434
12	6	0	-3.141113	1.294441	-0.233515
13	6	0	-3.078796	-1.089685	0.097494
14	6	0	-4.532636	1.263760	-0.155892
15	1	0	-2.642169	2.244100	-0.383821
16	6	0	-4.464824	-1.119391	0.172014
17	1	0	-2.514565	-2.010985	0.204110
18	6	0	-5.197075	0.059781	0.043131
19	1	0	-5.093097	2.186930	-0.251490
20	1	0	-4.974647	-2.062645	0.332510
21	1	0	-6.279537	0.037443	0.100500
22	16	0	2.880487	-1.288532	-1.036138
23	6	0	2.087513	-1.402452	1.530612
24	6	0	3.375316	-1.234738	0.731670
25	1	0	2.176161	-0.948729	2.519889

26	1	0	1.821979	-2.457497	1.636780
27	1	0	3.863017	-0.282009	0.941454
28	1	0	4.078076	-2.045733	0.914565
29	6	0	2.368668	1.839809	-0.046950
30	8	0	3.405773	2.113798	-0.615502
31	1	0	-0.259414	2.101548	0.442896
32	6	0	2.160976	2.201862	1.397833
33	1	0	3.128745	2.334663	1.880782
34	1	0	1.624176	3.156717	1.429294
35	1	0	1.557060	1.472689	1.939199

Structure **33** in 2-propanol:

Electronic Energy (Hartrees): -1582.12488094
Free Energy (Hartress): -1581.896036
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.366352	-0.142495	-0.035298
2	6	0	-1.924507	0.305658	0.262871
3	6	0	0.068979	1.191905	-0.805016
4	1	0	0.166549	0.995593	-1.875010
5	16	0	-0.611759	-0.012946	1.536470
6	7	0	-1.791230	-0.826545	-0.654931
7	6	0	-0.491858	-1.204593	-0.774063
8	8	0	-0.078923	-2.185938	-1.356154
9	6	0	1.812211	-0.528949	0.096690
10	6	0	2.662648	-0.354842	-0.998963
11	6	0	2.322798	-1.081330	1.271534
12	6	0	4.001749	-0.720862	-0.914284
13	1	0	2.280575	0.063504	-1.924335
14	6	0	3.663847	-1.443614	1.355719
15	1	0	1.679266	-1.233756	2.131852
16	6	0	4.506909	-1.262906	0.264149
17	1	0	4.650911	-0.580176	-1.771010
18	1	0	4.047483	-1.865717	2.277701
19	1	0	5.552035	-1.543452	0.330342
20	6	0	-1.404711	1.551413	-0.464726
21	6	0	1.030020	2.336585	-0.504749
22	8	0	1.515595	2.945484	-1.436345
23	16	0	-3.636076	0.301247	0.851414
24	6	0	-2.947670	-1.710120	-0.775322
25	6	0	-4.147900	-0.815997	-0.512346
26	1	0	-5.017533	-1.382111	-0.183375
27	1	0	-4.404924	-0.220848	-1.388038
28	1	0	-2.985577	-2.140760	-1.776391
29	1	0	-2.881405	-2.512639	-0.034165
30	1	0	-1.989476	1.730228	-1.368201
31	1	0	-1.478773	2.424595	0.184268
32	6	0	1.338146	2.710216	0.916801
33	1	0	1.971080	3.596765	0.925199
34	1	0	0.420841	2.899400	1.477674
35	1	0	1.857467	1.885579	1.413882

Structure **34** in 2-propanol:

Electronic Energy (Hartrees): -1582.12769570
Free Energy (Hartress): -1581.897468
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.485622	-0.089514	-0.224511
2	6	0	1.846583	-0.096766	-0.621656
3	6	0	-0.100578	1.355363	-0.635754
4	1	0	-0.637522	1.607388	-1.552468
5	6	0	1.430770	1.341454	-0.937606
6	1	0	1.628002	1.584900	-1.980401

7	16	0	0.508125	-1.106954	-1.436412
8	7	0	1.620666	-0.317523	0.807557
9	6	0	0.286782	-0.476937	1.063554
10	8	0	-0.181494	-0.913232	2.091549
11	6	0	-1.947647	-0.434185	-0.188846
12	6	0	-2.937699	0.529550	-0.382207
13	6	0	-2.332460	-1.757764	0.054324
14	6	0	-4.285179	0.177518	-0.335798
15	1	0	-2.680191	1.564635	-0.574815
16	6	0	-3.675265	-2.108274	0.097887
17	1	0	-1.575369	-2.519639	0.208294
18	6	0	-4.657948	-1.139524	-0.097293
19	1	0	-5.041460	0.939579	-0.486847
20	1	0	-3.954737	-3.138830	0.285855
21	1	0	-5.706905	-1.411888	-0.063121
22	16	0	3.556060	-0.583451	-0.969243
23	6	0	2.657325	-1.082956	1.497216
24	6	0	3.954229	-0.678780	0.820496
25	1	0	2.664028	-0.827163	2.556879
26	1	0	2.470250	-2.156231	1.383117
27	1	0	4.300385	0.295347	1.164405
28	1	0	4.738330	-1.421387	0.958177
29	6	0	-0.414012	2.409698	0.411751
30	8	0	-0.582589	2.115793	1.575954
31	1	0	1.994365	2.024402	-0.297407
32	6	0	-0.487592	3.821342	-0.089806
33	1	0	-1.423898	3.932420	-0.647494
34	1	0	-0.472955	4.526647	0.739720
35	1	0	0.328583	4.027116	-0.786833

Structure **35** in dichloromethane:

Electronic Energy (Hartrees): -2059.26945177
Free Energy (Hartress): -2058.907203
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.628934	-0.522959	-0.464177
2	6	0	0.525128	1.397727	-1.298541
3	6	0	0.508212	-1.049147	-1.416098
4	1	0	0.943843	-1.672674	-2.195327
5	6	0	-0.202603	0.197780	-1.973094
6	1	0	-0.171716	0.280161	-3.058383
7	16	0	2.298073	0.904098	-1.455818
8	7	0	0.283335	1.304511	0.132844
9	6	0	0.875536	0.215356	0.683185
10	8	0	0.773490	-0.168191	1.827927
11	6	0	2.684400	-1.482671	0.001900
12	6	0	2.758326	-2.796084	-0.458331
13	6	0	3.638355	-1.025797	0.918062
14	6	0	3.776444	-3.638024	-0.014856
15	1	0	2.019884	-3.181481	-1.150124
16	6	0	4.652355	-1.865413	1.358001
17	1	0	3.584256	-0.006459	1.286761
18	6	0	4.724703	-3.176280	0.890100
19	1	0	3.821702	-4.658233	-0.378024
20	1	0	5.384668	-1.497527	2.067464
21	1	0	5.514988	-3.833901	1.233783
22	16	0	0.081412	3.075630	-1.778229
23	6	0	-0.493320	2.349736	0.808744
24	6	0	-1.012538	3.268064	-0.315246
25	1	0	-1.353102	1.874387	1.293418
26	1	0	-2.025318	3.003561	-0.607233
27	1	0	-0.982020	4.317901	-0.025845
28	7	0	-1.749452	-1.077184	-0.722876
29	6	0	-0.571090	-1.826221	-0.677241
30	6	0	-1.639040	0.081729	-1.491206
31	8	0	-0.457481	-2.889628	-0.130444
32	8	0	-2.537127	0.855444	-1.694117
33	6	0	-2.943629	-1.457176	-0.033611
34	6	0	-4.113311	-1.683839	-0.749411
35	6	0	-2.903152	-1.587565	1.350591

36	6	0	-5.267081	-2.042894	-0.059884
37	1	0	-4.116579	-1.578908	-1.828000
38	6	0	-4.059175	-1.957707	2.028591
39	1	0	-1.975676	-1.399685	1.880805
40	6	0	-5.239895	-2.182881	1.325228
41	1	0	-6.185702	-2.219072	-0.607134
42	1	0	-4.037190	-2.066540	3.106498
43	1	0	-6.140272	-2.466409	1.857964
44	6	0	0.340806	3.063051	1.888209
45	1	0	0.726930	2.272794	2.538883
46	6	0	1.524953	3.834399	1.310999
47	1	0	2.160813	3.195482	0.691690
48	1	0	1.192993	4.678088	0.698580
49	1	0	2.137892	4.234591	2.122431
50	6	0	-0.558419	3.965955	2.731926
51	1	0	-1.388230	3.404970	3.170255
52	1	0	0.015314	4.411671	3.547794
53	1	0	-0.976862	4.784520	2.138762

Structure **36** in dichloromethane:

Electronic Energy (Hartrees): -2059.26893182
Free Energy (Hartress): -2058.904187
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.550911	1.780209	-1.025112
2	6	0	-1.930097	0.014113	-0.258407
3	6	0	-1.088808	0.600787	0.913535
4	6	0	-0.072984	0.549599	-1.830011
5	6	0	-0.937149	-0.604748	-1.303073
6	16	0	-2.394095	1.603543	-1.104621
7	16	0	0.106836	3.409565	-1.440501
8	7	0	-0.234189	1.528186	0.377982
9	6	0	0.415249	2.626537	1.116695
10	1	0	-0.370343	3.272511	1.527890
11	6	0	1.177002	3.402910	0.043301
12	1	0	1.343421	4.437382	0.338967
13	1	0	2.125939	2.929368	-0.207863
14	8	0	-1.167594	0.297385	2.080017
15	6	0	-3.083666	-0.870923	0.132771
16	6	0	-4.321992	-0.744681	-0.499756
17	6	0	-2.914528	-1.868961	1.097891
18	6	0	-5.377255	-1.589720	-0.170126
19	1	0	-4.473560	0.012714	-1.261755
20	6	0	-3.970674	-2.712589	1.424958
21	1	0	-1.960654	-1.991178	1.591834
22	6	0	-5.204551	-2.575850	0.795128
23	1	0	-6.332476	-1.473266	-0.668985
24	1	0	-3.826429	-3.480017	2.176898
25	1	0	-6.026026	-3.233479	1.055409
26	6	0	1.309113	2.133760	2.268850
27	1	0	0.634637	1.771285	3.047923
28	6	0	2.215483	0.976925	1.857761
29	1	0	1.625830	0.109276	1.557136
30	1	0	2.877626	1.245172	1.028757
31	1	0	2.842890	0.678210	2.701632
32	6	0	2.111136	3.304894	2.837930
33	1	0	1.466525	4.157208	3.072209
34	1	0	2.613445	3.000969	3.758892
35	1	0	2.880744	3.640931	2.136478
36	1	0	-1.521241	-1.096810	-2.080857
37	1	0	-0.168431	0.718928	-2.901839
38	6	0	0.050777	-1.609848	-0.731501
39	6	0	1.357143	0.164837	-1.495675
40	7	0	1.340906	-1.089766	-0.878623
41	6	0	2.522944	-1.795829	-0.491657
42	6	0	2.609226	-2.357617	0.779140
43	6	0	3.566840	-1.923599	-1.403769
44	6	0	3.757744	-3.056006	1.136071
45	1	0	1.787269	-2.252539	1.476347
46	6	0	4.713929	-2.616140	-1.032746

47	1	0	3.479130	-1.486995	-2.390977
48	6	0	4.810783	-3.184129	0.234709
49	1	0	3.828333	-3.498163	2.122973
50	1	0	5.528676	-2.716455	-1.740081
51	1	0	5.704269	-3.728232	0.518223
52	8	0	-0.204011	-2.679669	-0.246836
53	8	0	2.346733	0.812402	-1.709960

Structure **37** in dichloromethane:

Electronic Energy (Hartrees): -1982.92288410
Free Energy (Hartress): -1982.570956
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.612227	-0.639331	0.506501
2	6	0	-1.494347	0.380862	0.823766
3	6	0	0.891273	0.920042	0.535845
4	6	0	-0.509471	1.560812	0.717897
5	16	0	-0.610068	-0.837531	1.887600
6	7	0	-1.461440	-0.244007	-0.491181
7	6	0	-0.293132	-0.901815	-0.725468
8	8	0	-0.015313	-1.522653	-1.726731
9	6	0	1.865249	-1.462327	0.620696
10	6	0	2.297560	-1.934393	1.862274
11	6	0	2.663958	-1.688526	-0.505425
12	6	0	3.497524	-2.629095	1.978522
13	1	0	1.705671	-1.755249	2.754064
14	6	0	3.862488	-2.384858	-0.385820
15	1	0	2.350901	-1.319330	-1.473070
16	6	0	4.282502	-2.858651	0.853553
17	1	0	3.815515	-2.989252	2.950107
18	1	0	4.468875	-2.555811	-1.268020
19	1	0	5.217008	-3.400845	0.942518
20	16	0	-3.224655	0.756167	1.167259
21	6	0	-2.670976	-0.243830	-1.321730
22	6	0	-3.616344	0.747298	-0.627422
23	1	0	-2.404705	0.160425	-2.303921
24	1	0	-3.484562	1.755771	-1.016690
25	1	0	-4.662037	0.461590	-0.734918
26	6	0	-3.239143	-1.659511	-1.531013
27	1	0	-2.406383	-2.258471	-1.910446
28	6	0	-3.750934	-2.308561	-0.247772
29	1	0	-2.989205	-2.311220	0.536055
30	1	0	-4.634852	-1.791664	0.137463
31	1	0	-4.032749	-3.345328	-0.448650
32	6	0	-4.323541	-1.630056	-2.607568
33	1	0	-3.952474	-1.189375	-3.537116
34	1	0	-4.659748	-2.645679	-2.828672
35	1	0	-5.198337	-1.057854	-2.283541
36	1	0	1.480281	1.089184	1.439872
37	1	0	-0.788717	2.225013	-0.100319
38	7	0	-0.493245	2.454005	1.933299
39	8	0	0.143372	3.480152	1.819268
40	8	0	-1.081183	2.111978	2.931549
41	6	0	1.681960	1.415358	-0.651383
42	6	0	1.094819	1.615362	-1.903196
43	6	0	3.056839	1.611432	-0.509784
44	6	0	1.871425	1.995816	-2.992908
45	1	0	0.027084	1.472205	-2.040606
46	6	0	3.834379	1.994242	-1.598210
47	1	0	3.518734	1.455834	0.460332
48	6	0	3.242812	2.184066	-2.843771
49	1	0	1.403463	2.144962	-3.959334
50	1	0	4.900552	2.144304	-1.471805
51	1	0	3.846287	2.480797	-3.694062

Structure **38** in dichloromethane:

Electronic Energy (Hartrees): -1982.92293033

Free Energy (Hartress): -1982.570837
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.295818	-0.641360	-0.977093
2	6	0	-0.554939	0.682360	-0.335130
3	6	0	0.778269	1.341881	0.113009
4	6	0	0.442130	-1.560406	-0.085587
5	6	0	-0.688327	-0.663637	0.481296
6	16	0	-0.042462	0.117658	-2.022804
7	16	0	2.686945	-1.308147	-1.915952
8	7	0	1.790604	0.455588	-0.159779
9	6	0	3.194773	0.851536	-0.376999
10	1	0	3.211334	1.601375	-1.178668
11	6	0	3.896183	-0.412492	-0.877176
12	1	0	4.750488	-0.164814	-1.504866
13	1	0	4.206769	-1.060793	-0.060780
14	8	0	0.910446	2.437094	0.603139
15	6	0	-1.764143	1.566473	-0.255402
16	6	0	-2.675901	1.650658	-1.306056
17	6	0	-2.037335	2.239376	0.939492
18	6	0	-3.842421	2.398877	-1.170538
19	1	0	-2.493685	1.121125	-2.235809
20	6	0	-3.201796	2.986266	1.073162
21	1	0	-1.342274	2.174460	1.768240
22	6	0	-4.107838	3.068870	0.018424
23	1	0	-4.542861	2.453019	-1.995941
24	1	0	-3.402018	3.503995	2.004380
25	1	0	-5.017099	3.649405	0.125119
26	6	0	3.850101	1.462333	0.874301
27	1	0	3.363177	2.427165	1.031010
28	6	0	3.652632	0.622722	2.133735
29	1	0	2.593354	0.465351	2.350894
30	1	0	4.128495	-0.357640	2.048352
31	1	0	4.100310	1.136905	2.988140
32	6	0	5.333446	1.715008	0.600017
33	1	0	5.478826	2.283119	-0.323529
34	1	0	5.775320	2.286091	1.419531
35	1	0	5.887628	0.775383	0.513845
36	1	0	0.059632	-2.411423	-0.649587
37	1	0	-0.470421	-0.426276	1.526959
38	7	0	1.197178	-2.204924	1.055621
39	8	0	0.516851	-2.783825	1.875330
40	8	0	2.402507	-2.139584	1.083472
41	6	0	-2.074403	-1.263022	0.418354
42	6	0	-2.535288	-1.978278	-0.688738
43	6	0	-2.948976	-1.034353	1.483006
44	6	0	-3.845931	-2.446493	-0.730754
45	1	0	-1.881886	-2.172403	-1.531757
46	6	0	-4.258708	-1.500802	1.442071
47	1	0	-2.599171	-0.484111	2.350744
48	6	0	-4.712112	-2.206901	0.331560
49	1	0	-4.187438	-3.001138	-1.597485
50	1	0	-4.922625	-1.314008	2.278448
51	1	0	-5.731872	-2.572806	0.296709

Structure **39** in dichloromethane:

Electronic Energy (Hartrees): -1982.92317345
Free Energy (Hartress): -1982.570837
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.487158	-1.088966	0.018450
2	6	0	-0.679921	-0.503084	-0.726339
3	6	0	0.322050	0.642862	-1.011136
4	6	0	0.633768	-1.047369	1.294281
5	6	0	-0.805749	-0.705792	0.831826
6	16	0	0.391333	-1.935441	-1.217977

7	16	0	3.190307	-1.681352	0.157861
8	7	0	1.535619	0.301788	-0.438808
9	6	0	2.824053	0.701197	-1.050161
10	1	0	2.847281	0.308155	-2.075111
11	6	0	3.876210	-0.030929	-0.226574
12	1	0	4.794624	-0.174743	-0.793388
13	1	0	4.100094	0.488539	0.705230
14	8	0	0.109743	1.641628	-1.650287
15	6	0	-2.007873	-0.395650	-1.421628
16	6	0	-2.593525	-1.506688	-2.030508
17	6	0	-2.709981	0.814222	-1.396519
18	6	0	-3.853159	-1.411666	-2.615637
19	1	0	-2.073455	-2.458958	-2.050114
20	6	0	-3.967784	0.906422	-1.982111
21	1	0	-2.274922	1.682524	-0.917780
22	6	0	-4.542552	-0.204129	-2.594556
23	1	0	-4.291593	-2.283651	-3.086969
24	1	0	-4.499742	1.850626	-1.957720
25	1	0	-5.522584	-0.127478	-3.051712
26	6	0	3.041886	2.224795	-1.107180
27	1	0	2.385347	2.602897	-1.892845
28	6	0	2.675109	2.935788	0.192806
29	1	0	1.596051	2.923937	0.355186
30	1	0	3.163622	2.485226	1.062161
31	1	0	2.990081	3.981240	0.141918
32	6	0	4.487400	2.516177	-1.516167
33	1	0	4.774221	1.951902	-2.408378
34	1	0	4.603736	3.578776	-1.739833
35	1	0	5.187516	2.267172	-0.713074
36	1	0	1.045872	-0.333245	2.007939
37	1	0	-1.431304	-1.593851	0.947859
38	7	0	0.607200	-2.355373	2.045986
39	8	0	1.176211	-3.317292	1.585608
40	8	0	-0.010600	-2.346483	3.088493
41	6	0	-1.472232	0.442530	1.549440
42	6	0	-0.798015	1.635033	1.815649
43	6	0	-2.821219	0.334374	1.890641
44	6	0	-1.464417	2.706461	2.401606
45	1	0	0.254187	1.732256	1.569547
46	6	0	-3.488135	1.402984	2.481773
47	1	0	-3.350490	-0.590840	1.684636
48	6	0	-2.811899	2.593202	2.734115
49	1	0	-0.929377	3.627883	2.601917
50	1	0	-4.535392	1.305266	2.744174
51	1	0	-3.329631	3.426690	3.195034

Structure **40** in dichloromethane:

Electronic Energy (Hartrees): -1982.92514117
Free Energy (Hartress): -1982.572856
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.446640	0.121696	-0.135578
2	6	0	-0.707254	0.212703	-1.068234
3	6	0	0.842516	-1.299272	0.020590
4	6	0	-0.528576	-1.302877	-0.709203
5	16	0	0.911424	0.651673	-1.825451
6	7	0	-0.717787	0.973723	0.170706
7	6	0	0.491522	0.971023	0.776089
8	8	0	0.781055	1.460551	1.844566
9	6	0	2.901018	0.261146	0.211030
10	6	0	3.820885	0.805650	-0.682444
11	6	0	3.338036	-0.168819	1.466995
12	6	0	5.161198	0.922259	-0.327390
13	1	0	3.503805	1.135101	-1.666251
14	6	0	4.678184	-0.053159	1.819380
15	1	0	2.631465	-0.589486	2.174389
16	6	0	5.593024	0.493495	0.923514
17	1	0	5.866987	1.344216	-1.033558
18	1	0	5.006350	-0.389779	2.796026
19	1	0	6.637817	0.582036	1.198471

