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Thieme

Supporting Information

Remarkable Diastereoselectivity of the Thia-Michael Reaction on α,α′-Di((*E*)-benzylidene)alkanones: Exclusive Formation of a *meso* Product

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Contents

General

Mps were recorded on a Köfler block and are uncorrected. IR spectra were recorded on a Perkin Elmer FT-IR Spectrophotometer (Spectrum BX II) as KBr pellets. ^{1}H and ^{13}C NMR spectra were obtained in $CDCl_3$ on Bruker AV-300 (300 MHz), Bruker DPX-300 (300 MHz) spectrometers using TMS as an internal standard. Mass spectra were acquired on a Waters Xevo G2QTof HRMS spectrometer. Analytical samples were dried *in vacuo* at room temperature. Microanalytical data were recorded on a Perkin-Elmer 2400 Series II C, H, N analyzer. Column chromatography was performed on silica gel (100-200 mesh) using petroleum ether (60-80°C) and petroleum ether-ethyl acetate mixtures as eluents. TLC was done with silica gel G. The microwave assisted reactions were performed on a microwave oven (LG, DMO, Model No. MG-556P, 900 Watt) and mono-mode microwave reactor (manufactured by CEM, Discover, USA). X-ray crystallographic studies were done by using a Bruker APEX II single crystal X-ray diffractometer.

General procedure for synthesis of bis-β-aryl-β-mercaptoalkanones (3/5/8/10)

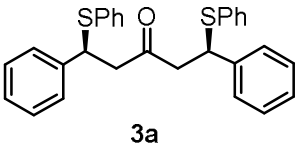
α,α'-Dibenzylidenealkanones (**1/4/9,** 1 mmol) was thoroughly mixed with neutral alumina (4 g) with added anhydrous K_2CO_3 (2 mmol) or amberlyst-15 (80 mg). The mass was cooled at 15 °C and thiophenol (**2**, 2 mmol) was added to it keeping the temperature constant. The resulting mixture was kept at 15 °C for 4 h under closed condition. The solid was then washed thoroughly with dichloromethane and the concentrate of the washings was subjected to column chromatography over silica gel using petroleum ether-ethyl acetate mixtures as eluents to get the bis-β-aryl-β-mercaptoalkanones **(3/5/8/10).**

General procedure for one-pot synthesis of bis-β-aryl-β-mercaptocyclohexanones (5/8) from cyclohexanones:

A mixture of cyclohexanone (**6**, 1 mmol) and aromatic aldehyde (**7**, 2mmol) was thoroughly ground over neutral alumina (4 g) with added anhydrous K_2CO_3 (1 mmol) or amberlyst-15 (80 mg) and the resulting powder was subjected to microwave irradiation at 540 W for 5 min (temp. 120-125°C). After cooling the mass at 15 °C, thiophenol (**2**, 2 mmol) was added to it keeping the temperature constant and thoroughly mixed. The mixture was kept at 15 °C for 4h under closed condition. The solid was then washed thoroughly with dichloromethane and the concentrate of the washings was subjected to column chromatography over silica gel using petroleum ether - ethyl acetate mixtures as eluents to get the bis-β-aryl-β-mercaptocyclohexanone (**5/8**) in pure state as a single diastereomer

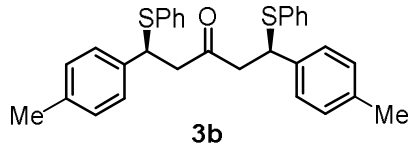
Spectral data of 3a-c

3a: Colourless crystals; Yield: 354 mg† (78%); mp 105-107 °C (lit.[1] 100-102°C); ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.93 (d, *J* = 7.8 Hz, 4H, 2 × CH_2), 4.62 (t, *J* = 6.9 Hz, 2H, 2 × CH), 7.12-7.26 (7.12-7.26, 2 × 10H, m, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 47.8 (2 × C_β), 49.4 (2 × C_α), 127.4, 127.6, 127.7, 128.5, 128.9, 132. 9, 133.9, 140.7, 204.5. Anal. Calcd. for $C_{29}H_{26}OS_2$: C, 76.61; H, 5.76. Found: C, 76.72; H, 5.52.



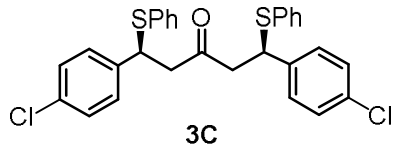
3a

3b: Colourless crystals; Yield: 347 mg† (72%); mp 72-74 °C; IR (KBr): υ_{max} = 1678 (C=O), 1492, 1325, 1226, 1015, 815 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.28 (s, 6H, 2 × Ar-CH_3), 2.89-2.92 (m, 4H, 2 × CH_2), 4.59 (dd, *J* = 8.0 and 6.8 Hz, 2H, 2 × CH), 6.97-7.02 (2 × 4H, m, Ar-H), 7.19-7.24 (2 × 5H, m, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.1, 47.5 (2 × C_β), 49.6(2 × C_α), 127.4, 127.5, 128.8, 129.1, 132.7, 134.2, 137.0, 137.6, 204.8. HRMS: *m/z* Calcd. for $C_{31}H_{30}NaOS_2$ $(M+Na)^+$: 505.1636; Found: 505.1673.



3b

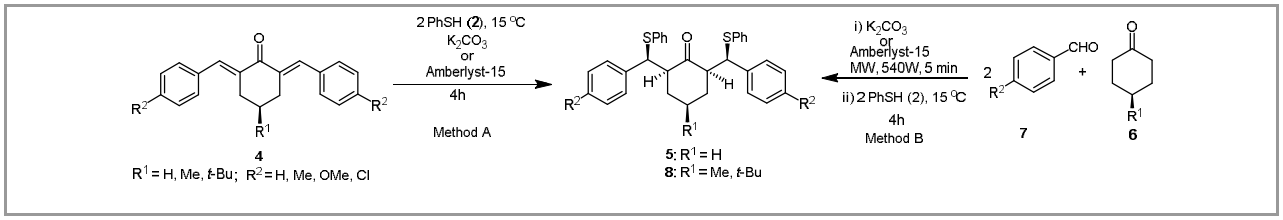
3c: Colourless crystals; Yield: 434 mg† (83%); mp 102-104 °C; IR (KBr): υ_{max} = 1670 (C=O), 1601, 1572, 1423, 1338, 1257, 1173, 1024, 984, 845, 750 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.83-3.02 (m, 4H, 2 × CH_2), 4.56 (dd, *J* = 7.4 and 6.3 Hz, 2H, 2 × CH), 6.98-7.12 (m, 2 × 4H, Ar-H), 7.15-7.30 (m, 2 × 5H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$): δ 47.2 (2 × C_β), 49.3 (2 × C_α), 127.9, 128.5, 128.9, 129.0, 132.9, 133.1, 139.1, 139.3, 204.1. Anal. Calcd. for $C_{29}H_{24}Cl_2OS_2$: C, 66.53; H, 4.62. Found: C, 66.72; H, 4.46.



3C

†Starting from the respective α,α′-di((*E*)-benzylidene)acetone (1 mmol)

Table 3. Yield of the Thia-Michael Reaction Products on α,α′-Di((*E*)-benzylidene)cyclohexanones



Entry	Cyclohexanone (6)	Benzaldehyde (7)	Product (5)	Yield[a] (%) Method A		Yield[b] (%) Method B		Diastereo-meric purity
				With K_2CO_3	With Amb.-15	With K_2CO_3	With Amb.-15	
1	**6a**: R^1 = H	**7a**: R^2 = H	**5a**	80 (396 mg)	65 (322 mg)	78 (386 mg)	68 (337 mg)	Pure
2	**6a**	**7b**: R^2 = Me	**5b**	75 (392 mg)	68 (356 mg)	72 (377 mg)	64 (335 mg)	Pure
3	**6a**	**7c**: R^2 = OMe	**5c**[c]	66 (366 mg)[d]	62 (344 mg)[d]	63 (350 mg)[d]	58 (322 mg)[d]	Mixture
4	**6a**	**7d**: R^2 = Cl	**5d**	85 (479 mg)	72 (406 mg)	83 (468 mg)	70 (395 mg)	Pure
5	**6b**: R^1 = Me	**7a**	**8a**	73 (372 mg)	66 (336 mg)	71 (361 mg)	64 (326 mg)	Pure
6	**6b**	**7b**	**8b**	69 (371 mg)	63 (338 mg)	67 (360 mg)	60 (322 mg)	Pure
7	**6b**	**7d**	**8c**	77 (445 mg)	72 (416 mg)	74 (428 mg)	69 (399 mg)	Pure
8	**6c**: R^1 = Me_3C	**7a**	**8d**[c]	69 (380 mg)[d]	63 (347 mg)[d]	67 (369 mg)[d]	61 (336 mg)[d]	Mixture
9	**6c**	**7d**	**8e**[c]	74 (458 mg)[d]	70 (433 mg)[d]	71 (439 mg)[d]	68 (421 mg)[d]	Mixture

[a]Isolated yield with respect to **4**, taken 1 mmol in each case.