20	16	0	-2.194653	0.690553	-1.963957
21	6	0	-1.951402	1.642210	0.594901
22	6	0	-3.027768	1.157293	-0.394388
23	1	0	-2.211245	1.270922	1.592368
24	1	0	-3.555688	0.285864	-0.007950
25	1	0	-3.748966	1.939885	-0.628108
26	6	0	-1.774372	3.168702	0.679317
27	1	0	-0.918985	3.328613	1.342859
28	6	0	-1.466222	3.816463	-0.668009
29	1	0	-0.592393	3.364159	-1.144506
30	1	0	-2.312182	3.729324	-1.356509
31	1	0	-1.260205	4.880595	-0.527423
32	6	0	-3.000142	3.803583	1.335360
33	1	0	-3.221500	3.340556	2.300945
34	1	0	-2.825147	4.868308	1.505921
35	1	0	-3.887548	3.713299	0.701857
36	1	0	-0.441155	-1.850975	-1.649717
37	1	0	0.760670	-1.574866	1.071011
38	7	0	1.705680	-2.391771	-0.564307
39	8	0	2.468538	-2.133815	-1.463321
40	8	0	1.534184	-3.497628	-0.094484
41	6	0	-1.694074	-1.856150	0.074523
42	6	0	-1.855541	-1.632978	1.444410
43	6	0	-2.699156	-2.530853	-0.622699
44	6	0	-3.005833	-2.064508	2.098421
45	1	0	-1.091085	-1.119335	2.018717
46	6	0	-3.850072	-2.961005	0.029527
47	1	0	-2.578177	-2.712983	-1.685525
48	6	0	-4.008454	-2.723457	1.392048
49	1	0	-3.116735	-1.884909	3.161756
50	1	0	-4.620993	-3.483385	-0.525436
51	1	0	-4.903833	-3.058179	1.903352

Structure **41** in dichloromethane:

Electronic Energy (Hartrees): -1982.92274142
Free Energy (Hartress): -1982.569916
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.272189	-0.013696	-0.214860
2	6	0	-1.054476	0.319981	-0.403685
3	6	0	0.576289	-1.124579	0.644743
4	6	0	-0.950071	-0.885584	0.590055
5	16	0	0.185869	-0.070984	-1.715079
6	7	0	-0.464786	1.475585	0.252783
7	6	0	0.878106	1.370732	0.387345
8	8	0	1.630237	2.178464	0.882694
9	6	0	2.740158	-0.246130	-0.434556
10	6	0	3.225518	-0.745035	-1.643739
11	6	0	3.634228	-0.010411	0.615159
12	6	0	4.583680	-1.000386	-1.806421
13	1	0	2.549985	-0.940152	-2.470169
14	6	0	4.989988	-0.271711	0.450914
15	1	0	3.277214	0.391416	1.556230
16	6	0	5.468456	-0.765885	-0.759377
17	1	0	4.946694	-1.382865	-2.753388
18	1	0	5.673144	-0.084529	1.271120
19	1	0	6.526226	-0.966044	-0.885837
20	16	0	-2.699074	0.831362	-0.930693
21	6	0	-1.329624	2.585744	0.661421
22	6	0	-2.759374	2.071260	0.423845
23	1	0	-1.191543	2.745076	1.735879
24	1	0	-3.160557	1.593726	1.316983
25	1	0	-3.437502	2.865583	0.114082
26	6	0	-0.971539	3.895414	-0.064453
27	1	0	0.098177	4.043535	0.110065
28	6	0	-1.208337	3.843514	-1.571292
29	1	0	-0.691861	2.998850	-2.034490
30	1	0	-2.273650	3.761518	-1.807085
31	1	0	-0.835560	4.761630	-2.032774
32	6	0	-1.715746	5.067782	0.573950

33	1	0	-1.533520	5.116690	1.651037
34	1	0	-1.380174	6.009345	0.133046
35	1	0	-2.795775	4.996005	0.412481
36	1	0	0.872979	-2.100539	0.270033
37	1	0	-1.300114	-0.507883	1.553364
38	7	0	1.090782	-1.092969	2.064236
39	6	0	-1.768584	-2.101664	0.221806
40	6	0	-1.377696	-3.006649	-0.767793
41	6	0	-2.986783	-2.306058	0.875333
42	6	0	-2.191113	-4.086611	-1.099192
43	1	0	-0.437981	-2.878730	-1.291881
44	6	0	-3.799817	-3.385801	0.546079
45	1	0	-3.298485	-1.613494	1.650941
46	6	0	-3.404170	-4.278804	-0.445534
47	1	0	-1.871037	-4.779234	-1.869227
48	1	0	-4.740236	-3.530232	1.065664
49	1	0	-4.033901	-5.122696	-0.703467
50	8	0	0.810003	-0.130479	2.746561
51	8	0	1.779647	-2.019719	2.426010

Structure **42** in dichloromethane:

Electronic Energy (Hartrees): -1982.92385923
Free Energy (Hartress): -1982.571493
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632251	0.050482	1.256955
2	6	0	1.474849	0.215707	0.232573
3	6	0	0.496634	1.290779	-0.345346
4	6	0	-0.443364	-1.343694	0.581588
5	6	0	0.857666	-1.150917	-0.218149
6	16	0	1.030189	0.356051	2.019279
7	16	0	-2.047775	0.252924	2.360486
8	7	0	-0.736795	1.069619	0.211792
9	6	0	-1.746589	2.118784	0.466826
10	1	0	-1.315867	2.830280	1.183654
11	6	0	-2.874126	1.365980	1.165858
12	1	0	-3.520285	2.035144	1.731097
13	1	0	-3.465608	0.770986	0.468211
14	8	0	0.793878	2.159661	-1.126019
15	6	0	2.916090	0.412228	-0.137747
16	6	0	3.913086	0.500968	0.831076
17	6	0	3.267473	0.462340	-1.490485
18	6	0	5.246194	0.651426	0.456382
19	1	0	3.662340	0.448086	1.885499
20	6	0	4.597288	0.608945	-1.861923
21	1	0	2.501315	0.382071	-2.253217
22	6	0	5.590020	0.707284	-0.888807
23	1	0	6.011960	0.722946	1.220046
24	1	0	4.859018	0.646416	-2.913153
25	1	0	6.627535	0.822611	-1.180853
26	6	0	-2.180135	2.906411	-0.780943
27	1	0	-1.321280	3.516335	-1.069682
28	6	0	-2.553165	2.027751	-1.970937
29	1	0	-1.697687	1.445077	-2.316875
30	1	0	-3.369106	1.339823	-1.731645
31	1	0	-2.884165	2.659736	-2.799279
32	6	0	-3.327322	3.847191	-0.406379
33	1	0	-3.089484	4.436624	0.484103
34	1	0	-3.524134	4.541606	-1.226027
35	1	0	-4.249878	3.291389	-0.213526
36	1	0	0.730918	-1.164235	-1.298584
37	1	0	-0.251667	-2.056513	1.384359
38	7	0	1.860178	-2.252926	0.038266
39	8	0	2.010552	-2.653385	1.170248
40	8	0	2.489831	-2.642069	-0.921358
41	6	0	-1.645382	-1.801783	-0.209901
42	6	0	-1.894168	-1.370130	-1.513305
43	6	0	-2.573691	-2.643109	0.409463
44	6	0	-3.047140	-1.768147	-2.183879
45	1	0	-1.194600	-0.713297	-2.016517

46	6	0	-3.728325	-3.039731	-0.257358
47	1	0	-2.388297	-2.986213	1.422009
48	6	0	-3.968573	-2.601279	-1.557040
49	1	0	-3.223968	-1.422950	-3.196455
50	1	0	-4.437625	-3.694215	0.236329
51	1	0	-4.866226	-2.910735	-2.080229

Structure **43** in dichloromethane:

Electronic Energy (Hartrees): -1982.92376039
Free Energy (Hartress): -1982.57249
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.992847	-0.178701	-0.793796
2	6	0	1.317359	0.050379	-0.378559
3	6	0	0.878750	-1.440204	-0.221123
4	6	0	-0.950164	0.733070	0.473972
5	6	0	0.571769	0.936927	0.666379
6	16	0	0.345989	0.494115	-1.890632
7	16	0	-2.582149	-0.471039	-1.597101
8	7	0	-0.472894	-1.477940	-0.384511
9	6	0	-1.279355	-2.663454	-0.713417
10	1	0	-0.956685	-3.034835	-1.693938
11	6	0	-2.706063	-2.129305	-0.834062
12	1	0	-3.315417	-2.751978	-1.486921
13	1	0	-3.191689	-2.035991	0.137115
14	8	0	1.614089	-2.380108	-0.039138
15	6	0	2.799904	0.292788	-0.423898
16	6	0	3.374929	1.103937	-1.402383
17	6	0	3.613935	-0.258443	0.571128
18	6	0	4.742751	1.359373	-1.391702
19	1	0	2.762285	1.546557	-2.180969
20	6	0	4.979434	0.004040	0.582332
21	1	0	3.187878	-0.906511	1.328102
22	6	0	5.547594	0.811701	-0.398679
23	1	0	5.175519	1.988131	-2.161102
24	1	0	5.599734	-0.429431	1.358250
25	1	0	6.612949	1.011303	-0.389787
26	6	0	-1.136207	-3.798583	0.317460
27	1	0	-0.125787	-4.195337	0.197006
28	6	0	-1.283937	-3.321915	1.760431
29	1	0	-0.532824	-2.569941	2.010629
30	1	0	-2.274608	-2.897740	1.951238
31	1	0	-1.155108	-4.167788	2.440497
32	6	0	-2.129752	-4.913896	-0.010445
33	1	0	-2.063969	-5.215663	-1.059958
34	1	0	-1.923029	-5.792636	0.604477
35	1	0	-3.159346	-4.602939	0.191611
36	1	0	-1.340803	0.120914	1.290320
37	1	0	0.882620	1.971280	0.540487
38	7	0	1.005503	0.577193	2.066384
39	6	0	-1.767595	2.000623	0.395712
40	6	0	-1.386371	3.112524	-0.359708
41	6	0	-2.985482	2.036350	1.078995
42	6	0	-2.212897	4.230922	-0.431936
43	1	0	-0.446304	3.115206	-0.899072
44	6	0	-3.810441	3.153690	1.009161
45	1	0	-3.288093	1.178153	1.670539
46	6	0	-3.426016	4.254711	0.249328
47	1	0	-1.905267	5.086568	-1.022419
48	1	0	-4.750316	3.163912	1.549004
49	1	0	-4.065340	5.128382	0.193546
50	8	0	1.553702	1.434382	2.719745
51	8	0	0.803222	-0.558375	2.443245

Structure **44** in dichloromethane:

Electronic Energy (Hartrees): -1864.97193373
Free Energy (Hartress): -1864.703226

No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.267814	-0.946460	0.496289
2	6	0	-2.389001	0.077999	-0.012260
3	6	0	0.078419	0.412305	-0.256151
4	6	0	-1.251099	1.029201	0.168693
5	1	0	-1.240973	1.324841	1.221714
6	16	0	-0.012450	-0.850529	2.314116
7	7	0	-2.190179	-1.203868	0.052399
8	6	0	-0.873282	-1.869287	0.205864
9	8	0	-0.876145	-3.060685	0.088990
10	6	0	1.589759	-1.547489	0.038323
11	6	0	2.728754	-1.484930	0.835504
12	6	0	1.693117	-2.066942	-1.254930
13	6	0	3.954010	-1.936771	0.349869
14	1	0	2.647316	-1.080163	1.837200
15	6	0	2.913088	-2.527884	-1.737714
16	1	0	0.815696	-2.111784	-1.893614
17	6	0	4.049583	-2.462213	-0.934582
18	1	0	4.834308	-1.880400	0.980434
19	1	0	2.976650	-2.937170	-2.739740
20	1	0	5.002151	-2.820437	-1.308683
21	16	0	-4.018140	0.569705	-0.203118
22	6	0	-3.420426	-2.020896	0.098386
23	6	0	-4.509456	-1.170715	-0.537349
24	1	0	-3.257237	-2.949623	-0.441834
25	1	0	-4.557148	-1.291292	-1.618315
26	1	0	-5.484671	-1.349602	-0.091282
27	8	0	-1.933574	3.246735	-0.014571
28	8	0	-1.360456	2.239614	-1.825409
29	1	0	0.004811	0.179779	-1.323639
30	6	0	1.224743	1.380902	-0.065715
31	6	0	1.391783	2.104726	1.116519
32	6	0	2.153103	1.539994	-1.097536
33	6	0	2.478283	2.962955	1.265929
34	1	0	0.685960	1.990052	1.930319
35	6	0	3.236959	2.397555	-0.948236
36	1	0	2.024466	0.984085	-2.021080
37	6	0	3.403657	3.109070	0.237396
38	1	0	2.599223	3.516373	2.190179
39	1	0	3.950459	2.510916	-1.756470
40	1	0	4.246879	3.780100	0.355728
41	7	0	-1.538405	2.285148	-0.631188
42	1	0	-3.615820	-2.233485	1.152753

Structure **45** in dichloromethane:

Electronic Energy (Hartrees): -1982.89334975
Free Energy (Hartress): -1982.544105
No imaginary frequencies.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.466810	0.869829	0.304865
2	6	0	1.724357	-0.892760	-0.398122
3	6	0	-0.749285	-0.537459	-0.319713
4	6	0	0.412446	-1.467001	0.027520
5	1	0	0.474374	-1.644368	1.105944
6	16	0	-0.022791	0.832803	2.088600
7	7	0	1.907473	0.393940	-0.384202
8	6	0	0.843678	1.407513	-0.183687
9	8	0	1.146994	2.538436	-0.435692
10	6	0	-1.614379	1.786424	-0.098299
11	6	0	-2.616083	2.138829	0.800474
12	6	0	-1.727164	2.188465	-1.432051
13	6	0	-3.716637	2.879266	0.373602
14	1	0	-2.528636	1.827017	1.834310
15	6	0	-2.818830	2.936925	-1.857558
16	1	0	-0.957528	1.914660	-2.147551

17	6	0	-3.821165	3.282025	-0.953594
18	1	0	-4.492747	3.142568	1.083504
19	1	0	-2.887436	3.248821	-2.893803
20	1	0	-4.675425	3.863569	-1.281834
21	16	0	3.081418	-1.840240	-0.820396
22	6	0	3.309734	0.852364	-0.578545
23	6	0	4.037127	-0.327654	-1.236803
24	1	0	3.277688	1.695789	-1.267117
25	1	0	4.056544	-0.251240	-2.322161
26	1	0	5.049575	-0.454334	-0.857424
27	8	0	0.270368	-3.790022	0.077622
28	6	0	3.887951	1.319760	0.767914
29	1	0	3.178449	2.055697	1.159268
30	6	0	4.027845	0.193590	1.790647
31	1	0	3.073592	-0.301340	1.991030
32	1	0	4.758410	-0.554967	1.468122
33	1	0	4.381097	0.608520	2.737449
34	6	0	5.222877	2.023069	0.525173
35	1	0	5.116817	2.843196	-0.189333
36	1	0	5.598986	2.435334	1.463622
37	1	0	5.977697	1.329033	0.143281
38	8	0	-0.007134	-2.821404	-1.821648
39	1	0	-0.751700	-0.409527	-1.407391
40	6	0	-2.081203	-1.127120	0.085345
41	6	0	-2.287893	-1.707226	1.339040
42	6	0	-3.145010	-1.064542	-0.817759
43	6	0	-3.544597	-2.197554	1.685782
44	1	0	-1.477843	-1.765416	2.056329
45	6	0	-4.399561	-1.552353	-0.470443
46	1	0	-2.987754	-0.620837	-1.796024
47	6	0	-4.602508	-2.118202	0.785967
48	1	0	-3.693410	-2.642655	2.663109
49	1	0	-5.215985	-1.492753	-1.181177
50	1	0	-5.579584	-2.499512	1.060332
51	7	0	0.211903	-2.814150	-0.632158

Cartesian coordinates for structures I_{14}, I_{24}, I_{27} and $I_{37\text{-}39}$ optimized at M06-2X/6-311++G(d,p) level in dichloromethane.

Structure $\mathbf{I_{14}}$:

Electronic Energy (Hartrees): -1864.95866400
Free Energy (Hartress): -1864.691104
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.002534	-1.429839	0.553163
2	6	0	-0.139277	-0.609463	-0.060337
3	6	0	2.110631	-0.281746	-1.124100
4	6	0	-0.306663	0.752703	0.830226
5	6	0	0.875697	1.649525	0.789287
6	16	0	0.512024	-0.095197	-1.720030
7	16	0	3.595325	0.256210	-1.776148
8	7	0	2.220296	-1.008779	-0.028708
9	8	0	0.944679	-2.293063	1.373249
10	6	0	-1.441797	-1.371989	-0.141734
11	6	0	-1.939116	-1.976699	1.017530
12	6	0	-2.219562	-1.392053	-1.300358
13	6	0	-3.179084	-2.604754	1.005609
14	1	0	-1.364291	-1.949363	1.933835
15	6	0	-3.462859	-2.016776	-1.307218
16	1	0	-1.877781	-0.917845	-2.214199
17	6	0	-3.946292	-2.627329	-0.155569
18	1	0	-3.548328	-3.070368	1.912166
19	1	0	-4.051398	-2.020821	-2.217241
20	1	0	-4.914251	-3.114902	-0.161788
21	6	0	3.581276	-1.366996	0.385470
22	1	0	3.813730	-2.354589	-0.018556
23	1	0	3.626026	-1.364691	1.472621
24	6	0	4.453425	-0.269853	-0.216125

25	1	0	5.449986	-0.619553	-0.473758
26	1	0	4.490060	0.612629	0.422685
27	1	0	0.919651	2.547057	0.193714
28	1	0	-0.435210	0.356001	1.842415
29	6	0	-1.578572	1.462089	0.408940
30	6	0	-2.755489	1.247794	1.130473
31	6	0	-1.621658	2.301157	-0.707577
32	6	0	-3.951383	1.838391	0.736486
33	1	0	-2.732978	0.607213	2.005643
34	6	0	-2.817937	2.894386	-1.103262
35	1	0	-0.721554	2.507311	-1.274958
36	6	0	-3.987454	2.659910	-0.387325
37	1	0	-4.854697	1.656205	1.307812
38	1	0	-2.831698	3.543340	-1.971728
39	1	0	-4.918536	3.120415	-0.697636
40	7	0	1.944588	1.404815	1.538253
41	8	0	1.972751	0.368880	2.279920
42	8	0	2.960188	2.169526	1.495522

Structure $\mathbf{I_{27}}$:

Electronic Energy (Hartrees): -1864.94858449
Free Energy (Hartress): -1864.682834
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.461803	-0.215611	1.317937
2	6	0	-0.108383	-0.601352	-0.038777
3	6	0	2.399197	-0.821848	0.192232
4	6	0	-0.397274	0.793456	-0.825589
5	6	0	0.822888	1.626140	-0.971808
6	16	0	1.298307	-1.431310	-0.934838
7	16	0	4.105610	-0.820948	0.156401
8	7	0	1.866358	-0.291573	1.290573
9	8	0	-0.129951	0.209703	2.267691
10	6	0	-1.313639	-1.516344	-0.043566
11	6	0	-2.035978	-1.823972	1.108105
12	6	0	-1.738091	-2.027052	-1.274864
13	6	0	-3.168212	-2.631826	1.023863
14	1	0	-1.737423	-1.429738	2.069886
15	6	0	-2.863761	-2.835707	-1.353521
16	1	0	-1.196831	-1.784209	-2.186040
17	6	0	-3.585916	-3.138012	-0.200922
18	1	0	-3.723942	-2.861294	1.925769
19	1	0	-3.179230	-3.224137	-2.314799
20	1	0	-4.468175	-3.764987	-0.258961
21	6	0	2.806085	0.349412	2.217730
22	1	0	2.476973	0.186848	3.242591
23	1	0	2.826694	1.418354	1.992652
24	6	0	4.146882	-0.324342	1.938733
25	1	0	4.280358	-1.234381	2.520851
26	1	0	4.987436	0.349316	2.085800
27	1	0	-0.696934	0.456854	-1.819019
28	1	0	1.174112	2.321548	-0.226099
29	7	0	1.538686	1.588364	-2.096019
30	8	0	1.206593	0.827394	-3.058380
31	8	0	2.574000	2.317272	-2.211598
32	6	0	-1.579984	1.501334	-0.186106
33	6	0	-2.871056	1.204139	-0.632709
34	6	0	-1.427181	2.449366	0.828741
35	6	0	-3.982644	1.824678	-0.071741
36	1	0	-3.005335	0.483362	-1.432310
37	6	0	-2.537174	3.071979	1.391301
38	1	0	-0.439859	2.712542	1.188864
39	6	0	-3.818473	2.758759	0.946892
40	1	0	-4.974680	1.582025	-0.435635
41	1	0	-2.398753	3.806959	2.176247
42	1	0	-4.682048	3.245402	1.386009