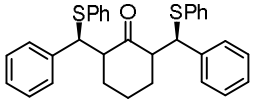
[b] Isolated yield with respect to **6**, taken 1 mmol in each case.

[c]Major product in the mixture.

[d]The given yield is the total yield of the diastereomers.

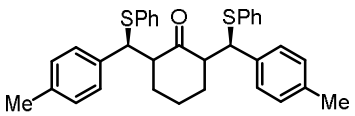
Spectral data of 5a,b,d and 8a-c

5a: Colourless crystals; mp 148-150 °C; IR (KBr): υ_{max} = 1677(C=O), 1597, 1462, 1251, 1167, 1036, 988, 872, 750 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 1.65-1.72 (3H, m, cyclohexanone H_A-3, H_A-4, H_A-5), 2.02-2.05 (1H, m, cyclohexanone H_B-4), 2.66 (br. s, 2H, cyclohexanone H_B-3, H_B-5), 2.87-2.95 (m, 2H, 2 × H_α), 4.64 (d, J = 7.8 Hz, 2H, 2 × H_β), 7.09-7.21 (m, 2 × 10H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 25.4, 32.9, 52.7, 57.3, 126.6, 127.0, 127.9, 128.0, 128.6, 132.4, 134.7, 142.0, 208.3 HRMS: *m/z* Calcd. for $C_{32}H_{30}NaOS_2$ $(M+Na)^+$: 517.1636; Found: 517.1698.



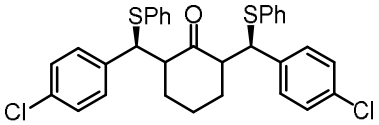
5a

5b: Colourless crystals; mp124-126 °C; IR (KBr): υ_{max} = 16 78 (C=O), 1514, 1344, 1219, 986, 822, 998 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 1.66-1.69 (m, 3H, cyclohexanone H_A-3, H_A-4, H_A-5), 2.00 (br. s, 1H, cyclohexanone H_B-4), 2.28 (s, 6H, 2 × Ar-CH_3),2.61 (br. s,2H, cyclohexanone H_B-3, H_B-5), 2.86 (t, J = 4.5 Hz, 2H, 2 × H_α), 4.62 (d, J = 7.5 Hz, 2H, 2 × H_β), 6.89 (2H, d, J = 8.1 Hz, 2 × Ar-H), 7.00 (d, J = 8.1 Hz, 2 × 2H, Ar-H), 7.12-7.23 (m, 5H, 2 × Ar-H).^{13}C NMR (75 MHz, $CDCl_3$): δ 21.0, 25.4, 32.8, 52.3, 57.5, 126.8, 127.8, 128.6, 128.7 132.1, 135.1, 136.0, 139.0, 208.4. HRMS: *m/z* Calcd. For $C_{34}H_{34}NaOS_2$ $(M+Na)^+$: 545.1933; Found: 545.1949.



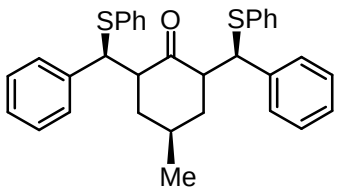
5b

5d: Colourless crystals; mp 162-164 °C; IR (KBr): υ_{max} = 16 75(C=O), 1521, 1328, 1214, 981, 822, 993 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 1.65-1.79 (m, 3H, cyclohexanone H_A-3, H_A-4, H_A-5), 2.03-2.08 (1H, m,cyclohexanoneH_B-4), 2.70-2.74 (m,2H, cyclohexanone H_B-3, H_B-5), 2.83-2.91 (m, 2H, 2 × H_α), 4.45 (d, J = 8.4 Hz, 2H, 2 × H_β), 6.92 (d, J = 8.4 Hz, 2 × 2H, Ar-H), 7.02 (d, J = 8.4 Hz, 2 × 2H, Ar-H), 7.15-7.19 (m, 2 × 5H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$): δ 25.6, 34.2, 52.4, 57.7, 127.7, 128.2, 128.9, 129.3, 132.5, 133.1, 133.9, 140.7, 209.1. HRMS: *m/z* Calcd. For $C_{32}H_{28}NaCl_2OS_2$ $(M+Na)^+$: 585.0856; Found: 585.0545.



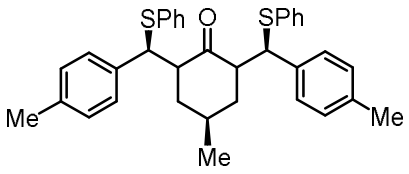
5d

8a: Colourless crystals; mp 142-144 °C; IR (KBr): υ_{max} = 16 73(C=O), 1515, 1333, 1215, 977, 818, 782 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 1.08 (d, J= 6.3 Hz, 3H, -CH_3), 1.45-1.57(m, 2H, cyclohexanone H_A-3, H_A-5), 1.99 (br.s, 1H, cyclohexa-none H-4), 2.49-2.54 (m, 2H, cyclohexanone H_B-3, H_B-5), 2.91-2.96 (m, 2H, 2 × H_α), 4.69 (d, J = 6.9 Hz, 2H, 2 × H_β), 7.07-7.28 (m, 2 × 10H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$): δ 21.3, 32.0, 39.8, 52.6, 56.0, 126.6, 127.0, 128.0, 128.04, 128.6, 132.2, 134.8, 141.9, 208.2 HRMS: *m/z* Calcd. for $C_{33}H_{32}NaOS_2$ $(M+Na)^+$: 531.1692; Found: 531.1564.



8a

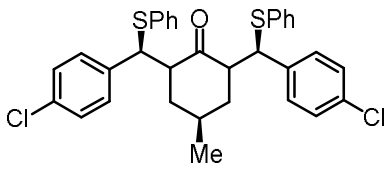
8b: Colourless crystals; mp158-160 °C; IR (KBr): υ_{max} = 16 77(C=O), 1505, 1488, 1447, 1254, 1038 cm^{-1}. ^1H NMR (300 MHz, $CDCl_3$): δ 1.05 (d,3H, J= 6.3 Hz, -CH_3), 1.42-1.54(m, 2H, cyclohexanone H_A-3, H_A-5), 1.95-1.96 (m, 1H, cyclohexanone H-4), 2.27 (s, 6H, 2 × Ar-CH_3), 2.45-2.49 (m, 2H, cyclohexanone H_B-3, H_B-5), 2.86-2.93 (m, 2H, 2 × H_α), 4.68 (d, J = 6.6 Hz, 2H, 2 × H_β), 6.95 (d, J = 7.8 Hz, 2 × 2H, Ar-H), 7.06 (d, J = 7.8 Hz, 2 × 2H, Ar-H), 7.14-7.15 (m, 2 × 3H, Ar-H) 7.20-



8b

7.22 (m, 2 × 2H, Ar-H).^{13}C NMR (75 MHz, $CDCl_3$): δ 21.0, 21.3, 32.0, 39.8, 52.3, 56.3, 126.8, 127.9, 128.6, 128.8, 132.0, 135.2, 136.1, 139.0, 208.2. HRMS: *m/z* Calcd. for $C_{35}H_{36}NaOS_2$ $(M+Na)^+$: 559.2105; Found: 559.1682.

8c: Colourless crystals; mp188-190 °C; IR (KBr): υ_{max} = 1706(C=O), 1493, 1437, 1087, 1014, 822, 749, 690, 532 cm^{-1}. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.08 (3H, d,J= 6.3 Hz, $-CH_3$), 1.41-1.54 (m, 2H, cyclohexanone H_A-3, H_A-5), 1.95-2.00 (m, 1H, cyclohexanone H-4), 2.55-2.60 (m, 2H, cyclohexanone H_B-3, H_B-5), 2.86-2.94 (m, 2H, 2 × H_α), 4.48 (d, *J* = 6.6 Hz, 2H, 2 × H_β), 6.96 (d, *J* = 8.4 Hz, 2 × 2H, Ar-H), 7.03 (d, *J* = 8.4 Hz, 2 × 2H, Ar-H), 7.15-7.40 (m,2 × 5H, Ar-H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.1, 32.1, 40.9, 52.1, 56.1, 127.4, 128.0, 128.6, 129.2, 132.3, 132.7, 133.8, 140.4, 208.8. HRMS: *m/z* Calcd. for $C_{33}H_{30}NaCl_2OS_2$ $(M+Na)^+$: Calcd: 599.1013; Found: 599.1005.