Structure $\mathbf{I_{24}}$:

Electronic Energy (Hartrees): -1982.87966868
Free Energy (Hartress): -1982.53032
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.522497	0.429170	-0.032353
2	6	0	-1.586483	-0.420293	-1.077512
3	6	0	1.022088	-0.890434	0.796417
4	6	0	0.097498	-2.046857	0.695987
5	1	0	0.269338	-2.886515	0.041955
6	16	0	-0.010347	-0.155870	-1.709742
7	7	0	-1.866213	0.249610	0.026182
8	6	0	-0.773962	0.916923	0.626329
9	8	0	-0.902377	1.708933	1.509479
10	6	0	1.606003	1.481280	-0.084575
11	6	0	2.346781	1.719127	-1.242980
12	6	0	1.961343	2.146519	1.093566
13	6	0	3.413449	2.612363	-1.231460
14	1	0	2.116651	1.207840	-2.171604
15	6	0	3.022782	3.044793	1.099515
16	1	0	1.420129	1.955537	2.010762
17	6	0	3.752365	3.282318	-0.061238
18	1	0	3.975706	2.781512	-2.142414
19	1	0	3.282139	3.555059	2.020054
20	1	0	4.582685	3.978964	-0.052255
21	16	0	-2.869504	-1.346978	-1.704309
22	6	0	-3.267703	0.242581	0.491463
23	6	0	-3.870629	-1.001411	-0.182963
24	1	0	-3.230826	0.083406	1.570035
25	1	0	-3.766609	-1.884916	0.445057
26	1	0	-4.905556	-0.856398	-0.487658
27	8	0	-1.791852	-3.102011	1.352090
28	6	0	-3.951199	1.580423	0.173529
29	1	0	-3.311024	2.351063	0.614583
30	6	0	-4.086449	1.857985	-1.322602
31	1	0	-3.122684	1.837925	-1.839918
32	1	0	-4.755668	1.137999	-1.803643
33	1	0	-4.514059	2.852117	-1.471376
34	6	0	-5.308499	1.635088	0.873156
35	1	0	-5.210033	1.452167	1.946055
36	1	0	-5.759224	2.620352	0.735576
37	1	0	-6.000831	0.895165	0.460671
38	8	0	-1.263235	-1.172620	2.261666
39	1	0	1.046490	-0.524287	1.827508
40	6	0	2.430985	-1.242532	0.362976
41	6	0	2.690685	-1.951387	-0.812802
42	6	0	3.510581	-0.819308	1.142165
43	6	0	4.000579	-2.207085	-1.210867
44	1	0	1.874507	-2.316009	-1.426318
45	6	0	4.819203	-1.076562	0.747909
46	1	0	3.321021	-0.280043	2.064201
47	6	0	5.068521	-1.766257	-0.435432
48	1	0	4.184538	-2.757240	-2.126857
49	1	0	5.643432	-0.740342	1.366949
50	1	0	6.087696	-1.966984	-0.745820
51	7	0	-0.992803	-2.118735	1.452962

Structure $\mathbf{I_{37}}$:

Electronic Energy (Hartrees): -1982.87005149
Free Energy (Hartress): -1982.522609
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.522024	0.219446	-0.594822
2	6	0	-1.940167	-0.172201	-0.964030
3	6	0	1.104781	-1.233942	-0.131129
4	6	0	0.030989	-2.209104	0.176599
5	16	0	-0.617844	-0.120348	-2.024839

6	7	0	-1.714862	0.310529	0.255790
7	6	0	-0.388675	0.690559	0.527658
8	8	0	-0.072584	1.196048	1.567168
9	6	0	1.627643	1.156543	-1.028497
10	6	0	2.359694	0.821053	-2.173186
11	6	0	1.974060	2.300402	-0.310526
12	6	0	3.415737	1.617967	-2.594807
13	1	0	2.119077	-0.076561	-2.737986
14	6	0	3.039543	3.092460	-0.732911
15	1	0	1.435945	2.575598	0.585745
16	6	0	3.761821	2.757294	-1.871395
17	1	0	3.971215	1.345921	-3.484785
18	1	0	3.301153	3.976096	-0.162149
19	1	0	4.589958	3.377298	-2.194752
20	16	0	-3.532276	-0.700074	-1.245789
21	6	0	-2.876467	0.443233	1.157572
22	6	0	-3.935698	-0.490867	0.544826
23	1	0	-2.573905	0.056503	2.132992
24	1	0	-3.904247	-1.486229	0.984511
25	1	0	-4.942852	-0.084761	0.617707
26	6	0	-3.291295	1.916572	1.294812
27	1	0	-2.395103	2.447694	1.630672
28	6	0	-3.758312	2.533699	-0.022445
29	1	0	-2.998791	2.465173	-0.807713
30	1	0	-4.677371	2.062258	-0.383903
31	1	0	-3.972381	3.593806	0.129759
32	6	0	-4.355575	2.049568	2.383170
33	1	0	-4.013046	1.623307	3.329442
34	1	0	-4.583683	3.104224	2.550115
35	1	0	-5.286372	1.551175	2.097374
36	1	0	1.630181	-1.584015	-1.020713
37	1	0	-0.488932	-2.252182	1.121044
38	7	0	-0.337988	-3.128106	-0.716115
39	8	0	-1.266031	-3.948712	-0.427997
40	8	0	0.219523	-3.198428	-1.854920
41	6	0	2.122692	-1.037774	0.979629
42	6	0	1.765751	-1.034212	2.330306
43	6	0	3.469344	-0.871475	0.644262
44	6	0	2.730009	-0.858262	3.318292
45	1	0	0.731874	-1.172754	2.624013
46	6	0	4.436128	-0.699883	1.630204
47	1	0	3.764301	-0.885903	-0.399841
48	6	0	4.067449	-0.688099	2.971988
49	1	0	2.434484	-0.858839	4.361581
50	1	0	5.476333	-0.581372	1.348501
51	1	0	4.817917	-0.555775	3.743274

Structure $\mathbf{I_{38}}$:

Electronic Energy (Hartrees): -1982.86973863
Free Energy (Hartress): -1982.52042
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.409536	-0.593433	1.456303
2	6	0	0.571955	0.389371	0.235500
3	6	0	-0.789881	1.093805	0.039563
4	6	0	-0.114308	-1.640945	-1.238019
5	6	0	0.919435	-0.603363	-0.989719
6	16	0	0.277010	-0.654801	1.732097
7	16	0	-2.597837	-1.398853	2.373776
8	7	0	-1.843496	0.247916	0.536114
9	6	0	-3.321809	0.507207	0.548173
10	1	0	-3.462574	1.404086	1.163022
11	6	0	-3.893078	-0.733235	1.257737
12	1	0	-4.767967	-0.497708	1.858549
13	1	0	-4.125443	-1.521385	0.541064
14	8	0	-0.977117	2.216255	-0.302400
15	6	0	1.691116	1.391136	0.435224
16	6	0	2.579639	1.325124	1.507762
17	6	0	1.904032	2.349131	-0.562221
18	6	0	3.654561	2.206090	1.591488

19	1	0	2.461626	0.584151	2.290844
20	6	0	2.972733	3.232536	-0.472185
21	1	0	1.239586	2.400340	-1.415693
22	6	0	3.852220	3.165008	0.605018
23	1	0	4.336279	2.136275	2.431011
24	1	0	3.119632	3.972368	-1.250677
25	1	0	4.687263	3.852757	0.671840
26	6	0	-4.011354	0.680971	-0.816962
27	1	0	-3.725475	-0.178865	-1.430192
28	6	0	-5.529668	0.672861	-0.582003
29	1	0	-5.903843	-0.278214	-0.199263
30	1	0	-5.819497	1.465248	0.116767
31	1	0	-6.037333	0.862916	-1.529339
32	6	0	-3.640082	1.965817	-1.555368
33	1	0	-2.619311	1.943628	-1.924052
34	1	0	-4.308591	2.078261	-2.412878
35	1	0	-3.770417	2.841059	-0.910851
36	1	0	0.000989	-2.684711	-0.996328
37	1	0	0.954936	0.077869	-1.844930
38	7	0	-1.226312	-1.295002	-1.866992
39	8	0	-1.401775	-0.067823	-2.181732
40	8	0	-2.135146	-2.141545	-2.137822
41	6	0	2.300249	-1.198180	-0.780305
42	6	0	2.509920	-2.324874	0.019742
43	6	0	3.406583	-0.594798	-1.385167
44	6	0	3.795891	-2.818278	0.228455
45	1	0	1.672170	-2.834345	0.481943
46	6	0	4.690930	-1.087076	-1.179843
47	1	0	3.257418	0.271514	-2.020783
48	6	0	4.890623	-2.198238	-0.365019
49	1	0	3.938497	-3.694125	0.851460
50	1	0	5.534591	-0.603517	-1.659409
51	1	0	5.890618	-2.584467	-0.203231

Structure $\mathbf{I_{39}}$:

Electronic Energy (Hartrees): -1982.86986882
Free Energy (Hartress): -1982.522171
No imaginary frequencies.
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.606825	-1.568484	-0.391913
2	6	0	-0.734412	-0.584563	-0.135159
3	6	0	0.234456	0.189369	-1.023288
4	6	0	-0.033595	0.104125	2.288736
5	6	0	-1.037185	0.281169	1.211144
6	16	0	0.186150	-2.148175	0.320055
7	16	0	3.154943	-2.283175	-0.447937
8	7	0	1.520959	-0.383928	-0.986236
9	6	0	2.762320	0.212903	-1.518163
10	1	0	2.543500	0.572551	-2.525430
11	6	0	3.751083	-0.965351	-1.598724
12	1	0	3.782045	-1.404197	-2.593704
13	1	0	4.756858	-0.687509	-1.288444
14	8	0	0.005718	1.180494	-1.652205
15	6	0	-2.034106	-0.984398	-0.814255
16	6	0	-2.910034	-1.793058	-0.079007
17	6	0	-2.395940	-0.573555	-2.095891
18	6	0	-4.128428	-2.180991	-0.617271
19	1	0	-2.631274	-2.115372	0.921757
20	6	0	-3.625466	-0.960017	-2.628199
21	1	0	-1.743102	0.056742	-2.684481
22	6	0	-4.492945	-1.759893	-1.895094
23	1	0	-4.794109	-2.809661	-0.037270
24	1	0	-3.899955	-0.629790	-3.623418
25	1	0	-5.446933	-2.058009	-2.314700
26	6	0	3.198027	1.391784	-0.634838
27	1	0	2.329182	2.057967	-0.588039
28	6	0	3.567845	0.966492	0.785093
29	1	0	2.769282	0.401885	1.275723
30	1	0	4.478321	0.358832	0.796367
31	1	0	3.761775	1.852696	1.393809

32	6	0	4.339305	2.151415	-1.308644
33	1	0	4.065800	2.468796	-2.318003
34	1	0	4.585357	3.042481	-0.727395
35	1	0	5.245394	1.541475	-1.371997
36	1	0	0.738449	0.808469	2.547475
37	1	0	-1.969860	-0.160641	1.563455
38	7	0	-0.154698	-0.950414	3.087233
39	8	0	-1.066225	-1.818622	2.855953
40	8	0	0.633971	-1.124730	4.067226
41	6	0	-1.319628	1.725338	0.849303
42	6	0	-0.332412	2.711407	0.907378
43	6	0	-2.602468	2.082416	0.428417
44	6	0	-0.620940	4.025759	0.555736
45	1	0	0.675572	2.457614	1.220307
46	6	0	-2.892196	3.395475	0.069020
47	1	0	-3.380092	1.325711	0.384316
48	6	0	-1.901626	4.371160	0.132367
49	1	0	0.155624	4.780468	0.612985
50	1	0	-3.894221	3.657454	-0.251680
51	1	0	-2.127531	5.395865	-0.140770

Cartesian coordinates for structures TS_{8-9}, TS_{11-12}, TS_{16-17}, TS_{20-24}, TS_{30-36}, TS_{40-43}, $TS1_{14}$, $TS1_{15}$, $TS1_{24}$, $TS1_{26}$, $TS1_{27}$, $TS1_{37-39}$, $TS2_{14}$, $TS2_{15}$, $TS2_{24}$, $TS2_{14}$, $TS2_{27}$ and $TS2_{37-39}$ optimized at M06-2X/6-311++G(d,p).

Structure $\mathbf{TS_8}$ in dichloromethane:

Electronic Energy (Hartrees) : -1941.27707790
Free Energy (Hartress): -1940.999976
One imaginary frequency (cm^{-1}): 438.4500i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.870751	0.312890	0.200214
2	6	0	0.391340	2.233718	0.128975
3	6	0	0.657571	-0.075586	-1.588165
4	1	0	1.558426	-0.344157	-2.122343
5	6	0	-0.120339	1.059853	-1.806681
6	1	0	0.101900	1.883182	-2.468063
7	16	0	2.089542	2.024604	-0.167440
8	7	0	-0.047219	1.298205	1.004018
9	6	0	0.753903	0.167438	1.140854
10	8	0	0.453468	-0.766116	1.868598
11	6	0	3.026543	-0.596428	0.160892
12	6	0	2.908460	-1.916796	0.619733
13	6	0	4.249948	-0.179104	-0.383300
14	6	0	3.995020	-2.781776	0.545344
15	1	0	1.968907	-2.259578	1.028949
16	6	0	5.330656	-1.047671	-0.449899
17	1	0	4.372038	0.832505	-0.757165
18	6	0	5.208809	-2.354322	0.016672
19	1	0	3.887829	-3.798438	0.905923
20	1	0	6.269847	-0.700574	-0.865069
21	1	0	6.052839	-3.032411	-0.033221
22	16	0	-0.487609	3.738079	0.251196
23	6	0	-1.249406	1.602907	1.779311
24	6	0	-1.835844	2.892862	1.189724
25	1	0	-1.957636	0.776065	1.704330
26	1	0	-0.951576	1.730457	2.821825
27	1	0	-2.644946	2.691230	0.494232
28	1	0	-2.172622	3.572336	1.969239
29	7	0	-1.512074	-0.577562	-0.947161
30	6	0	-0.249232	-1.164356	-1.114783
31	6	0	-1.511142	0.739987	-1.455266
32	8	0	0.013453	-2.321260	-0.906806
33	8	0	-2.495862	1.439359	-1.535663
34	6	0	-2.646449	-1.245551	-0.408472
35	6	0	-3.864966	-1.208267	-1.082904
36	6	0	-2.519497	-1.930891	0.798956
37	6	0	-4.968365	-1.851983	-0.531638

38	1	0	-3.944582	-0.680643	-2.024878
39	6	0	-3.625922	-2.583732	1.331409
40	1	0	-1.562366	-1.938484	1.308588
41	6	0	-4.851936	-2.541575	0.672095
42	1	0	-5.918859	-1.819871	-1.051612
43	1	0	-3.529307	-3.119758	2.268581
44	1	0	-5.713675	-3.044876	1.095140

Structure **TS_9** in dichloromethane:

Electronic Energy (Hartrees) : -1941.27596675
Free Energy (Hartress): -1940.998367
One imaginary frequency (cm^{-1}): 424.7471i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266347	1.084091	-0.262308
2	6	0	-1.929545	-1.223466	-0.588616
3	6	0	-0.495408	0.014750	1.573122
4	1	0	-1.042209	0.643222	2.263789
5	16	0	-0.836102	-0.172321	-1.415349
6	7	0	-2.919480	-0.496172	-0.004424
7	6	0	-2.624135	0.834603	0.246317
8	8	0	-3.373287	1.570855	0.870830
9	6	0	-0.646694	2.409924	-0.376333
10	6	0	-1.212146	3.530240	0.250521
11	6	0	0.554037	2.570618	-1.084425
12	6	0	-0.592998	4.771961	0.154556
13	1	0	-2.133403	3.425579	0.805791
14	6	0	1.160461	3.813925	-1.182596
15	1	0	1.034768	1.717470	-1.554161
16	6	0	0.589113	4.922908	-0.562818
17	1	0	-1.044825	5.627864	0.643107
18	1	0	2.087145	3.913987	-1.735727
19	1	0	1.065064	5.893995	-0.636558
20	6	0	-0.709320	-1.338477	1.322303
21	7	0	1.492442	-0.870402	0.784432
22	6	0	0.556791	-1.925929	0.844741
23	6	0	0.943559	0.303103	1.319435
24	8	0	0.800502	-3.071787	0.550255
25	8	0	1.547845	1.327298	1.519082
26	6	0	2.830218	-1.005896	0.323677
27	6	0	3.886348	-0.557374	1.114262
28	6	0	3.072309	-1.598006	-0.914380
29	6	0	5.191235	-0.694930	0.652824
30	1	0	3.685196	-0.106788	2.077974
31	6	0	4.381683	-1.745357	-1.358843
32	1	0	2.240854	-1.943334	-1.517158
33	6	0	5.442691	-1.291252	-0.579711
34	1	0	6.013348	-0.342981	1.265257
35	1	0	4.570223	-2.212890	-2.318445
36	1	0	6.461721	-1.402744	-0.931577
37	16	0	-2.479127	-2.811354	-1.079338
38	6	0	-4.137673	-1.217036	0.360505
39	6	0	-3.799452	-2.701404	0.202442
40	1	0	-4.654427	-3.282503	-0.136042
41	1	0	-3.408168	-3.127922	1.124812
42	1	0	-4.415351	-0.979230	1.387800
43	1	0	-4.937256	-0.905706	-0.314656
44	1	0	-1.458590	-1.966093	1.781349

Structure **TS_{11}** in toluene:

Electronic Energy (Hartrees) : -1885.13388969
Free Energy (Hartress): -1884.866526
One imaginary frequency (cm^{-1}): 436.1444i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.040785	-2.111171	0.565560
2	6	0	-0.677734	-1.165923	-0.288554
3	6	0	1.723177	-0.872954	-0.490386
4	6	0	0.134177	0.482767	1.406525
5	1	0	-0.021854	-0.165459	2.260635
6	6	0	1.414118	0.710657	0.931746
7	1	0	2.242382	0.333698	1.525999
8	16	0	0.365730	-0.513960	-1.506585
9	16	0	3.439007	-0.909169	-0.932384
10	7	0	1.398057	-1.930194	0.312552
11	8	0	-0.377576	-2.900673	1.400085
12	6	0	-2.129856	-1.030591	-0.378837
13	6	0	-2.964976	-1.610251	0.588984
14	6	0	-2.716124	-0.261937	-1.397253
15	6	0	-4.340822	-1.429855	0.524096
16	1	0	-2.528289	-2.194884	1.386645
17	6	0	-4.091238	-0.090916	-1.456043
18	1	0	-2.096406	0.211456	-2.152357
19	6	0	-4.911758	-0.674283	-0.494064
20	1	0	-4.970317	-1.881475	1.282061
21	1	0	-4.523149	0.501797	-2.254460
22	1	0	-5.985910	-0.537532	-0.537628
23	6	0	2.521276	-2.584018	0.962570
24	1	0	2.234775	-3.600102	1.231277
25	1	0	2.800466	-2.035064	1.868763
26	6	0	3.627600	-2.538702	-0.088143
27	6	0	1.781070	1.947097	0.152415
28	6	0	-1.028053	1.334492	1.101471
29	8	0	2.203176	1.971931	-0.974265
30	8	0	-2.006142	1.423982	1.801412
31	8	0	-0.883248	2.008032	-0.053502
32	8	0	1.639491	3.039024	0.908387
33	6	0	1.893152	4.282953	0.248106
34	1	0	1.710075	5.055055	0.991793
35	1	0	2.924659	4.330304	-0.102277
36	1	0	1.215067	4.400626	-0.598909
37	6	0	-1.922223	2.935747	-0.368281
38	1	0	-2.896559	2.448503	-0.327379
39	1	0	-1.903734	3.770644	0.335512
40	1	0	-1.712081	3.288019	-1.376299
41	1	0	3.505055	-3.332728	-0.824131
42	1	0	4.622594	-2.588501	0.349982

Structure **TS_{12}** in toluene:

Electronic Energy (Hartrees) : -1885.12837563
Free Energy (Hartress): -1884.859655
One imaginary frequency (cm^{-1}): 414.9738i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.207331	-0.675638	1.260635
2	6	0	-1.051713	-0.826120	0.065775
3	6	0	1.173034	-1.762927	-0.279911
4	6	0	-0.235389	0.738757	-1.130704
5	1	0	-1.027930	0.560075	-1.853636
6	6	0	1.057549	0.409095	-1.537409
7	1	0	1.230706	-0.088721	-2.480660
8	16	0	-0.372640	-2.142048	-0.927129
9	16	0	2.713488	-2.534858	-0.537236
10	7	0	1.066868	-1.165882	0.914078
11	6	0	-2.521669	-0.682162	0.069022
12	6	0	-3.197764	-0.161471	1.179552
13	6	0	-3.262427	-1.019121	-1.072494
14	6	0	-4.578243	-0.008001	1.146538
15	1	0	-2.632077	0.135678	2.050992
16	6	0	-4.642693	-0.864643	-1.097348
17	1	0	-2.762045	-1.402883	-1.957016
18	6	0	-5.308019	-0.359273	0.014905
19	1	0	-5.085720	0.396670	2.014750
20	1	0	-5.196224	-1.134702	-1.989312
21	1	0	-6.384472	-0.235047	-0.002775
22	6	0	2.241005	0.979873	-0.921925

23	6	0	-0.517441	1.994314	-0.337514
24	8	0	-1.201941	2.080765	0.642730
25	8	0	3.352594	1.016553	-1.405799
26	8	0	0.042618	3.055353	-0.939298
27	8	0	1.987463	1.458538	0.325168
28	6	0	3.027092	2.219746	0.931171
29	1	0	3.279730	3.082926	0.311974
30	1	0	2.638012	2.547790	1.893497
31	1	0	3.927427	1.617191	1.073846
32	6	0	-0.131844	4.299052	-0.257213
33	1	0	0.402403	5.039687	-0.848069
34	1	0	-1.189445	4.558258	-0.192164
35	1	0	0.287284	4.239559	0.748912
36	8	0	-0.421594	-0.192819	2.352077
37	6	0	2.244109	-1.198694	1.773551
38	6	0	3.414202	-1.532694	0.846310
39	1	0	2.093464	-1.970365	2.532504
40	1	0	2.366845	-0.230812	2.258640
41	1	0	4.177111	-2.127327	1.344911
42	1	0	3.865411	-0.643982	0.408245

Structure **TS1$_{14}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.95198000
Free Energy (Hartress): -1864.684164
One imaginary frequency (cm^{-1}): 400.6128i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.952454	-1.462263	-0.593811
2	6	0	0.125083	-0.781984	0.150557
3	6	0	-2.127356	-0.389696	1.101778
4	6	0	0.197820	0.937626	-0.904504
5	6	0	-0.946981	1.735768	-0.659787
6	16	0	-0.546446	-0.231340	1.726615
7	16	0	-3.647451	0.088435	1.743523
8	7	0	-2.191714	-1.068297	-0.029850
9	8	0	-0.897230	-2.184356	-1.558592
10	6	0	1.490854	-1.355891	0.174655
11	6	0	1.994654	-2.031525	-0.944885
12	6	0	2.349203	-1.125040	1.258158
13	6	0	3.315764	-2.468498	-0.967076
14	1	0	1.359040	-2.206932	-1.801626
15	6	0	3.668239	-1.557384	1.226963
16	1	0	2.003232	-0.591764	2.138177
17	6	0	4.160033	-2.231620	0.112202
18	1	0	3.685464	-2.990409	-1.842618
19	1	0	4.312544	-1.361528	2.076541
20	1	0	5.190206	-2.567528	0.086874
21	6	0	-3.532154	-1.433408	-0.495662
22	1	0	-3.742814	-2.451322	-0.160746
23	1	0	-3.557620	-1.370775	-1.581430
24	6	0	-4.458316	-0.405564	0.149724
25	1	0	-5.438059	-0.817055	0.380068
26	1	0	-4.544402	0.498956	-0.450197
27	1	0	-0.982795	2.551938	0.042695
28	1	0	0.223778	0.437750	-1.871166
29	6	0	1.512352	1.478814	-0.467456
30	6	0	2.649138	1.195672	-1.231567
31	6	0	1.659780	2.211456	0.715136
32	6	0	3.906602	1.620750	-0.818934
33	1	0	2.541602	0.631452	-2.151467
34	6	0	2.918827	2.635428	1.128880
35	1	0	0.795014	2.451891	1.323577
36	6	0	4.046081	2.335146	0.368335
37	1	0	4.777774	1.386957	-1.420658
38	1	0	3.018669	3.198517	2.049950
39	1	0	5.026342	2.661929	0.696228
40	7	0	-2.104696	1.551480	-1.358958
41	8	0	-2.192745	0.628206	-2.198588
42	8	0	-3.079246	2.305574	-1.134194

Structure **TS2$_{14}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.95714211
Free Energy (Hartress): -1864.68781
One imaginary frequency (cm^{-1}): 224.6333i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.934367	-1.521447	-0.543618
2	6	0	0.178996	-0.691679	0.111235
3	6	0	-2.056865	-0.247787	1.015026
4	6	0	0.230779	0.716320	-0.715267
5	6	0	-0.996617	1.528409	-0.519261
6	16	0	-0.500118	-0.265254	1.775463
7	16	0	-3.564478	0.316334	1.601155
8	7	0	-2.154395	-1.096328	-0.013719
9	8	0	-0.835918	-2.352558	-1.399732
10	6	0	1.515430	-1.386147	0.143929
11	6	0	2.049939	-1.868224	-1.055454
12	6	0	2.273045	-1.485505	1.310726
13	6	0	3.310300	-2.453138	-1.076591
14	1	0	1.485621	-1.780013	-1.975196
15	6	0	3.537627	-2.066508	1.285402
16	1	0	1.895406	-1.111196	2.256857
17	6	0	4.058587	-2.555343	0.092830
18	1	0	3.708944	-2.826153	-2.013135
19	1	0	4.111186	-2.133858	2.202452
20	1	0	5.042361	-3.009861	0.073350
21	6	0	-3.505373	-1.478016	-0.430638
22	1	0	-3.740842	-2.442785	0.023664
23	1	0	-3.538564	-1.541510	-1.516441
24	6	0	-4.408040	-0.363317	0.094752
25	1	0	-5.385849	-0.732401	0.395257
26	1	0	-4.496510	0.461432	-0.609256
27	1	0	-1.026148	2.395558	0.121239
28	1	0	0.298182	0.397364	-1.759350
29	6	0	1.488799	1.481682	-0.353188
30	6	0	2.587165	1.432687	-1.214618
31	6	0	1.592595	2.227181	0.824152
32	6	0	3.766432	2.103292	-0.905050
33	1	0	2.514489	0.867341	-2.137889
34	6	0	2.773928	2.893945	1.138158
35	1	0	0.749809	2.304325	1.501282
36	6	0	3.865543	2.830734	0.277651
37	1	0	4.606367	2.057116	-1.589070
38	1	0	2.835777	3.469139	2.055097
39	1	0	4.783018	3.354186	0.521307
40	7	0	-2.041882	1.416876	-1.361080
41	8	0	-2.070677	0.474623	-2.199398
42	8	0	-3.018805	2.206356	-1.255060

Structure **TS1$_{15}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.96772339
Free Energy (Hartress): -1864.698174
One imaginary frequency (cm^{-1}): 148.6953i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.175871	-0.897052	0.307784
2	6	0	-2.312360	0.147393	0.197683
3	6	0	0.119897	0.517032	-0.363612
4	6	0	-1.215357	1.164794	0.032739
5	1	0	-1.149416	1.798532	0.911982
6	16	0	-0.378511	-0.810081	2.063149
7	7	0	-2.217019	-1.071133	-0.303894
8	6	0	-0.925371	-1.747891	-0.289444
9	8	0	-0.896491	-2.892192	-0.631127
10	6	0	1.537423	-1.513838	0.036204
11	6	0	2.512564	-1.596342	1.026009

12	6	0	1.860752	-1.899991	-1.268661
13	6	0	3.790969	-2.059222	0.719950
14	1	0	2.266121	-1.288762	2.034839
15	6	0	3.134001	-2.365174	-1.574061
16	1	0	1.116580	-1.832440	-2.056225
17	6	0	4.105368	-2.445614	-0.577993
18	1	0	4.540646	-2.116830	1.501296
19	1	0	3.368733	-2.663998	-2.589600
20	1	0	5.099924	-2.806216	-0.815270
21	16	0	-3.880756	0.601918	0.700973
22	6	0	-3.418355	-1.900392	-0.090874
23	6	0	-4.582348	-0.926225	-0.041149
24	1	0	-3.519411	-2.617309	-0.902250
25	1	0	-4.948151	-0.660592	-1.032011
26	1	0	-5.396560	-1.284685	0.583777
27	8	0	-1.330832	3.259179	-0.988215
28	8	0	-2.165996	1.599975	-2.071398
29	1	0	0.100230	0.347663	-1.446637
30	6	0	1.314055	1.391455	-0.052013
31	6	0	1.479311	2.011618	1.188567
32	6	0	2.309852	1.538280	-1.020164
33	6	0	2.628464	2.749395	1.457061
34	1	0	0.722794	1.906012	1.957054
35	6	0	3.458459	2.275857	-0.751959
36	1	0	2.186682	1.063064	-1.988236
37	6	0	3.621552	2.881566	0.490682
38	1	0	2.746448	3.222128	2.425632
39	1	0	4.222301	2.379657	-1.514304
40	1	0	4.515059	3.457267	0.704254
41	7	0	-1.620147	2.094628	-1.109624
42	1	0	-3.285472	-2.426923	0.859825

Structure **TS2$_{15}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.96200751
Free Energy (Hartress): -1864.696301
One imaginary frequency (cm^{-1}): 1279.7499i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.255478	-0.882862	0.466234
2	6	0	-2.390113	0.019403	-0.143993
3	6	0	0.036579	0.405560	-0.422932
4	6	0	-1.305288	0.935460	0.069159
5	1	0	-1.069882	0.740022	1.329680
6	16	0	-0.083506	-0.448535	2.226201
7	7	0	-2.138727	-1.286212	-0.116487
8	6	0	-0.858375	-1.867228	0.191696
9	8	0	-0.793576	-3.062028	0.267972
10	6	0	1.612315	-1.491366	0.165749
11	6	0	2.704612	-1.305858	1.008334
12	6	0	1.799360	-2.152673	-1.051073
13	6	0	3.965726	-1.769123	0.639955
14	1	0	2.570016	-0.787249	1.949845
15	6	0	3.056604	-2.618822	-1.418241
16	1	0	0.962000	-2.298443	-1.726698
17	6	0	4.146337	-2.426090	-0.572536
18	1	0	4.807131	-1.612136	1.305313
19	1	0	3.185130	-3.130401	-2.365493
20	1	0	5.128143	-2.785911	-0.858718
21	16	0	-4.061530	0.402828	-0.319765
22	6	0	-3.331341	-2.156662	-0.115530
23	6	0	-4.428111	-1.336874	-0.767821
24	1	0	-3.114461	-3.066066	-0.670298
25	1	0	-4.410735	-1.413047	-1.853971
26	1	0	-5.414460	-1.592861	-0.387018
27	8	0	-2.653824	2.771628	0.320491
28	8	0	-1.024038	2.931303	-1.071136
29	1	0	-0.043332	0.079068	-1.465200
30	6	0	1.202890	1.363114	-0.304326
31	6	0	1.345984	2.265136	0.751226
32	6	0	2.208467	1.288195	-1.269028
33	6	0	2.481779	3.064916	0.843050

34	1	0	0.574508	2.357328	1.507443
35	6	0	3.347070	2.081167	-1.174451
36	1	0	2.103074	0.594075	-2.096248
37	6	0	3.488947	2.970228	-0.113353
38	1	0	2.577482	3.764684	1.665543
39	1	0	4.120251	2.003336	-1.930538
40	1	0	4.373738	3.592175	-0.037241
41	7	0	-1.680016	2.321926	-0.258540
42	1	0	-3.558851	-2.404219	0.924475

Structure **TS_{16}** in *N*,*N*-dimethylformamide:

Electronic Energy (Hartrees) : -1521.65988739
Free Energy (Hartress): -1521.474666
One imaginary frequency (cm^{-1}): 374.4590i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.737268	-0.030242	-0.066429
2	6	0	1.511725	-1.022511	0.171223
3	6	0	-0.358438	0.950911	-1.630444
4	1	0	-1.119278	0.485323	-2.252579
5	6	0	0.967181	0.847169	-2.127568
6	1	0	1.246206	0.083594	-2.840466
7	16	0	0.026435	-1.633138	-0.387903
8	7	0	1.406790	0.120130	0.839463
9	6	0	0.122732	0.701743	0.877123
10	8	0	-0.092633	1.728444	1.483681
11	6	0	-2.218044	-0.059481	0.085560
12	6	0	-2.885064	0.696380	1.054701
13	6	0	-2.974363	-0.832247	-0.806284
14	6	0	-4.275121	0.663858	1.133151
15	1	0	-2.322407	1.308161	1.746380
16	6	0	-4.359738	-0.868215	-0.717251
17	1	0	-2.481648	-1.409800	-1.583670
18	6	0	-5.017377	-0.117296	0.254085
19	1	0	-4.776976	1.252479	1.892913
20	1	0	-4.925482	-1.478733	-1.411692
21	1	0	-6.098960	-0.139796	0.321899
22	16	0	3.081155	-1.722540	0.181203
23	6	0	2.606344	0.569346	1.553248
24	6	0	3.769871	-0.146775	0.870433
25	1	0	2.697532	1.650695	1.461752
26	1	0	2.504185	0.282985	2.601809
27	1	0	4.163702	0.424988	0.033164
28	1	0	4.563165	-0.400229	1.569467
29	1	0	-0.676863	1.922009	-1.249476
30	6	0	1.975294	1.692009	-1.659151
31	7	0	2.804647	2.396115	-1.240339

Structure **TS_{17}** in *N*,*N*-dimethylformamide:

Electronic Energy (Hartrees) : -1521.65913284
Free Energy (Hartress): -1521.473611
One imaginary frequency (cm^{-1}): 394.5216i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.708153	-0.143022	-0.031139
2	6	0	-1.611783	-0.150691	0.754670
3	6	0	0.232520	0.940250	-1.546419
4	1	0	0.653757	0.277627	-2.300850
5	16	0	-0.210878	0.651730	1.292574
6	7	0	-1.349986	-1.206064	-0.019008
7	6	0	-0.019355	-1.354221	-0.435445
8	8	0	0.332362	-2.267111	-1.157007
9	6	0	2.187845	-0.104575	0.097588
10	6	0	2.987584	-1.219622	-0.173737
11	6	0	2.806335	1.097883	0.466312

12	6	0	4.372980	-1.129475	-0.066956
13	1	0	2.530012	-2.154701	-0.467146
14	6	0	4.187976	1.178818	0.581245
15	1	0	2.207288	1.982079	0.666180
16	6	0	4.978488	0.063898	0.311957
17	1	0	4.979043	-2.002989	-0.280157
18	1	0	4.646816	2.115691	0.875945
19	1	0	6.057449	0.127008	0.395750
20	6	0	-1.146110	1.233619	-1.654196
21	16	0	-3.256516	-0.009231	1.243564
22	6	0	-2.493793	-2.059073	-0.351915
23	6	0	-3.723045	-1.187920	-0.100274
24	1	0	-4.580441	-1.768789	0.231211
25	1	0	-3.985678	-0.590702	-0.972158
26	1	0	-2.428567	-2.364470	-1.395536
27	1	0	-2.471225	-2.937238	0.296128
28	1	0	-1.821543	0.579933	-2.192509
29	1	0	0.889095	1.771574	-1.302504
30	6	0	-1.690810	2.415625	-1.139892
31	7	0	-2.152661	3.396484	-0.716321

Structure **TS_{20}** in 2-propanol:

Electronic Energy (Hartrees) : -1582.05498530
Free Energy (Hartress): -1581.831363
One imaginary frequency (cm^{-1}): 413.7144i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.874700	-0.248105	0.050614
2	6	0	-1.426638	-0.518373	0.841828
3	6	0	0.304709	0.991081	-1.394206
4	1	0	0.792788	0.428561	-2.187853
5	16	0	-0.094134	0.344080	1.430756
6	7	0	-1.106187	-1.436144	-0.073032
7	6	0	0.221683	-1.429076	-0.512452
8	8	0	0.633205	-2.227771	-1.339049
9	6	0	2.347832	-0.127833	0.131746
10	6	0	3.140658	-0.575973	-0.934513
11	6	0	2.975674	0.494990	1.217430
12	6	0	4.522014	-0.418348	-0.898715
13	1	0	2.677162	-1.047846	-1.790644
14	6	0	4.356187	0.653812	1.244372
15	1	0	2.398722	0.856749	2.062510
16	6	0	5.137281	0.194922	0.188219
17	1	0	5.118472	-0.774389	-1.731390
18	1	0	4.819938	1.135514	2.097702
19	1	0	6.214035	0.317421	0.210886
20	6	0	-1.086833	1.173375	-1.462865
21	6	0	-1.739156	2.248990	-0.791181
22	8	0	-1.146035	3.098742	-0.096478
23	16	0	-3.066267	-0.586369	1.375436
24	6	0	-2.191374	-2.321943	-0.502558
25	6	0	-3.470931	-1.576557	-0.131320
26	1	0	-4.291572	-2.249760	0.105735
27	1	0	-3.769125	-0.870624	-0.906033
28	1	0	-2.120670	-2.488592	-1.577080
29	1	0	-2.096734	-3.271142	0.028952
30	1	0	-1.693767	0.493523	-2.051132
31	1	0	0.889303	1.829516	-1.022650
32	6	0	-3.243015	2.357794	-0.930058
33	1	0	-3.501250	3.358342	-1.287015
34	1	0	-3.660689	1.614795	-1.610720
35	1	0	-3.700998	2.237276	0.057052

Structure **TS_{21}** in dichloromethane:

Electronic Energy (Hartrees) : -2059.19404441
Free Energy (Hartress): -2058.839601
One imaginary frequency (cm^{-1}): 419.5816i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.605870	1.190465	-0.134120
2	6	0	-1.399901	-1.071616	-0.459674
3	6	0	0.227143	0.184216	1.617820
4	1	0	-0.205981	0.887935	2.317553
5	16	0	-0.270490	-0.084077	-1.308613
6	7	0	-2.345959	-0.305252	0.142313
7	6	0	-1.953933	1.000143	0.426504
8	8	0	-2.612190	1.760174	1.116987
9	6	0	0.034058	2.504766	-0.286856
10	6	0	-0.300384	3.564471	0.568563
11	6	0	1.038550	2.705123	-1.243954
12	6	0	0.350545	4.787933	0.454169
13	1	0	-1.065097	3.426599	1.320145
14	6	0	1.680760	3.930296	-1.355384
15	1	0	1.334277	1.902145	-1.912262
16	6	0	1.339340	4.979493	-0.506255
17	1	0	0.080979	5.597008	1.123504
18	1	0	2.451875	4.062347	-2.105545
19	1	0	1.842079	5.935979	-0.591272
20	6	0	-0.092684	-1.166152	1.491464
21	7	0	2.090786	-0.907968	0.779675
22	6	0	1.081809	-1.881036	0.981171
23	6	0	1.669503	0.339285	1.247776
24	8	0	1.225691	-3.060456	0.756932
25	8	0	2.356242	1.327998	1.319631
26	6	0	3.374348	-1.181769	0.235896
27	6	0	4.519047	-0.775190	0.918186
28	6	0	3.474344	-1.863860	-0.975058
29	6	0	5.770547	-1.045921	0.375010
30	1	0	4.424572	-0.253350	1.862256
31	6	0	4.730497	-2.142088	-1.502250
32	1	0	2.574729	-2.175059	-1.492566
33	6	0	5.879715	-1.731077	-0.831964
34	1	0	6.661891	-0.727289	0.903027
35	1	0	4.809638	-2.676517	-2.441914
36	1	0	6.857207	-1.944535	-1.248972
37	16	0	-1.965504	-2.675536	-0.836457
38	6	0	-3.616017	-0.972049	0.478252
39	6	0	-3.253016	-2.464626	0.468949
40	1	0	-4.098042	-3.097461	0.206398
41	1	0	-2.828936	-2.797213	1.415425
42	1	0	-3.911058	-0.654686	1.482133
43	1	0	-0.878707	-1.694041	2.009453
44	6	0	-4.730481	-0.642462	-0.536296
45	1	0	-4.511804	-1.207983	-1.450282
46	6	0	-6.071809	-1.110888	0.030805
47	1	0	-6.860654	-0.972907	-0.711795
48	1	0	-6.066888	-2.165527	0.315975
49	1	0	-6.334232	-0.521699	0.915083
50	6	0	-4.806522	0.838965	-0.897611
51	1	0	-4.993613	1.451142	-0.012243
52	1	0	-3.889661	1.195650	-1.372928
53	1	0	-5.625949	0.995561	-1.603234

Structure **TS_{22}** in dichloromethane:

Electronic Energy (Hartrees) : -2059.19495891
Free Energy (Hartress): -2058.835804
One imaginary frequency (cm^{-1}): 416.6556i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.461442	-0.859537	-0.971187
2	6	0	0.467728	1.298271	-0.536012
3	6	0	1.913880	1.304908	-0.262003
4	6	0	0.539098	-1.156450	1.099099
5	6	0	0.138389	0.146560	1.378141
6	16	0	0.092766	-0.029122	-1.619258
7	16	0	2.162098	-2.341410	-1.577053

8	7	0	2.395950	0.023274	-0.520346
9	6	0	3.789065	-0.474489	-0.469346
10	1	0	4.279162	-0.102986	-1.376165
11	6	0	3.652903	-1.999655	-0.562105
12	1	0	4.510582	-2.452716	-1.054900
13	1	0	3.506546	-2.458310	0.415992
14	8	0	2.601078	2.209705	0.183309
15	6	0	-0.374819	2.499842	-0.527441
16	6	0	-1.585996	2.526315	-1.232701
17	6	0	-0.024880	3.615513	0.248253
18	6	0	-2.416196	3.637360	-1.181742
19	1	0	-1.896558	1.672769	-1.827886
20	6	0	-0.865028	4.722087	0.300875
21	1	0	0.899650	3.610895	0.808426
22	6	0	-2.059791	4.741920	-0.412433
23	1	0	-3.345739	3.635496	-1.738909
24	1	0	-0.581649	5.575027	0.907374
25	1	0	-2.709237	5.608556	-0.368502
26	6	0	4.591573	-0.005915	0.754417
27	1	0	4.728896	1.070097	0.635548
28	6	0	3.879650	-0.245866	2.082817
29	1	0	2.924007	0.280929	2.130644
30	1	0	3.703167	-1.308614	2.272486
31	1	0	4.502660	0.130170	2.898103
32	6	0	5.967879	-0.673775	0.732338
33	1	0	6.460428	-0.545163	-0.235799
34	1	0	6.608200	-0.229073	1.496928
35	1	0	5.896954	-1.745413	0.941254
36	1	0	0.654523	0.871648	1.993856
37	1	0	1.443214	-1.642372	1.435252
38	6	0	-1.349187	0.190890	1.304940
39	6	0	-0.659694	-1.951666	0.778779
40	7	0	-1.758803	-1.065748	0.835976
41	8	0	-2.085083	1.105312	1.580481
42	8	0	-0.743041	-3.127233	0.512174
43	6	0	-3.095322	-1.411072	0.502752
44	6	0	-3.350685	-2.096059	-0.684398
45	6	0	-4.140019	-1.060238	1.356226
46	6	0	-4.658490	-2.435351	-1.012598
47	1	0	-2.530025	-2.360901	-1.339679
48	6	0	-5.446229	-1.389485	1.009110
49	1	0	-3.929147	-0.534843	2.278441
50	6	0	-5.709196	-2.078913	-0.171041
51	1	0	-4.855921	-2.972614	-1.933062
52	1	0	-6.259360	-1.111586	1.669707
53	1	0	-6.728299	-2.338607	-0.433687

Structure **TS1$_{24}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.87297322
Free Energy (Hartress): -1982.524066
One imaginary frequency (cm^{-1}): 395.0010i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470195	0.574343	0.142973
2	6	0	1.618202	-0.346477	1.097577
3	6	0	-0.944970	-1.098807	-0.893950
4	6	0	-0.026061	-2.142229	-0.626209
5	1	0	-0.186682	-2.925871	0.095723
6	16	0	0.048319	-0.101787	1.726974
7	7	0	1.853480	0.307727	-0.026558
8	6	0	0.737965	0.963114	-0.608709
9	8	0	0.845559	1.645542	-1.598767
10	6	0	-1.661433	1.453934	0.149584
11	6	0	-2.544818	1.458369	1.237409
12	6	0	-1.995986	2.205243	-0.985763
13	6	0	-3.722898	2.192174	1.196348
14	1	0	-2.331615	0.877146	2.129330
15	6	0	-3.175495	2.943158	-1.018251
16	1	0	-1.342265	2.203399	-1.846638
17	6	0	-4.045471	2.939760	0.066384
18	1	0	-4.390676	2.175445	2.050079

19	1	0	-3.415444	3.518690	-1.905369
20	1	0	-4.965732	3.511392	0.033930
21	16	0	2.948778	-1.227084	1.720660
22	6	0	3.243627	0.335690	-0.515983
23	6	0	3.908841	-0.867275	0.175947
24	1	0	3.199843	0.153768	-1.590431
25	1	0	3.847790	-1.765734	-0.435044
26	1	0	4.940316	-0.668824	0.462434
27	8	0	1.920199	-3.202724	-1.053616
28	6	0	3.883048	1.705716	-0.242543
29	1	0	3.206572	2.441172	-0.689705
30	6	0	4.033040	2.022385	1.244302
31	1	0	3.078586	1.982790	1.777433
32	1	0	4.732320	1.335183	1.730121
33	1	0	4.430391	3.032814	1.364259
34	6	0	5.225420	1.792408	-0.967152
35	1	0	5.113706	1.591911	-2.035609
36	1	0	5.649167	2.792253	-0.850664
37	1	0	5.946847	1.078813	-0.557893
38	8	0	1.455564	-1.398035	-2.175195
39	1	0	-0.842409	-0.621370	-1.866593
40	6	0	-2.353015	-1.306050	-0.463400
41	6	0	-2.677453	-1.962648	0.728900
42	6	0	-3.386301	-0.785864	-1.248938
43	6	0	-4.004517	-2.083706	1.128430
44	1	0	-1.897923	-2.380956	1.356157
45	6	0	-4.712500	-0.908636	-0.850003
46	1	0	-3.143692	-0.274804	-2.174384
47	6	0	-5.025150	-1.553680	0.343850
48	1	0	-4.240271	-2.594991	2.054924
49	1	0	-5.500463	-0.496413	-1.470145
50	1	0	-6.058285	-1.646427	0.658836
51	7	0	1.149739	-2.250764	-1.313027

Structure **TS2$_{24}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.87830279
Free Energy (Hartress): -1982.528205
One imaginary frequency (cm^{-1}): 220.1760i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.526768	0.497635	0.056383
2	6	0	1.525293	-0.489338	0.968687
3	6	0	-0.940659	-0.871557	-0.743209
4	6	0	0.042457	-1.959948	-0.522165
5	1	0	-0.136482	-2.785585	0.147934
6	16	0	0.027719	-0.059243	1.730404
7	7	0	1.838440	0.303522	-0.062868
8	6	0	0.758555	0.999302	-0.614700
9	8	0	0.868327	1.791430	-1.507024
10	6	0	-1.654169	1.497370	0.092727
11	6	0	-2.434497	1.665702	1.237581
12	6	0	-2.008206	2.182713	-1.073635
13	6	0	-3.537042	2.513343	1.226731
14	1	0	-2.205526	1.131541	2.154293
15	6	0	-3.108114	3.034741	-1.079582
16	1	0	-1.435156	2.045061	-1.980795
17	6	0	-3.875331	3.204530	0.068078
18	1	0	-4.128843	2.629171	2.127248
19	1	0	-3.366748	3.562433	-1.990483
20	1	0	-4.734221	3.865716	0.058918
21	16	0	2.821341	-1.437705	1.547693
22	6	0	3.239827	0.322813	-0.518226
23	6	0	3.857234	-0.949695	0.090539
24	1	0	3.220252	0.227201	-1.604499
25	1	0	3.823148	-1.787229	-0.602101
26	1	0	4.871838	-0.787934	0.450302
27	8	0	1.850514	-3.122517	-1.201222
28	6	0	3.916466	1.642946	-0.118933
29	1	0	3.276057	2.435909	-0.518811
30	6	0	4.035195	1.831145	1.392293
31	1	0	3.065841	1.770729	1.895751

32	1	0	4.705261	1.089088	1.837636
33	1	0	4.452297	2.818103	1.605760
34	6	0	5.279097	1.744384	-0.802327
35	1	0	5.190270	1.625602	-1.885174
36	1	0	5.725232	2.721248	-0.603677
37	1	0	5.971331	0.983663	-0.429380
38	8	0	1.340332	-1.258947	-2.229127
39	1	0	-0.927750	-0.566135	-1.793498
40	6	0	-2.352510	-1.267241	-0.360685
41	6	0	-2.640156	-1.957680	0.819074
42	6	0	-3.410655	-0.891025	-1.191954
43	6	0	-3.957645	-2.245266	1.167530
44	1	0	-1.841117	-2.278732	1.477400
45	6	0	-4.726840	-1.176658	-0.845178
46	1	0	-3.199137	-0.363241	-2.116061
47	6	0	-5.004898	-1.851088	0.340604
48	1	0	-4.163075	-2.782311	2.086724
49	1	0	-5.534125	-0.874435	-1.502760
50	1	0	-6.029850	-2.075743	0.613472
51	7	0	1.087610	-2.131445	-1.353784

Structure **TS1$_{26}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.88357277
Free Energy (Hartress): -1982.532574
One imaginary frequency (cm^{-1}): 176.5338i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.393966	0.741557	0.160872
2	6	0	1.658035	-0.982888	0.073239
3	6	0	-0.805912	-0.673581	-0.375781
4	6	0	0.302893	-1.646283	0.044289
5	1	0	0.108406	-2.160420	0.980171
6	16	0	0.227508	0.604023	1.887280
7	7	0	1.896430	0.161736	-0.549110
8	6	0	0.853256	1.161818	-0.605139
9	8	0	1.084422	2.198177	-1.155107
10	6	0	-1.536069	1.713679	-0.084632
11	6	0	-2.354077	2.153109	0.953098
12	6	0	-1.858318	2.075370	-1.397157
13	6	0	-3.473245	2.940178	0.687348
14	1	0	-2.116559	1.866263	1.970108
15	6	0	-2.970630	2.865072	-1.662776
16	1	0	-1.242990	1.733789	-2.222847
17	6	0	-3.785364	3.298787	-0.618930
18	1	0	-4.101504	3.269378	1.507476
19	1	0	-3.203767	3.138135	-2.685971
20	1	0	-4.656413	3.910290	-0.826221
21	16	0	3.061055	-1.899582	0.429162
22	6	0	3.327056	0.554756	-0.675000
23	6	0	4.085265	-0.773796	-0.602963
24	1	0	3.440062	0.979421	-1.673709
25	1	0	4.175053	-1.249211	-1.578581
26	1	0	5.068614	-0.672025	-0.148383
27	8	0	-0.187701	-3.791344	-0.736973
28	6	0	3.766304	1.602547	0.366296
29	1	0	2.983583	2.364378	0.401516
30	6	0	3.955973	1.048092	1.779188
31	1	0	3.057166	0.549443	2.144942
32	1	0	4.801080	0.354956	1.832058
33	1	0	4.174008	1.876571	2.457859
34	6	0	5.049927	2.268609	-0.131675
35	1	0	4.898984	2.755160	-1.098541
36	1	0	5.379856	3.025338	0.583137
37	1	0	5.858808	1.538426	-0.237999
38	8	0	0.888212	-2.491708	-2.070362
39	1	0	-0.795970	-0.611145	-1.470760
40	6	0	-2.183273	-1.126690	0.053296
41	6	0	-2.449306	-1.585301	1.345261
42	6	0	-3.234792	-1.034622	-0.861399
43	6	0	-3.746766	-1.927410	1.716107
44	1	0	-1.650691	-1.661371	2.073536

45	6	0	-4.531146	-1.377207	-0.491347
46	1	0	-3.036281	-0.683840	-1.869119
47	6	0	-4.790881	-1.820684	0.802028
48	1	0	-3.939933	-2.277313	2.723902
49	1	0	-5.335304	-1.298325	-1.214153
50	1	0	-5.799941	-2.088707	1.094207
51	7	0	0.350353	-2.747726	-1.015390

Structure **TS2$_{26}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.88221849
Free Energy (Hartress): -1982.534712
One imaginary frequency (cm^{-1}): 1299.3065i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.488284	-0.792493	0.284919
2	6	0	-1.731216	0.862283	-0.443400
3	6	0	0.723754	0.564044	-0.487118
4	6	0	-0.465145	1.414396	-0.054428
5	1	0	-0.422843	1.054627	1.208227
6	16	0	0.103422	-0.409420	2.046518
7	7	0	-1.875421	-0.459455	-0.464929
8	6	0	-0.821808	-1.398445	-0.174584
9	8	0	-1.071003	-2.567842	-0.264010
10	6	0	1.649720	-1.736583	0.035836
11	6	0	2.665172	-1.909675	0.972886
12	6	0	1.768479	-2.352282	-1.213426
13	6	0	3.782487	-2.683498	0.667643
14	1	0	2.585952	-1.425807	1.938942
15	6	0	2.880784	-3.129065	-1.517387
16	1	0	0.992511	-2.220376	-1.960936
17	6	0	3.893647	-3.296554	-0.575814
18	1	0	4.565751	-2.805779	1.407219
19	1	0	2.956832	-3.602950	-2.489613
20	1	0	4.762251	-3.900823	-0.812206
21	16	0	-3.163519	1.733732	-0.834634
22	6	0	-3.258468	-0.966336	-0.671141
23	6	0	-3.998052	0.187040	-1.351940
24	1	0	-3.189518	-1.811519	-1.355724
25	1	0	-3.941644	0.126948	-2.437314
26	1	0	-5.039938	0.248159	-1.042258
27	8	0	-1.249086	3.543388	0.272270
28	6	0	-3.867837	-1.446888	0.657638
29	1	0	-3.149476	-2.154190	1.082400
30	6	0	-4.093516	-0.326792	1.671806
31	1	0	-3.171298	0.214240	1.901219
32	1	0	-4.844159	0.389360	1.323324
33	1	0	-4.459481	-0.756457	2.607304
34	6	0	-5.163655	-2.206372	0.371850
35	1	0	-4.997061	-3.027898	-0.329663
36	1	0	-5.559490	-2.626866	1.298583
37	1	0	-5.931235	-1.547977	-0.045936
38	8	0	0.463919	3.311082	-1.004554
39	1	0	0.667521	0.346671	-1.559394
40	6	0	2.086510	1.149909	-0.182966
41	6	0	2.351567	1.898246	0.964974
42	6	0	3.133104	0.872628	-1.063774
43	6	0	3.643797	2.339313	1.234816
44	1	0	1.555178	2.147901	1.656669
45	6	0	4.425758	1.308634	-0.793292
46	1	0	2.934146	0.301142	-1.964705
47	6	0	4.686260	2.038112	0.363026
48	1	0	3.834937	2.919283	2.130686
49	1	0	5.227482	1.078099	-1.485648
50	1	0	5.692565	2.378934	0.578708
51	7	0	-0.401127	2.867388	-0.284556

Structure **TS1$_{27}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.94380753

Free Energy (Hartress): -1864.679261
One imaginary frequency (cm^{-1}): 368.7695i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.270107	0.199039	-1.414620
2	6	0	0.195880	-0.771766	-0.411004
3	6	0	-2.261588	-0.695461	-0.608367
4	6	0	0.268836	0.422717	1.164619
5	6	0	-1.037296	0.787109	1.586614
6	16	0	-1.186236	-1.857837	-0.010551
7	16	0	-3.976507	-0.603062	-0.534363
8	7	0	-1.682364	0.242598	-1.353524
9	8	0	0.359339	0.967474	-2.104505
10	6	0	1.517020	-1.442571	-0.494605
11	6	0	2.466948	-1.096227	-1.459795
12	6	0	1.849880	-2.397954	0.475100
13	6	0	3.719628	-1.704028	-1.453306
14	1	0	2.235973	-0.346421	-2.204259
15	6	0	3.098436	-3.004722	0.472353
16	1	0	1.134863	-2.661134	1.250489
17	6	0	4.041295	-2.656400	-0.492406
18	1	0	4.447805	-1.424431	-2.206256
19	1	0	3.336344	-3.742888	1.229581
20	1	0	5.019291	-3.123642	-0.491823
21	6	0	-2.572255	1.286843	-1.865298
22	1	0	-2.239392	1.598650	-2.853818
23	1	0	-2.541483	2.134645	-1.176123
24	6	0	-3.951388	0.633022	-1.910556
25	1	0	-4.113414	0.087797	-2.838954
26	1	0	-4.753585	1.347969	-1.745639
27	1	0	0.714745	-0.346584	1.789487
28	1	0	-1.568232	1.677176	1.290237
29	7	0	-1.708020	0.014765	2.497021
30	8	0	-1.185539	-1.021652	2.961113
31	8	0	-2.852469	0.366825	2.855986
32	6	0	1.242616	1.480423	0.776688
33	6	0	2.609534	1.232222	0.943098
34	6	0	0.842212	2.719406	0.264475
35	6	0	3.553053	2.198520	0.610069
36	1	0	2.932569	0.276380	1.343577
37	6	0	1.783699	3.686838	-0.063317
38	1	0	-0.210495	2.935582	0.117835
39	6	0	3.142229	3.429256	0.106947
40	1	0	4.607803	1.990947	0.750594
41	1	0	1.456081	4.643841	-0.453324
42	1	0	3.875270	4.186166	-0.148344

Structure **TS2$_{27}$** in dichloromethane:

Electronic Energy (Hartrees) : -1864.94801605
Free Energy (Hartress): -1864.680113
One imaginary frequency (cm^{-1}): 111.2547i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330796	-0.136601	-1.452148
2	6	0	0.218015	-0.719650	-0.162011
3	6	0	-2.242522	-0.836823	-0.348241
4	6	0	0.241904	0.552068	0.891683
5	6	0	-1.102372	1.131004	1.103671
6	16	0	-1.121390	-1.828629	0.466520
7	16	0	-3.940034	-0.759151	-0.210935
8	7	0	-1.731003	-0.177766	-1.400826
9	8	0	0.265010	0.424671	-2.330941
10	6	0	1.538779	-1.446668	-0.195526
11	6	0	2.398499	-1.410181	-1.292855
12	6	0	1.924275	-2.148877	0.951852
13	6	0	3.622922	-2.073376	-1.238899
14	1	0	2.130197	-0.857900	-2.182811
15	6	0	3.141933	-2.813890	0.998406

16	1	0	1.276801	-2.171349	1.824658
17	6	0	3.997728	-2.776442	-0.100104
18	1	0	4.283975	-2.036395	-2.097078
19	1	0	3.421638	-3.358638	1.892604
20	1	0	4.950401	-3.292199	-0.065586
21	6	0	-2.668374	0.704926	-2.099300
22	1	0	-2.424418	0.737307	-3.159450
23	1	0	-2.587810	1.704530	-1.663234
24	6	0	-4.042726	0.085493	-1.854520
25	1	0	-4.286155	-0.677141	-2.592121
26	1	0	-4.830395	0.833963	-1.806807
27	1	0	0.561683	0.080506	1.821458
28	1	0	-1.524590	1.919005	0.499993
29	7	0	-1.819890	0.827646	2.201448
30	8	0	-1.402085	-0.026664	3.030373
31	8	0	-2.938592	1.384709	2.380429
32	6	0	1.308785	1.537685	0.451723
33	6	0	2.619896	1.360457	0.902262
34	6	0	1.030943	2.617861	-0.389330
35	6	0	3.630915	2.235784	0.519123
36	1	0	2.848865	0.529871	1.561999
37	6	0	2.039991	3.495693	-0.772637
38	1	0	0.023303	2.785991	-0.752319
39	6	0	3.343391	3.306496	-0.322131
40	1	0	4.640460	2.083529	0.883682
41	1	0	1.804976	4.330684	-1.422966
42	1	0	4.128315	3.992072	-0.620755

Structure **TS_{28}** in dichloromethane:

Electronic Energy (Hartrees) : -1864.93842258
Free Energy (Hartress): -1864.671942
One imaginary frequency (cm^{-1}): 433.0652
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.371956	0.824618	1.313352
2	6	0	1.334929	0.657059	0.201661
3	6	0	-0.868428	1.235462	-0.616246
4	6	0	0.261516	-1.337136	-0.375124
5	6	0	-0.950126	-0.954663	-0.951606
6	16	0	0.750132	1.475213	-1.211689
7	16	0	-2.303961	2.068581	-1.202236
8	7	0	-0.832568	1.208479	0.757109
9	8	0	0.534164	0.632600	2.509183
10	6	0	2.757502	0.355682	0.366354
11	6	0	3.249648	-0.153531	1.579469
12	6	0	3.644188	0.502830	-0.712252
13	6	0	4.592280	-0.487689	1.703043
14	1	0	2.577354	-0.284848	2.415516
15	6	0	4.983981	0.166907	-0.578856
16	1	0	3.291493	0.878776	-1.667448
17	6	0	5.464814	-0.329190	0.630100
18	1	0	4.957751	-0.877400	2.646431
19	1	0	5.652710	0.289618	-1.422723
20	1	0	6.510994	-0.593213	0.733081
21	6	0	-2.044012	1.656390	1.444873
22	1	0	-1.753429	2.104503	2.395184
23	1	0	-2.715323	0.816956	1.625892
24	6	0	-2.666915	2.680499	0.498923
25	1	0	-2.210468	3.663017	0.611116
26	1	0	-3.745966	2.749484	0.620574
27	1	0	-0.975161	-0.888908	-2.033609
28	1	0	0.358665	-1.816573	0.587963
29	7	0	1.359528	-1.698384	-1.229943
30	8	0	1.387309	-1.278703	-2.378095
31	8	0	2.238937	-2.395276	-0.745612
32	6	0	-2.230270	-1.270357	-0.291812
33	6	0	-3.412149	-1.176241	-1.037216
34	6	0	-2.316801	-1.646029	1.055839
35	6	0	-4.645492	-1.447725	-0.454755
36	1	0	-3.357549	-0.893991	-2.083219
37	6	0	-3.549479	-1.918755	1.636155

38	1	0	-1.423733	-1.714383	1.667915
39	6	0	-4.719292	-1.818065	0.884919
40	1	0	-5.549091	-1.373837	-1.049319
41	1	0	-3.596575	-2.208517	2.679887
42	1	0	-5.679484	-2.031404	1.340695

Structure **TS_{29}** in dichloromethane:

Electronic Energy (Hartrees) : -1864.93873707
Free Energy (Hartress): -1864.670889
One imaginary frequency (cm^{-1}): 458.1796i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.127493	-1.710034	-0.249670
2	6	0	-1.300044	-0.305803	-0.649165
3	6	0	1.022367	-0.977345	-0.812456
4	6	0	-0.130751	0.344792	1.324855
5	6	0	1.210030	0.114091	1.033833
6	16	0	0.032704	0.192235	-1.648607
7	16	0	2.610905	-1.573136	-1.310747
8	7	0	0.218525	-2.004289	-0.398411
9	8	0	-1.944666	-2.492953	0.208598
10	6	0	-2.555875	0.442243	-0.621455
11	6	0	-3.719231	-0.121035	-0.073629
12	6	0	-2.601278	1.766850	-1.089149
13	6	0	-4.892554	0.624056	-0.013159
14	1	0	-3.698304	-1.135705	0.297106
15	6	0	-3.776273	2.499429	-1.027542
16	1	0	-1.711121	2.232880	-1.499785
17	6	0	-4.929620	1.930069	-0.488528
18	1	0	-5.783470	0.175630	0.411361
19	1	0	-3.792126	3.518446	-1.396262
20	1	0	-5.847981	2.503810	-0.439944
21	6	0	0.920613	-3.225053	-0.026820
22	1	0	0.233308	-4.066879	-0.098855
23	1	0	1.285062	-3.133216	1.000435
24	6	0	2.063213	-3.316673	-1.033554
25	1	0	1.727579	-3.726184	-1.985419
26	1	0	2.909214	-3.885271	-0.653110
27	1	0	-0.626943	1.302415	1.270329
28	1	0	1.660470	-0.743320	1.524234
29	6	0	2.141997	1.211818	0.703010
30	6	0	3.514728	0.996109	0.877342
31	6	0	1.715882	2.453841	0.212799
32	6	0	4.437344	1.990280	0.568217
33	1	0	3.856520	0.043020	1.266354
34	6	0	2.638554	3.446649	-0.091891
35	1	0	0.660173	2.654191	0.066459
36	6	0	4.002880	3.218897	0.080898
37	1	0	5.495571	1.804309	0.712979
38	1	0	2.290856	4.403364	-0.465071
39	1	0	4.719246	3.996486	-0.157991
40	7	0	-0.818683	-0.544505	2.225656
41	8	0	-0.299615	-1.607976	2.533484
42	8	0	-1.915924	-0.187459	2.628230

Structure **TS_{30}** in *N*,*N*-dimethylformamide:

Electronic Energy (Hartrees) : -1521.65684460
Free Energy (Hartress): -1521.469153
One imaginary frequency (cm^{-1}): 499.8059i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.455265	-0.306700	0.311588
2	6	0	-1.865832	0.406856	0.343432
3	6	0	-0.122618	0.984341	-1.764288

4	1	0	0.054942	0.140600	-2.421307
5	16	0	-0.445210	0.830941	1.263187
6	7	0	-1.725964	-0.881292	-0.092094
7	6	0	-0.422716	-1.331458	-0.247630
8	8	0	-0.141309	-2.388486	-0.800725
9	6	0	1.909115	-0.390581	0.385017
10	6	0	2.615930	-1.258348	-0.465038
11	6	0	2.637303	0.436882	1.254266
12	6	0	4.004347	-1.295323	-0.431574
13	1	0	2.071448	-1.896488	-1.147710
14	6	0	4.024457	0.390852	1.283915
15	1	0	2.123734	1.121446	1.922127
16	6	0	4.715719	-0.475923	0.441585
17	1	0	4.534087	-1.969517	-1.095305
18	1	0	4.565944	1.035162	1.967064
19	1	0	5.798834	-0.510998	0.464426
20	6	0	-1.401327	1.420223	-1.451331
21	16	0	-3.551725	0.760834	0.757105
22	6	0	-2.955603	-1.514450	-0.548748
23	6	0	-4.021428	-0.991181	0.408952
24	1	0	-4.017777	-1.541016	1.348906
25	1	0	-5.016559	-1.000058	-0.030506
26	1	0	-3.158412	-1.222381	-1.584076
27	1	0	-2.844963	-2.596142	-0.487383
28	1	0	-2.236944	0.967145	-1.973333
29	1	0	-1.553673	2.434975	-1.102089
30	6	0	1.001959	1.821104	-1.521817
31	7	0	1.913586	2.495434	-1.303573

Structure **TS_{31}** in *N*,*N*-dimethylformamide:

Electronic Energy (Hartrees) : -1521.65331988
Free Energy (Hartress): -1521.465673
One imaginary frequency (cm^{-1}): 509.2062i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.570765	-0.367848	0.294347
2	6	0	1.787835	-0.736258	-0.123603
3	6	0	0.109355	0.694548	-1.831041
4	1	0	-0.722324	0.146347	-2.257722
5	6	0	1.417600	0.252145	-1.964464
6	1	0	1.613791	-0.599335	-2.603949
7	16	0	0.375884	-1.760323	-0.141934
8	7	0	1.573256	0.293502	0.746028
9	6	0	0.248044	0.599210	1.019609
10	8	0	-0.088604	1.549873	1.714692
11	6	0	-2.031308	-0.388028	0.280013
12	6	0	-2.753587	0.776877	0.589995
13	6	0	-2.740399	-1.540395	-0.094375
14	6	0	-4.142309	0.777286	0.525691
15	1	0	-2.220368	1.673187	0.877645
16	6	0	-4.127120	-1.532062	-0.149747
17	1	0	-2.212161	-2.456571	-0.339293
18	6	0	-4.835787	-0.372805	0.159642
19	1	0	-4.685014	1.684998	0.764993
20	1	0	-4.656320	-2.434563	-0.433710
21	1	0	-5.918841	-0.368185	0.116703
22	16	0	3.471876	-1.275225	-0.059961
23	6	0	2.753606	0.955392	1.295140
24	6	0	3.938126	0.418320	0.491410
25	1	0	2.662137	2.036823	1.188405
26	1	0	2.829533	0.697371	2.353867
27	1	0	4.132617	1.022576	-0.393212
28	1	0	4.842856	0.346700	1.091449
29	1	0	2.229193	0.963193	-1.851711
30	6	0	-0.181491	2.042138	-1.475766
31	7	0	-0.427717	3.133089	-1.189137

Structure **TS_{32}** in 2-propanol:

Electronic Energy (Hartrees) : -1582.05725406
Free Energy (Hartress): -1581.832848
One imaginary frequency (cm^{-1}): 430.9670i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.938359	-0.090420	-0.046195
2	6	0	1.267666	-1.015311	-0.626604
3	6	0	-0.339577	1.792411	-0.220478
4	1	0	-1.160155	2.066643	-0.877217
5	6	0	0.962575	1.943526	-0.726644
6	1	0	1.122751	2.039822	-1.794434
7	16	0	-0.196479	-0.863215	-1.482720
8	7	0	1.134494	-0.836620	0.680903
9	6	0	-0.131197	-0.411527	1.126259
10	8	0	-0.375154	-0.255494	2.309948
11	6	0	-2.422194	-0.069039	-0.019000
12	6	0	-3.119326	0.288428	-1.181799
13	6	0	-3.150396	-0.373209	1.136184
14	6	0	-4.507339	0.322919	-1.195651
15	1	0	-2.575363	0.547608	-2.086099
16	6	0	-4.541799	-0.325750	1.119282
17	1	0	-2.633758	-0.650341	2.045065
18	6	0	-5.225679	0.018347	-0.041725
19	1	0	-5.028083	0.593873	-2.107115
20	1	0	-5.091780	-0.566042	2.022431
21	1	0	-6.309193	0.050298	-0.049187
22	16	0	2.824897	-1.571619	-1.121797
23	6	0	2.285256	-1.202590	1.510469
24	6	0	3.482214	-1.176836	0.562957
25	1	0	2.394159	-0.475382	2.312718
26	1	0	2.106879	-2.200211	1.917380
27	1	0	3.942786	-0.191922	0.511311
28	1	0	4.227085	-1.926093	0.820998
29	6	0	2.097303	1.998690	0.130442
30	8	0	2.034516	1.810824	1.363162
31	1	0	-0.508471	2.054622	0.823267
32	6	0	3.437193	2.289731	-0.518062
33	1	0	4.226538	2.318128	0.233393
34	1	0	3.672305	1.525089	-1.266097
35	1	0	3.405211	3.248743	-1.041937

Structure **TS_{33}** in 2-propanol:

Electronic Energy (Hartrees) : -1582.04996619
Free Energy (Hartress): -1581.825413
One imaginary frequency (cm^{-1}): 517.5797i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.358505	-0.512574	0.376100
2	6	0	-1.954120	0.205936	0.536494
3	6	0	-0.269260	1.090875	-1.489942
4	1	0	-0.298359	0.330098	-2.265718
5	16	0	-0.547816	0.406504	1.540294
6	7	0	-1.822899	-0.966856	-0.157803
7	6	0	-0.529156	-1.399431	-0.366982
8	8	0	-0.257513	-2.354793	-1.097661
9	6	0	1.811159	-0.619404	0.456213
10	6	0	2.523354	-1.406008	-0.463401
11	6	0	2.535046	0.124392	1.403166
12	6	0	3.911829	-1.456703	-0.416092
13	1	0	1.987016	-1.965495	-1.217066
14	6	0	3.920577	0.068247	1.442959
15	1	0	2.019279	0.754628	2.121135
16	6	0	4.617317	-0.725542	0.534224
17	1	0	4.444659	-2.069021	-1.134934
18	1	0	4.457184	0.646407	2.186616
19	1	0	5.700040	-0.768122	0.565055
20	6	0	-1.456594	1.582005	-0.965028
21	6	0	1.047638	1.717519	-1.324537

22	8	0	1.992916	1.346258	-2.011821
23	16	0	-3.632234	0.441497	1.049648
24	6	0	-3.044959	-1.568411	-0.684671
25	6	0	-4.167035	-0.565623	-0.397590
26	1	0	-5.100116	-1.061787	-0.138985
27	1	0	-4.333665	0.106471	-1.237682
28	1	0	-2.943141	-1.748449	-1.755995
29	1	0	-3.207545	-2.519016	-0.172562
30	1	0	-2.373808	1.371383	-1.505653
31	1	0	-1.462163	2.501986	-0.389446
32	6	0	1.214786	2.843514	-0.339493
33	1	0	0.777580	3.751711	-0.767262
34	1	0	0.700583	2.651689	0.604231
35	1	0	2.275789	3.013015	-0.158831

Structure **TS_{34}** in 2-propanol:

Electronic Energy (Hartrees) : -1582.05272562
Free Energy (Hartress): -1581.828067
One imaginary frequency (cm^{-1}): 527.6075i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.578837	-0.554421	0.279809
2	6	0	1.774839	-0.883630	-0.200219
3	6	0	0.227828	0.879509	-1.659268
4	1	0	-0.648199	0.471558	-2.151055
5	6	0	1.485638	0.335299	-1.861757
6	1	0	1.626711	-0.424127	-2.621502
7	16	0	0.345976	-1.866495	-0.382032
8	7	0	1.566818	-0.002685	0.827029
9	6	0	0.248934	0.281692	1.127808
10	8	0	-0.081227	1.148789	1.942324
11	6	0	-2.041225	-0.581518	0.259690
12	6	0	-2.719838	-1.154657	-0.827592
13	6	0	-2.790152	-0.015166	1.302000
14	6	0	-4.106768	-1.168466	-0.867177
15	1	0	-2.157690	-1.577299	-1.654353
16	6	0	-4.180058	-0.029482	1.251998
17	1	0	-2.281705	0.429490	2.146714
18	6	0	-4.843874	-0.603559	0.172222
19	1	0	-4.613450	-1.615087	-1.715161
20	1	0	-4.745183	0.410717	2.066036
21	1	0	-5.927367	-0.610695	0.138502
22	16	0	3.451801	-1.460030	-0.190174
23	6	0	2.752122	0.553528	1.475051
24	6	0	3.933315	0.131187	0.601478
25	1	0	2.670042	1.638830	1.535591
26	1	0	2.821617	0.133024	2.481166
27	1	0	4.134057	0.860162	-0.182222
28	1	0	4.836242	-0.037079	1.185060
29	6	0	0.075063	2.175977	-0.980589
30	8	0	1.031468	2.746354	-0.468195
31	1	0	2.348823	0.959349	-1.651507
32	6	0	-1.308379	2.760090	-0.937397
33	1	0	-2.010326	2.034378	-0.515219
34	1	0	-1.317914	3.675939	-0.347632
35	1	0	-1.641386	2.974597	-1.957688

Structure **TS_{35}** in dichloromethane:

Electronic Energy (Hartrees) : -2059.19817531
Free Energy (Hartress): -2058.838811
One imaginary frequency (cm^{-1}): 449.8717i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.974072	0.231345	-0.064611
2	6	0	0.385926	1.855322	-0.907334

3	6	0	0.964129	-0.870879	-1.662570
4	1	0	1.925881	-1.218460	-2.013730
5	6	0	0.129468	0.036090	-2.314175
6	1	0	0.351004	0.596403	-3.209590
7	16	0	2.114746	1.719026	-1.004757
8	7	0	-0.067897	1.265671	0.224783
9	6	0	0.783159	0.312660	0.787467
10	8	0	0.471913	-0.363121	1.757004
11	6	0	3.183831	-0.530977	0.280522
12	6	0	4.401430	-0.266740	-0.364831
13	6	0	3.129905	-1.578342	1.211986
14	6	0	5.536437	-1.011002	-0.073493
15	1	0	4.475914	0.525876	-1.102896
16	6	0	4.271467	-2.321285	1.495447
17	1	0	2.196432	-1.806411	1.705546
18	6	0	5.477126	-2.043065	0.860092
19	1	0	6.467779	-0.784778	-0.579756
20	1	0	4.211864	-3.126017	2.219527
21	1	0	6.363245	-2.624063	1.088561
22	16	0	-0.604793	3.190270	-1.430618
23	6	0	-1.374176	1.696341	0.753613
24	6	0	-1.967265	2.637453	-0.316708
25	1	0	-2.008996	0.809797	0.844463
26	1	0	-2.706783	2.132724	-0.930931
27	1	0	-2.405118	3.530306	0.126336
28	7	0	-1.214094	-1.335297	-1.020791
29	6	0	0.097795	-1.816336	-0.895113
30	6	0	-1.261075	-0.279229	-1.957117
31	8	0	0.423436	-2.800116	-0.281564
32	8	0	-2.281950	0.250039	-2.335780
33	6	0	-2.343935	-1.902377	-0.369398
34	6	0	-3.484018	-2.224077	-1.103350
35	6	0	-2.290518	-2.134461	1.004253
36	6	0	-4.582272	-2.773745	-0.450181
37	1	0	-3.506526	-2.044721	-2.170692
38	6	0	-3.389695	-2.698532	1.643041
39	1	0	-1.394158	-1.869416	1.553567
40	6	0	-4.537489	-3.014818	0.920380
41	1	0	-5.471422	-3.022424	-1.018172
42	1	0	-3.349026	-2.886625	2.709760
43	1	0	-5.393109	-3.451521	1.422495
44	6	0	-1.200588	2.337872	2.141221
45	1	0	-0.690840	1.589458	2.753726
46	6	0	-0.341291	3.600309	2.102351
47	1	0	0.635759	3.417440	1.645110
48	1	0	-0.833188	4.407765	1.551537
49	1	0	-0.166660	3.958352	3.119698
50	6	0	-2.569832	2.605127	2.764086
51	1	0	-3.174017	1.694569	2.800676
52	1	0	-2.449027	2.972284	3.785732
53	1	0	-3.127062	3.363736	2.206321

Structure **TS_{36}** in dichloromethane:

Electronic Energy (Hartrees) : -2059.18755619
Free Energy (Hartress): -2058.828375
One imaginary frequency (cm^{-1}): 433.6898i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.749725	2.139340	-0.683074
2	6	0	-2.111320	0.284171	0.062851
3	6	0	-1.009116	0.555152	0.997186
4	6	0	-0.121632	0.386963	-2.101565
5	6	0	-0.918486	-0.623454	-1.585888
6	16	0	-2.418362	1.729686	-0.891101
7	16	0	0.006396	3.638453	-1.158894
8	7	0	-0.261634	1.626499	0.480012
9	6	0	0.667831	2.546958	1.199269
10	1	0	0.014940	3.224649	1.763740
11	6	0	1.330940	3.343200	0.078249
12	1	0	1.684008	4.311111	0.427561
13	1	0	2.137074	2.793548	-0.407176

14	8	0	-0.703702	-0.043874	2.015343
15	6	0	-3.199393	-0.669267	0.321968
16	6	0	-4.370654	-0.641869	-0.452179
17	6	0	-3.060214	-1.675375	1.290194
18	6	0	-5.376820	-1.577408	-0.254926
19	1	0	-4.504796	0.112265	-1.221682
20	6	0	-4.072547	-2.610403	1.479718
21	1	0	-2.160960	-1.721189	1.886578
22	6	0	-5.233160	-2.567810	0.714601
23	1	0	-6.273780	-1.534427	-0.862111
24	1	0	-3.946902	-3.379702	2.233281
25	1	0	-6.017610	-3.299931	0.867573
26	6	0	1.649315	1.895675	2.179534
27	1	0	1.046151	1.502255	3.000533
28	6	0	2.426444	0.737861	1.571792
29	1	0	1.742274	-0.060043	1.292644
30	1	0	2.998867	1.033827	0.687316
31	1	0	3.130124	0.334842	2.305122
32	6	0	2.579397	2.974956	2.739073
33	1	0	2.020936	3.840385	3.107552
34	1	0	3.156140	2.567012	3.571510
35	1	0	3.289085	3.320974	1.981607
36	1	0	-1.858492	-0.974788	-1.987245
37	1	0	-0.328475	1.014852	-2.954229
38	6	0	-0.032930	-1.612514	-0.906056
39	6	0	1.273932	0.112700	-1.710341
40	7	0	1.271503	-1.093747	-0.969964
41	6	0	2.429357	-1.811140	-0.559808
42	6	0	2.424224	-2.503003	0.651591
43	6	0	3.554909	-1.842202	-1.383234
44	6	0	3.548000	-3.226891	1.033819
45	1	0	1.547702	-2.472011	1.286173
46	6	0	4.678015	-2.558618	-0.983231
47	1	0	3.550909	-1.313356	-2.326829
48	6	0	4.679438	-3.253255	0.222456
49	1	0	3.538161	-3.767021	1.973446
50	1	0	5.551776	-2.577816	-1.624401
51	1	0	5.554992	-3.815512	0.526107
52	8	0	-0.342048	-2.669481	-0.417920
53	8	0	2.262679	0.765602	-1.951107

Structure **TS1$_{37}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86519536
Free Energy (Hartress): -1982.518716
One imaginary frequency (cm^{-1}): 369.6798i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.570081	0.377481	0.752773
2	6	0	-1.829959	0.896680	0.525966
3	6	0	0.984175	0.801696	-1.142064
4	6	0	-0.189036	1.168210	-1.852433
5	16	0	-0.522806	1.737571	1.205623
6	7	0	-1.586587	-0.393152	0.303172
7	6	0	-0.263432	-0.819704	0.553393
8	8	0	0.057588	-1.983518	0.460913
9	6	0	1.867639	0.339855	1.470941
10	6	0	2.537031	1.544342	1.728798
11	6	0	2.484726	-0.865169	1.821450
12	6	0	3.783469	1.545692	2.340188
13	1	0	2.092805	2.492343	1.435970
14	6	0	3.737238	-0.857133	2.428915
15	1	0	1.994984	-1.805257	1.607725
16	6	0	4.391012	0.341920	2.691030
17	1	0	4.284118	2.487440	2.533562
18	1	0	4.204332	-1.799178	2.693019
19	1	0	5.366917	0.341159	3.162566
20	16	0	-3.429471	1.407308	0.196650
21	6	0	-2.725716	-1.224694	-0.125663
22	6	0	-3.764075	-0.207048	-0.634964
23	1	0	-2.385046	-1.839566	-0.962030
24	1	0	-3.667948	-0.031311	-1.705168

25	1	0	-4.785996	-0.500135	-0.400670
26	6	0	-3.194592	-2.142548	1.014219
27	1	0	-2.309202	-2.710467	1.316057
28	6	0	-3.720235	-1.376158	2.226653
29	1	0	-2.987243	-0.663158	2.616493
30	1	0	-4.639916	-0.832152	1.990422
31	1	0	-3.951244	-2.078742	3.030554
32	6	0	-4.232343	-3.130793	0.483521
33	1	0	-3.850747	-3.684084	-0.378438
34	1	0	-4.489819	-3.851927	1.261960
35	1	0	-5.154862	-2.624373	0.185597
36	1	0	1.602757	1.654976	-0.876808
37	1	0	-0.813486	0.489402	-2.410268
38	7	0	-0.575821	2.478750	-1.946334
39	8	0	-1.611816	2.749092	-2.592494
40	8	0	0.092406	3.385559	-1.405754
41	6	0	1.781956	-0.371449	-1.594627
42	6	0	1.202584	-1.469554	-2.240457
43	6	0	3.163638	-0.373212	-1.375250
44	6	0	1.986493	-2.537762	-2.659121
45	1	0	0.133325	-1.496259	-2.419580
46	6	0	3.948954	-1.442244	-1.793975
47	1	0	3.624600	0.474280	-0.877837
48	6	0	3.361554	-2.528547	-2.435714
49	1	0	1.522359	-3.380581	-3.158620
50	1	0	5.018693	-1.424570	-1.619179
51	1	0	3.971507	-3.363301	-2.762361

Structure **TS2$_{37}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86959173
Free Energy (Hartress): -1982.52012
One imaginary frequency (cm^{-1}): 52.6560i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.590284	-0.322111	-0.617248
2	6	0	1.819172	0.111764	-0.977338
3	6	0	-0.982828	1.209499	-0.139578
4	6	0	0.206786	2.063999	0.061388
5	16	0	0.527417	-0.088187	-2.074213
6	7	0	1.623397	-0.461154	0.219313
7	6	0	0.310702	-0.869907	0.478220
8	8	0	-0.003649	-1.429371	1.494412
9	6	0	-1.814914	-1.113306	-1.007026
10	6	0	-2.515158	-0.712266	-2.150744
11	6	0	-2.300918	-2.179793	-0.251148
12	6	0	-3.673988	-1.371829	-2.538294
13	1	0	-2.165792	0.130897	-2.741234
14	6	0	-3.468325	-2.833824	-0.640003
15	1	0	-1.787509	-2.495298	0.645886
16	6	0	-4.156698	-2.436022	-1.779705
17	1	0	-4.201588	-1.050847	-3.428738
18	1	0	-3.837424	-3.658451	-0.041273
19	1	0	-5.063770	-2.949578	-2.076428
20	16	0	3.376559	0.736565	-1.232077
21	6	0	2.782900	-0.536710	1.126540
22	6	0	3.782038	0.487088	0.552571
23	1	0	2.450296	-0.201347	2.111654
24	1	0	3.687165	1.462040	1.027591
25	1	0	4.812866	0.143289	0.618259
26	6	0	3.295141	-1.982136	1.225568
27	1	0	2.434426	-2.577514	1.546432
28	6	0	3.793917	-2.531959	-0.109586
29	1	0	3.029739	-2.479346	-0.890852
30	1	0	4.684202	-1.999063	-0.456322
31	1	0	4.067303	-3.582821	0.008208
32	6	0	4.369873	-2.079644	2.307054
33	1	0	4.010290	-1.693423	3.264158
34	1	0	4.656602	-3.123487	2.450178
35	1	0	5.270862	-1.525463	2.028729
36	1	0	-1.537288	1.590644	-0.997354
37	1	0	0.761382	2.112098	0.985047

38	7	0	0.602463	2.946144	-0.870150
39	8	0	1.610249	3.675832	-0.639288
40	8	0	0.001804	3.036996	-1.977088
41	6	0	-1.921101	1.124807	1.051045
42	6	0	-1.457118	1.107944	2.368450
43	6	0	-3.298887	1.057605	0.825534
44	6	0	-2.348579	1.020184	3.433206
45	1	0	-0.394416	1.165065	2.575818
46	6	0	-4.192339	0.970875	1.888487
47	1	0	-3.673021	1.078542	-0.192801
48	6	0	-3.718627	0.948849	3.196984
49	1	0	-1.970685	1.009984	4.449191
50	1	0	-5.257595	0.925591	1.692492
51	1	0	-4.412491	0.883211	4.027300

Structure **TS1$_{38}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.85889688
Free Energy (Hartress): -1982.511161
One imaginary frequency (cm^{-1}): 388.9346i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.492609	-0.526202	1.348091
2	6	0	0.519987	0.543291	0.429624
3	6	0	-0.740378	1.185710	-0.017796
4	6	0	-0.151029	-1.920821	-0.825362
5	6	0	0.781804	-0.871588	-1.000962
6	16	0	0.141547	-0.491642	1.844485
7	16	0	-2.801805	-1.489747	1.900014
8	7	0	-1.832647	0.445269	0.503768
9	6	0	-3.296557	0.754190	0.552122
10	1	0	-3.423368	1.270786	1.512092
11	6	0	-3.909336	-0.634447	0.688746
12	1	0	-4.910492	-0.607379	1.112977
13	1	0	-3.882200	-1.207392	-0.239491
14	8	0	-0.886604	2.138602	-0.743301
15	6	0	1.759661	1.352490	0.498769
16	6	0	2.746317	1.087267	1.457487
17	6	0	2.026470	2.316651	-0.483408
18	6	0	3.959499	1.763462	1.438159
19	1	0	2.585880	0.339572	2.228320
20	6	0	3.239157	2.998055	-0.491646
21	1	0	1.292352	2.524275	-1.248939
22	6	0	4.212511	2.725086	0.462928
23	1	0	4.707902	1.537425	2.189165
24	1	0	3.422105	3.741427	-1.259498
25	1	0	5.158628	3.253536	0.448642
26	6	0	-3.889051	1.675684	-0.519661
27	1	0	-3.372807	2.632089	-0.404862
28	6	0	-3.744683	1.220446	-1.965802
29	1	0	-2.701429	1.176311	-2.270426
30	1	0	-4.186889	0.234202	-2.126008
31	1	0	-4.268667	1.934460	-2.607549
32	6	0	-5.366759	1.889102	-0.168927
33	1	0	-5.506219	2.161689	0.880979
34	1	0	-5.774683	2.693611	-0.783869
35	1	0	-5.952475	0.987659	-0.372077
36	1	0	0.041519	-2.829124	-0.278541
37	1	0	0.583097	-0.202061	-1.834811
38	7	0	-1.392342	-1.870919	-1.395974
39	8	0	-1.730150	-0.879109	-2.070966
40	8	0	-2.183757	-2.823269	-1.216208
41	6	0	2.220768	-1.194296	-0.808210
42	6	0	2.659358	-2.107804	0.157083
43	6	0	3.174117	-0.524459	-1.581998
44	6	0	4.019150	-2.329280	0.352109
45	1	0	1.946466	-2.650519	0.767572
46	6	0	4.532453	-0.744446	-1.385800
47	1	0	2.842187	0.178203	-2.338603
48	6	0	4.959584	-1.643633	-0.411921
49	1	0	4.344528	-3.038144	1.105187
50	1	0	5.256689	-0.211099	-1.991206

51	1	0	6.018404	-1.814291	-0.253530

Structure **TS2$_{38}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86929001
Free Energy (Hartress): -1982.518729
One imaginary frequency (cm^{-1}): 207.0378i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.397208	-0.616271	1.313269
2	6	0	0.563736	0.470108	0.337688
3	6	0	-0.768145	1.164322	0.006327
4	6	0	-0.230360	-1.763942	-0.696821
5	6	0	0.779412	-0.682211	-0.798322
6	16	0	0.218828	-0.435796	1.907162
7	16	0	-2.646363	-1.637450	1.887024
8	7	0	-1.815599	0.396078	0.539971
9	6	0	-3.300135	0.565453	0.487165
10	1	0	-3.554327	1.138532	1.387827
11	6	0	-3.802108	-0.865281	0.668632
12	1	0	-4.805778	-0.896095	1.086758
13	1	0	-3.732890	-1.457044	-0.243129
14	8	0	-0.916198	2.160843	-0.638348
15	6	0	1.748366	1.400834	0.420471
16	6	0	2.686594	1.288407	1.447991
17	6	0	1.990950	2.302891	-0.620311
18	6	0	3.837105	2.070296	1.447224
19	1	0	2.545589	0.581482	2.259377
20	6	0	3.137818	3.090175	-0.613567
21	1	0	1.293456	2.385773	-1.442708
22	6	0	4.064678	2.977094	0.417706
23	1	0	4.554265	1.965689	2.252914
24	1	0	3.308389	3.788246	-1.425091
25	1	0	4.960383	3.587581	0.416976
26	6	0	-3.831181	1.303036	-0.757770
27	1	0	-3.129609	1.113016	-1.571073
28	6	0	-5.207005	0.772027	-1.170869
29	1	0	-5.174225	-0.272125	-1.487816
30	1	0	-5.932163	0.868830	-0.356527
31	1	0	-5.576634	1.360599	-2.013566
32	6	0	-3.932763	2.804296	-0.480980
33	1	0	-2.994751	3.219264	-0.112093
34	1	0	-4.201369	3.337754	-1.396032
35	1	0	-4.714071	2.996758	0.261818
36	1	0	-0.017793	-2.728519	-0.264154
37	1	0	0.644685	-0.141667	-1.739694
38	7	0	-1.373350	-1.708157	-1.403352
39	8	0	-1.685407	-0.645796	-2.006918
40	8	0	-2.161009	-2.694207	-1.401955
41	6	0	2.202213	-1.200738	-0.724853
42	6	0	2.601178	-2.153114	0.216066
43	6	0	3.161249	-0.675994	-1.595174
44	6	0	3.933443	-2.550626	0.299683
45	1	0	1.878690	-2.594156	0.893190
46	6	0	4.491946	-1.071584	-1.512602
47	1	0	2.861220	0.056232	-2.337528
48	6	0	4.883949	-2.006595	-0.558579
49	1	0	4.226623	-3.289563	1.037018
50	1	0	5.221189	-0.650696	-2.195725
51	1	0	5.920854	-2.315621	-0.490536

Structure **TS1$_{39}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86342035
Free Energy (Hartress): -1982.516301
One imaginary frequency (cm^{-1}): 390.6695i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.530288	1.553368	-0.655283
2	6	0	0.792728	0.657178	-0.476038
3	6	0	-0.151258	-0.252976	-1.145149
4	6	0	-0.113275	0.401067	2.217454
5	6	0	0.913417	-0.091307	1.376058
6	16	0	-0.035752	2.250895	-0.275851
7	16	0	-3.103899	2.236855	-0.656196
8	7	0	-1.461925	0.297951	-1.068970
9	6	0	-2.716722	-0.352282	-1.496657
10	1	0	-2.525326	-0.790788	-2.478257
11	6	0	-3.726663	0.804066	-1.643713
12	1	0	-3.803711	1.142397	-2.674764
13	1	0	-4.715143	0.545401	-1.268593
14	8	0	0.034901	-1.343757	-1.628577
15	6	0	2.206289	0.764370	-0.929557
16	6	0	3.048985	1.679991	-0.283504
17	6	0	2.735054	-0.054338	-1.932071
18	6	0	4.385888	1.786141	-0.644409
19	1	0	2.656944	2.301031	0.518892
20	6	0	4.078964	0.050267	-2.281004
21	1	0	2.105933	-0.778332	-2.431942
22	6	0	4.907878	0.967123	-1.643322
23	1	0	5.021767	2.502411	-0.136896
24	1	0	4.476395	-0.593528	-3.057498
25	1	0	5.953463	1.042318	-1.919009
26	6	0	-3.119210	-1.464156	-0.519998
27	1	0	-2.231069	-2.096594	-0.419623
28	6	0	-3.511525	-0.929495	0.855884
29	1	0	-2.768265	-0.237751	1.261291
30	1	0	-4.472863	-0.407654	0.818411
31	1	0	-3.617467	-1.756809	1.561789
32	6	0	-4.233833	-2.312355	-1.129544
33	1	0	-3.933661	-2.726248	-2.095590
34	1	0	-4.473942	-3.144400	-0.464006
35	1	0	-5.149593	-1.730719	-1.273280
36	1	0	-1.002355	-0.129504	2.511840
37	1	0	1.862830	0.412232	1.526997
38	7	0	0.026169	1.639172	2.777096
39	8	0	1.033390	2.339003	2.514500
40	8	0	-0.860086	2.066141	3.549128
41	6	0	1.064696	-1.553992	1.173797
42	6	0	-0.014451	-2.437127	1.279569
43	6	0	2.328625	-2.066713	0.863934
44	6	0	0.165556	-3.800504	1.081151
45	1	0	-1.003041	-2.061841	1.522079
46	6	0	2.508555	-3.431056	0.660584
47	1	0	3.174645	-1.390513	0.792270
48	6	0	1.427329	-4.301042	0.767420
49	1	0	-0.679368	-4.474192	1.170178
50	1	0	3.494985	-3.814415	0.425496
51	1	0	1.567477	-5.364818	0.612063

Structure **TS2$_{39}$** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86391509
Free Energy (Hartress): -1982.514533
One imaginary frequency (cm^{-1}): 127.4522i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.760445	-1.323500	-0.335260
2	6	0	-0.609447	-0.690330	-0.478686
3	6	0	0.348738	0.303445	-1.150929
4	6	0	0.566057	-0.135948	1.763478
5	6	0	-0.752410	-0.292520	1.110700
6	16	0	0.343719	-2.270234	-0.421371
7	16	0	3.334935	-1.833159	0.042832
8	7	0	1.664777	-0.099736	-0.896396
9	6	0	2.973010	0.482369	-1.309267
10	1	0	3.162544	0.094988	-2.316296
11	6	0	3.972154	-0.149344	-0.333744
12	1	0	4.960465	-0.252372	-0.776370

13	1	0	4.033080	0.384282	0.614779
14	8	0	0.067157	1.319894	-1.726421
15	6	0	-1.971080	-0.877280	-1.107589
16	6	0	-2.648413	-2.083540	-0.904196
17	6	0	-2.630185	0.162599	-1.768617
18	6	0	-3.945126	-2.259973	-1.371868
19	1	0	-2.179838	-2.900149	-0.362400
20	6	0	-3.928647	-0.018668	-2.236891
21	1	0	-2.143834	1.117863	-1.903727
22	6	0	-4.590467	-1.225912	-2.043694
23	1	0	-4.448913	-3.205094	-1.205786
24	1	0	-4.425325	0.798356	-2.747795
25	1	0	-5.602441	-1.359513	-2.408219
26	6	0	3.035900	2.013035	-1.349667
27	1	0	2.319443	2.331891	-2.109303
28	6	0	2.669989	2.677872	-0.027629
29	1	0	2.655900	3.762396	-0.157407
30	1	0	1.681496	2.373329	0.314588
31	1	0	3.390622	2.449335	0.761912
32	6	0	4.435704	2.431771	-1.805645
33	1	0	4.452039	3.505567	-2.001722
34	1	0	5.183056	2.224356	-1.034185
35	1	0	4.731962	1.915560	-2.722767
36	1	0	1.143063	0.774500	1.718805
37	1	0	-1.237396	-1.174097	1.531214
38	7	0	1.078922	-1.077808	2.574447
39	8	0	0.478777	-2.169816	2.770414
40	8	0	2.202076	-0.870137	3.117853
41	6	0	-1.705235	0.877844	1.253289
42	6	0	-3.037933	0.615437	1.581804
43	6	0	-1.316717	2.200587	1.037758
44	6	0	-3.963430	1.648408	1.686531
45	1	0	-3.351152	-0.409957	1.751955
46	6	0	-2.241634	3.236298	1.136977
47	1	0	-0.289391	2.435390	0.789270
48	6	0	-3.568095	2.963617	1.458697
49	1	0	-4.992579	1.424510	1.944405
50	1	0	-1.922708	4.258020	0.963949
51	1	0	-4.287585	3.770811	1.537294

Structure **TS_{40}** in dichloromethane:

Electronic Energy (Hartrees) : -1982.86155378
Free Energy (Hartress): -1982.512349
One imaginary frequency (cm^{-1}): 458.3967i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.499119	0.488553	-0.145530
2	6	0	-0.682149	0.262895	-1.164417
3	6	0	0.772438	-1.651115	0.290140
4	6	0	-0.402035	-1.799769	-0.451720
5	16	0	0.931575	0.454233	-1.794181
6	7	0	-0.765330	0.885223	0.054018
7	6	0	0.432308	0.995569	0.740189
8	8	0	0.510756	1.387457	1.895540
9	6	0	2.930437	0.551696	0.154754
10	6	0	3.882055	0.372991	-0.861811
11	6	0	3.378111	0.708594	1.476624
12	6	0	5.239268	0.371579	-0.569869
13	1	0	3.568409	0.235914	-1.891679
14	6	0	4.738009	0.703329	1.759608
15	1	0	2.658512	0.829789	2.273921
16	6	0	5.673685	0.537756	0.742247
17	1	0	5.958089	0.237164	-1.369745
18	1	0	5.067251	0.825589	2.785209
19	1	0	6.733515	0.534505	0.969798
20	16	0	-2.167312	0.424103	-2.084558
21	6	0	-2.059556	1.458720	0.456984
22	6	0	-3.079008	0.911242	-0.559154
23	1	0	-2.306687	1.080395	1.451347
24	1	0	-3.596184	0.032693	-0.177764
25	1	0	-3.810433	1.665624	-0.846037

26	6	0	-1.969325	2.994157	0.519851
27	1	0	-1.137197	3.214912	1.194977
28	6	0	-1.674054	3.632341	-0.835839
29	1	0	-0.763709	3.227486	-1.287608
30	1	0	-2.500314	3.486137	-1.537842
31	1	0	-1.530786	4.708644	-0.713106
32	6	0	-3.243134	3.561548	1.144854
33	1	0	-3.430526	3.124521	2.129356
34	1	0	-3.149056	4.642865	1.268008
35	1	0	-4.119533	3.375944	0.516707
36	1	0	-0.300627	-2.251680	-1.432121
37	1	0	0.808736	-1.604424	1.369572
38	7	0	2.000502	-2.193080	-0.232797
39	8	0	2.113637	-2.363983	-1.437287
40	8	0	2.891426	-2.429853	0.568964
41	6	0	-1.697506	-2.003573	0.219364
42	6	0	-1.935033	-1.590607	1.537404
43	6	0	-2.744426	-2.598134	-0.497452
44	6	0	-3.186858	-1.761342	2.116290
45	1	0	-1.147812	-1.117777	2.116481
46	6	0	-3.996324	-2.769604	0.084347
47	1	0	-2.568413	-2.927736	-1.515803
48	6	0	-4.223870	-2.346846	1.391597
49	1	0	-3.353886	-1.433879	3.136372
50	1	0	-4.794124	-3.234895	-0.483573
51	1	0	-5.199074	-2.479021	1.846306

Structure **TS_{41}** in dichloromethane:

Electronic Energy (Hartrees) : -1982.85745898
Free Energy (Hartress): -1982.511592
One imaginary frequency (cm^{-1}): 478.2896i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.302829	0.442511	-0.521628
2	6	0	-1.091515	0.116332	-0.632253
3	6	0	0.621055	-0.853926	1.307909
4	6	0	-0.709953	-1.177976	1.050735
5	16	0	0.250125	-0.432706	-1.602404
6	7	0	-0.769096	1.327175	-0.079728
7	6	0	0.584850	1.591117	0.048366
8	8	0	1.032303	2.571949	0.623978
9	6	0	2.756787	0.300576	-0.600113
10	6	0	3.329718	-0.768176	-1.310640
11	6	0	3.603450	1.186907	0.084335
12	6	0	4.705268	-0.936454	-1.348493
13	1	0	2.700498	-1.480167	-1.835592
14	6	0	4.982130	1.006528	0.043849
15	1	0	3.176679	2.007031	0.643458
16	6	0	5.539228	-0.048013	-0.670817
17	1	0	5.128860	-1.764723	-1.904707
18	1	0	5.622497	1.698637	0.578652
19	1	0	6.614416	-0.182133	-0.698652
20	16	0	-2.796411	0.041708	-1.062386
21	6	0	-1.870778	2.180702	0.384221
22	6	0	-3.130193	1.305824	0.236379
23	1	0	-1.701128	2.391442	1.443375
24	1	0	-3.358056	0.780544	1.162986
25	1	0	-4.002091	1.879836	-0.073721
26	6	0	-1.895525	3.509115	-0.391046
27	1	0	-0.897495	3.939130	-0.266498
28	6	0	-2.163258	3.329132	-1.883524
29	1	0	-1.457352	2.630612	-2.342040
30	1	0	-3.177677	2.962720	-2.067710
31	1	0	-2.060396	4.290058	-2.393706
32	6	0	-2.902819	4.464346	0.247136
33	1	0	-2.697707	4.607014	1.311411
34	1	0	-2.851262	5.440907	-0.239583
35	1	0	-3.928305	4.097417	0.142109
36	1	0	1.461703	-1.509530	1.134497
37	1	0	-1.445548	-0.662926	1.659630
38	7	0	0.918498	0.109530	2.339873

39	6	0	-1.111668	-2.518417	0.582722
40	6	0	-0.234136	-3.398631	-0.064737
41	6	0	-2.435972	-2.924496	0.787724
42	6	0	-0.672490	-4.646794	-0.490160
43	1	0	0.798586	-3.115409	-0.237889
44	6	0	-2.873444	-4.174159	0.361400
45	1	0	-3.121640	-2.255093	1.296854
46	6	0	-1.993670	-5.039036	-0.281903
47	1	0	0.020821	-5.317343	-0.985249
48	1	0	-3.901859	-4.471077	0.533812
49	1	0	-2.331532	-6.013381	-0.615810
50	8	0	0.017163	0.797958	2.795759
51	8	0	2.083457	0.200518	2.696915

Structure **TS_{42}** in dichloromethane:

Electronic Energy (Hartrees) : -1982.85094858
Free Energy (Hartress): -1982.502566
One imaginary frequency (cm^{-1}): 432.8683i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.540772	0.039189	1.363291
2	6	0	1.642738	0.477472	0.418277
3	6	0	0.618640	1.376543	-0.150387
4	6	0	-0.440690	-1.714268	0.049483
5	6	0	0.627995	-1.336056	-0.764818
6	16	0	1.093696	-0.135010	1.944312
7	16	0	-1.962992	0.002852	2.400165
8	7	0	-0.603125	1.069606	0.445251
9	6	0	-1.752914	1.993654	0.641961
10	1	0	-1.440495	2.680555	1.439600
11	6	0	-2.841457	1.088606	1.209378
12	1	0	-3.593747	1.649720	1.760439
13	1	0	-3.313087	0.468575	0.443604
14	8	0	0.762673	2.228280	-1.011179
15	6	0	3.067374	0.523725	0.096852
16	6	0	3.996275	-0.165048	0.894489
17	6	0	3.530485	1.189015	-1.051118
18	6	0	5.345142	-0.170762	0.569074
19	1	0	3.669132	-0.706901	1.775657
20	6	0	4.882456	1.177084	-1.368941
21	1	0	2.829634	1.712538	-1.685155
22	6	0	5.795385	0.502523	-0.563175
23	1	0	6.044444	-0.705683	1.201036
24	1	0	5.222736	1.698151	-2.256629
25	1	0	6.849289	0.498042	-0.817007
26	6	0	-2.156651	2.841281	-0.570433
27	1	0	-1.329628	3.532323	-0.743470
28	6	0	-2.382005	2.044708	-1.847904
29	1	0	-1.486869	1.485069	-2.125829
30	1	0	-3.216256	1.346883	-1.745826
31	1	0	-2.617196	2.731052	-2.665742
32	6	0	-3.396577	3.660882	-0.203687
33	1	0	-3.265114	4.189524	0.744891
34	1	0	-3.591834	4.404959	-0.978855
35	1	0	-4.283352	3.025026	-0.122519
36	1	0	0.529663	-0.880049	-1.739825
37	1	0	-0.202342	-2.425050	0.832950
38	7	0	1.880255	-2.023357	-0.641889
39	8	0	2.131276	-2.637768	0.386751
40	8	0	2.663140	-1.935470	-1.578085
41	6	0	-1.828315	-1.793583	-0.444514
42	6	0	-2.232510	-1.282913	-1.683000
43	6	0	-2.782425	-2.433482	0.359911
44	6	0	-3.557160	-1.386386	-2.091719
45	1	0	-1.513610	-0.810454	-2.341211
46	6	0	-4.107788	-2.530449	-0.046451
47	1	0	-2.472710	-2.863139	1.306084
48	6	0	-4.502141	-1.999527	-1.272586
49	1	0	-3.852296	-0.987960	-3.056146
50	1	0	-4.830710	-3.027788	0.590338
51	1	0	-5.534045	-2.078196	-1.595351

Structure **TS_{43}** in dichloromethane:

Electronic Energy (Hartrees) : -1982.84983319
Free Energy (Hartress): -1982.502631
One imaginary frequency (cm^{-1}): 452.3331i
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.954082	0.048967	-1.036500
2	6	0	-1.429286	0.189130	-0.681644
3	6	0	-0.784846	1.504386	-0.513783
4	6	0	0.878098	-0.844717	0.976987
5	6	0	-0.475685	-0.663534	1.251016
6	16	0	-0.411563	-0.824709	-1.667217
7	16	0	2.551467	-0.004740	-1.765143
8	7	0	0.583295	1.322239	-0.687042
9	6	0	1.622319	2.370294	-0.834556
10	1	0	1.394934	2.863505	-1.786849
11	6	0	2.939921	1.597583	-0.965462
12	1	0	3.660043	2.125699	-1.587548
13	1	0	3.383396	1.382023	0.004704
14	8	0	-1.304436	2.567480	-0.215089
15	6	0	-2.865489	-0.073613	-0.569109
16	6	0	-3.380745	-1.331995	-0.924349
17	6	0	-3.742232	0.887486	-0.041642
18	6	0	-4.729348	-1.615279	-0.775347
19	1	0	-2.724051	-2.102300	-1.316146
20	6	0	-5.093787	0.592560	0.107722
21	1	0	-3.363865	1.857448	0.246230
22	6	0	-5.594441	-0.651413	-0.258257
23	1	0	-5.105730	-2.590704	-1.061101
24	1	0	-5.758223	1.345718	0.515649
25	1	0	-6.648926	-0.872920	-0.140608
26	6	0	1.644976	3.440127	0.277089
27	1	0	0.602877	3.650716	0.518873
28	6	0	2.363918	3.007336	1.555750
29	1	0	2.064689	2.010185	1.879450
30	1	0	3.450467	3.028660	1.428590
31	1	0	2.114730	3.701065	2.362232
32	6	0	2.282468	4.712530	-0.284546
33	1	0	1.716529	5.102826	-1.134083
34	1	0	2.317377	5.486655	0.485491
35	1	0	3.309899	4.524611	-0.613665
36	1	0	1.552056	-0.096671	1.380100
37	1	0	-1.210122	-1.455757	1.252775
38	7	0	-0.903990	0.422798	2.098107
39	6	0	1.475655	-2.173803	0.757027
40	6	0	0.728540	-3.307767	0.408080
41	6	0	2.865100	-2.302971	0.882551
42	6	0	1.356865	-4.529039	0.195803
43	1	0	-0.348848	-3.246298	0.299779
44	6	0	3.492014	-3.525957	0.670358
45	1	0	3.454808	-1.433962	1.157177
46	6	0	2.739803	-4.644611	0.324538
47	1	0	0.762888	-5.396565	-0.069276
48	1	0	4.568264	-3.604107	0.776526
49	1	0	3.224961	-5.599837	0.159655
50	8	0	-2.048911	0.374437	2.523483
51	8	0	-0.134049	1.340798	2.335605

Summaries of reaction paths corresponding to the IRCs of transition structures $TS_{8\text{-}9}$, TS_{16},$TS_{28\text{-}29}$, $TS1_{14}$, $TS2_{14}$ $TS1_{27}$, $TS2_{27}$ and TS_{32} calculated at M06-2X/6-311++G(d,p) level in dichloromethane.

Structure **TS_8**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.02361	-6.70603
2	-0.02338	-6.37119
3	-0.02309	-6.03628
4	-0.02273	-5.70129
5	-0.02227	-5.36617
6	-0.02169	-5.03095
7	-0.02097	-4.69567
8	-0.02009	-4.36035
9	-0.01905	-4.02499
10	-0.01782	-3.68960
11	-0.01640	-3.35421
12	-0.01479	-3.01883
13	-0.01298	-2.68347
14	-0.01100	-2.34811
15	-0.00889	-2.01271
16	-0.00676	-1.67729
17	-0.00470	-1.34184
18	-0.00287	-1.00637
19	-0.00138	-0.67092
20	-0.00037	-0.33550
21	0.00000	0.00000
22	-0.00044	0.33553
23	-0.00187	0.67096
24	-0.00448	1.00643
25	-0.00830	1.34190
26	-0.01324	1.67737
27	-0.01918	2.01284
28	-0.02567	2.34832
29	-0.03249	2.68379
30	-0.03931	3.01924
31	-0.04582	3.35467
32	-0.05165	3.69003
33	-0.05647	4.02518
34	-0.05998	4.35948
35	-0.06218	4.69138
36	-0.06345	5.02177
37	-0.06438	5.35461
38	-0.06509	5.68907
39	-0.06567	6.02383
40	-0.06613	6.35849
41	-0.06650	6.69306

Structure **TS_9**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.06641	-6.72689
2	-0.06587	-6.39024
3	-0.06524	-6.05369
4	-0.06451	-5.71733
5	-0.06363	-5.38154
6	-0.06252	-5.04732
7	-0.06094	-4.71447
8	-0.05847	-4.37985
9	-0.05481	-4.04374
10	-0.05003	-3.70708
11	-0.04442	-3.37021
12	-0.03813	-3.03326
13	-0.03154	-2.69627
14	-0.02495	-2.35925
15	-0.01865	-2.02222

16	-0.01292	-1.68518
17	-0.00805	-1.34815
18	-0.00431	-1.01111
19	-0.00179	-0.67408
20	-0.00041	-0.33709
21	0.00000	0.00000
22	-0.00035	0.33705
23	-0.00129	0.67403
24	-0.00266	1.01105
25	-0.00435	1.34809
26	-0.00624	1.68512
27	-0.00824	2.02212
28	-0.01022	2.35908
29	-0.01208	2.69599
30	-0.01375	3.03285
31	-0.01521	3.36973
32	-0.01649	3.70665
33	-0.01759	4.04358
34	-0.01853	4.38049
35	-0.01931	4.71734
36	-0.01995	5.05411
37	-0.02047	5.39077
38	-0.02088	5.72742
39	-0.02121	6.06401
40	-0.02151	6.40047
41	-0.02170	6.73667

Structure **$TS1_{14}$**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.00659	-6.73888
2	-0.00653	-6.40084
3	-0.00645	-6.06272
4	-0.00637	-5.72456
5	-0.00628	-5.38635
6	-0.00619	-5.04822
7	-0.00610	-4.71022
8	-0.00602	-4.37213
9	-0.00594	-4.03400
10	-0.00585	-3.69599
11	-0.00576	-3.35826
12	-0.00565	-3.02100
13	-0.00552	-2.68431
14	-0.00535	-2.34891
15	-0.00509	-2.01642
16	-0.00464	-1.68712
17	-0.00377	-1.35228
18	-0.00253	-1.01454
19	-0.00126	-0.67643
20	-0.00034	-0.33828
21	0.00000	0.00000
22	-0.00035	0.33830
23	-0.00130	0.67646
24	-0.00265	1.01465
25	-0.00423	1.35284
26	-0.00587	1.69104
27	-0.00758	2.02924
28	-0.00928	2.36743
29	-0.01089	2.70558
30	-0.01237	3.04366
31	-0.01367	3.38167
32	-0.01481	3.71967
33	-0.01580	4.05767
34	-0.01670	4.39569
35	-0.01744	4.73376
36	-0.01806	5.07186
37	-0.01858	5.40997
38	-0.01902	5.74813
39	-0.01938	6.08629
40	-0.01968	6.42443
41	-0.01992	6.76245

Structure **TS2$_{14}$**:

```
--------------------------------------------------------------------------------
    Summary of reaction path following
 --------------------------------------------------------------------------------
                        Electronic Energy    RxCoord
   1                   -0.04324  -6.23784
   2                   -0.04243  -5.92587
   3                   -0.04147  -5.61400
   4                   -0.04031  -5.30255
   5                   -0.03888  -4.99230
   6                   -0.03696  -4.68254
   7                   -0.03430  -4.37132
   8                   -0.03091  -4.05936
   9                   -0.02700  -3.74719
  10                   -0.02282  -3.43494
  11                   -0.01859  -3.12266
  12                   -0.01455  -2.81037
  13                   -0.01090  -2.49807
  14                   -0.00781  -2.18577
  15                   -0.00538  -1.87347
  16                   -0.00346  -1.56118
  17                   -0.00205  -1.24890
  18                   -0.00107  -0.93663
  19                   -0.00044  -0.62438
  20                   -0.00010  -0.31219
  21                    0.00000   0.00000
  22                   -0.00008   0.31183
  23                   -0.00026   0.62357
  24                   -0.00046   0.93475
  25                   -0.00065   1.24614
  26                   -0.00082   1.55775
  27                   -0.00096   1.86938
  28                   -0.00108   2.18123
  29                   -0.00119   2.49300
  30                   -0.00128   2.80522
  31                   -0.00137   3.11748
  32                   -0.00145   3.42974
  33                   -0.00151   3.74196
  34                   -0.00156   4.05406
 --------------------------------------------------------------------------------
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Structure **TS$_{16}$**:

```
--------------------------------------------------------------------------------
    Summary of reaction path following
 --------------------------------------------------------------------------------
                        Electronic Energy    RxCoord
   1                   -0.02339  -9.20392
   2                   -0.02334  -8.87517
   3                   -0.02327  -8.54637
   4                   -0.02320  -8.21765
   5                   -0.02312  -7.88917
   6                   -0.02302  -7.56113
   7                   -0.02290  -7.23347
   8                   -0.02275  -6.90561
   9                   -0.02254  -6.57729
  10                   -0.02228  -6.24864
  11                   -0.02194  -5.91985
  12                   -0.02152  -5.59099
  13                   -0.02101  -5.26212
  14                   -0.02040  -4.93325
  15                   -0.01968  -4.60441
  16                   -0.01883  -4.27560
  17                   -0.01783  -3.94682
  18                   -0.01666  -3.61805
  19                   -0.01530  -3.28925
  20                   -0.01376  -2.96041
  21                   -0.01206  -2.63151
  22                   -0.01024  -2.30259
  23                   -0.00833  -1.97367
  24                   -0.00637  -1.64474
  25                   -0.00443  -1.31581
  26                   -0.00263  -0.98687
  27                   -0.00122  -0.65793
```

28	-0.00030	-0.32901
29	0.00000	0.00000
30	-0.00025	0.32892
31	-0.00082	0.65757
32	-0.00134	0.98461
33	-0.00159	1.29758
34	-0.00173	1.62202
35	-0.00187	1.94921
36	-0.00205	2.27639
37	-0.00236	2.60453
38	-0.00288	2.93327
39	-0.00367	3.26217
40	-0.00477	3.59111
41	-0.00619	3.92007
42	-0.00798	4.24904
43	-0.01017	4.57801
44	-0.01278	4.90699
45	-0.01583	5.23596
46	-0.01930	5.56494
47	-0.02317	5.89392
48	-0.02741	6.22290
49	-0.03194	6.55187
50	-0.03662	6.88082
51	-0.04128	7.20975
52	-0.04574	7.53862
53	-0.04982	7.86736
54	-0.05335	8.19584
55	-0.05626	8.52392
56	-0.05859	8.85187
57	-0.06044	9.18009
58	-0.06192	9.50841
59	-0.06308	9.83659

Structure **$TS1_{27}$**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.00422	-6.34214
2	-0.00418	-6.00695
3	-0.00412	-5.67173
4	-0.00406	-5.33649
5	-0.00393	-5.00126
6	-0.00386	-4.66605
7	-0.00379	-4.33091
8	-0.00371	-3.99582
9	-0.00363	-3.66075
10	-0.00354	-3.32569
11	-0.00346	-2.99068
12	-0.00336	-2.65569
13	-0.00326	-2.32119
14	-0.00315	-1.99029
15	-0.00297	-1.66725
16	-0.00257	-1.33887
17	-0.00184	-1.00541
18	-0.00098	-0.67047
19	-0.00028	-0.33532
20	0.00000	0.00000
21	-0.00029	0.33534
22	-0.00110	0.67058
23	-0.00238	1.00581
24	-0.00392	1.34106
25	-0.00565	1.67630
26	-0.00732	2.01153
27	-0.00898	2.34677
28	-0.01058	2.68198
29	-0.01208	3.01716
30	-0.01344	3.35228
31	-0.01465	3.68738
32	-0.01573	4.02249
33	-0.01668	4.35762
34	-0.01753	4.69279
35	-0.01828	5.02799
36	-0.01894	5.36320

37	-0.01952	5.69843
38	-0.02004	6.03364
39	-0.02053	6.36885
40	-0.02092	6.70403

Structure **TS2$_{27}$**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.04532	-6.90492
2	-0.04414	-6.55939
3	-0.04279	-6.21412
4	-0.04121	-5.86977
5	-0.03922	-5.52714
6	-0.03650	-5.18318
7	-0.03293	-4.83797
8	-0.02870	-4.49236
9	-0.02413	-4.14663
10	-0.01952	-3.80085
11	-0.01515	-3.45505
12	-0.01129	-3.10925
13	-0.00806	-2.76344
14	-0.00549	-2.41765
15	-0.00354	-2.07187
16	-0.00211	-1.72610
17	-0.00111	-1.38034
18	-0.00054	-1.03468
19	-0.00018	-0.68928
20	-0.00003	-0.34477
21	0.00000	0.00000
22	-0.00002	0.34210

Structure **TS$_{28}$**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.02745	-6.86681
2	-0.02691	-6.52349
3	-0.02628	-6.18015
4	-0.02557	-5.83680
5	-0.02475	-5.49344
6	-0.02382	-5.15010
7	-0.02278	-4.80676
8	-0.02161	-4.46342
9	-0.02031	-4.12010
10	-0.01885	-3.77679
11	-0.01724	-3.43351
12	-0.01544	-3.09026
13	-0.01345	-2.74701
14	-0.01129	-2.40371
15	-0.00905	-2.06036
16	-0.00683	-1.71698
17	-0.00474	-1.37358
18	-0.00289	-1.03017
19	-0.00140	-0.68678
20	-0.00038	-0.34344
21	0.00000	0.00000
22	-0.00044	0.34347
23	-0.00188	0.68684
24	-0.00441	1.03024
25	-0.00795	1.37362
26	-0.01233	1.71700
27	-0.01738	2.06035
28	-0.02289	2.40366
29	-0.02865	2.74695
30	-0.03443	3.09018
31	-0.04003	3.43339
32	-0.04525	3.77659
33	-0.04984	4.11972
34	-0.05353	4.46251

35	-0.05614	4.80383
36	-0.05787	5.14245
37	-0.05918	5.48369
38	-0.06027	5.82653
39	-0.06120	6.16962
40	-0.06200	6.51273
41	-0.06269	6.85580

Structure **TS_{29}**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.06045	-6.84386
2	-0.05991	-6.50181
3	-0.05925	-6.15952
4	-0.05842	-5.81708
5	-0.05740	-5.47503
6	-0.05611	-5.13560
7	-0.05425	-4.79688
8	-0.05144	-4.45528
9	-0.04767	-4.11278
10	-0.04317	-3.77008
11	-0.03828	-3.42738
12	-0.03309	-3.08473
13	-0.02783	-2.74217
14	-0.02261	-2.39960
15	-0.01756	-2.05696
16	-0.01278	-1.71425
17	-0.00840	-1.37146
18	-0.00478	-1.02864
19	-0.00209	-0.68579
20	-0.00049	-0.34294
21	0.00000	0.00000
22	-0.00042	0.34290
23	-0.00152	0.68571
24	-0.00314	1.02858
25	-0.00512	1.37145
26	-0.00735	1.71433
27	-0.00969	2.05718
28	-0.01201	2.39999
29	-0.01420	2.74274
30	-0.01616	3.08541
31	-0.01788	3.42802
32	-0.01937	3.77065
33	-0.02066	4.11332
34	-0.02186	4.45605
35	-0.02285	4.79881
36	-0.02372	5.14159
37	-0.02448	5.48436
38	-0.02513	5.82715
39	-0.02568	6.16995
40	-0.02613	6.51275
41	-0.02651	6.85555

Structure **TS_{32}**:

Summary of reaction path following

	Electronic Energy	RxCoord
1	-0.06193	-9.97038
2	-0.06063	-9.63802
3	-0.05894	-9.30572
4	-0.05674	-8.97359
5	-0.05394	-8.64130
6	-0.05047	-8.30855
7	-0.04644	-7.97549
8	-0.04202	-7.64230
9	-0.03741	-7.30906
10	-0.03280	-6.97580
11	-0.02840	-6.64251
12	-0.02437	-6.30922

13	-0.02078	-5.97594
14	-0.01766	-5.64265
15	-0.01502	-5.30937
16	-0.01282	-4.97609
17	-0.01102	-4.64281
18	-0.00958	-4.30955
19	-0.00846	-3.97630
20	-0.00764	-3.64312
21	-0.00705	-3.31014
22	-0.00665	-2.97796
23	-0.00637	-2.64658
24	-0.00611	-2.31643
25	-0.00579	-1.98786
26	-0.00525	-1.66253
27	-0.00426	-1.33248
28	-0.00285	-0.99971
29	-0.00143	-0.66654
30	-0.00038	-0.33334
31	0.00000	0.00000
32	-0.00037	0.33332
33	-0.00143	0.66651
34	-0.00292	0.99971
35	-0.00463	1.33294
36	-0.00642	1.66616
37	-0.00819	1.99938
38	-0.00989	2.33257
39	-0.01148	2.66573
40	-0.01291	2.99885
41	-0.01417	3.33193
42	-0.01526	3.66502
43	-0.01621	3.99814
44	-0.01703	4.33132
45	-0.01775	4.66451
46	-0.01835	4.99769
47	-0.01886	5.33084
48	-0.01928	5.66396
49	-0.01962	5.99704
50	-0.01990	6.33005
51	-0.02011	6.66292
52	-0.02027	6.99560
53	-0.02040	7.32794
54	-0.02049	7.65998
55	-0.02057	7.99201
56	-0.02063	8.32450
57	-0.02069	8.65736
58	-0.02074	8.99020