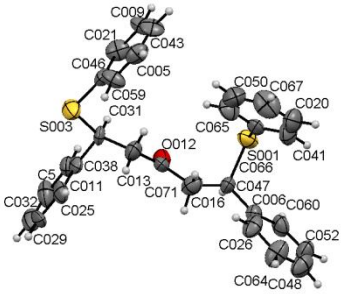


8c

Crystallographic Data Collection and Refinement

A suitable single crystal of compound **3a** (crystallized from acetone-petroleum ether) was mounted on a thin glass fibre with commercially available super glue. X-ray single crystal data collection was performed at room temperature using "Bruker SMART" diffractometer, equipped with a normal focus, sealed tube X-ray source with graphite monochromated Mo-Kα radiation (λ = 0.71073 Å). The structure was solved by SHELXS 97. Structure refinement was carried out using SHELXL 97. The relevant data are given in **Table 1** (**CCDC 1582432**) contains the supplementary crystallographic data. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre.

Table 1. Crystallographic data for compound 3a

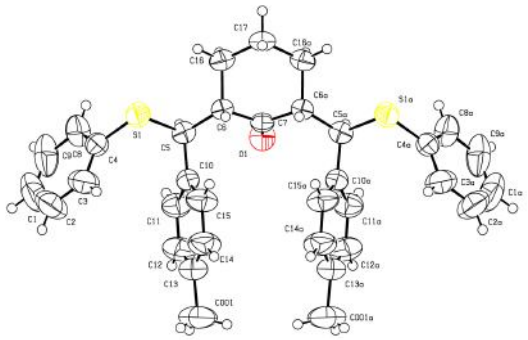


Molecular formula	$C_{29}H_{26}OS_2$
Formula weight	454.65
Temperature (K)	296.0
Wavelength (Mo-Kα)	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pca2_1$
Cell axes (Å)	10.979(9), 12.790(11), 33.90(3)
Cell angles (deg)	90.00, 90.00, 90.00
Volume (Å^3)	4761(7)
Z	8
Density (mg/mm^3)	1.263
Absorption coefficient (mm^{-1})	0.243
F (000)	1906
Theta range for data collection	1.59 to 27.41°

Index ranges	$-13 \le h \le 11, -16 \le k \le 16, -43 \le l \le 43$
Reflection collected	29755
Independent reflection	10192[R(int) = 0.2568]
Refinement method	Full-matrix least square on F^2
Data/restraints/parameter	10192/1/577
Goodness of fit on F^2	0.941
Final *R* indices [$I>2\sigma(I)$]	$R_1 = 0.0906$, $wR_2 = 0.1767$
R indices (all data)	$R_1 = 0.2931$, $wR_2 = 0.2499$
$\Delta\rho$ (e Å^{-3}) min. and max.	0.295/-0.473

A suitable single crystal of compound **5b** (crystallized from acetone-*n*-hexane) was also analysed using similar method (**CCDC 1419463**). **Table 2** contains the data obtained.

Table 2. Crystallographic data for compound 5b

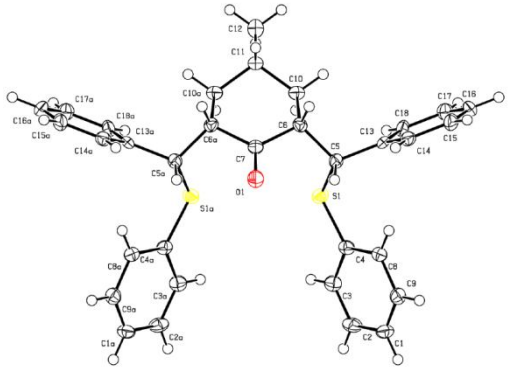


Molecular formula	$C_{34}H_{34}OS_2$
Formula weight	520.72
Temperature (K)	273.0
Wavelength (Mo-Kα)	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Cell axes (Å)	24.0948(10), 12.4204(6), 9.9484(5)
Cell angles (deg)	90.00, 90.00, 90.00
Volume (Å^3)	2977.2(2)

Z	4
Density (mg/mm^3)	1.162
Absorption coefficient (mm^{-1})	0.203
F (000)	1104
Theta range for data collection	1.69 to 27.16°
Index ranges	-30 ≤ h ≤ 27, -15 ≤ k ≤ 13, -12 ≤ l ≤ 12
Reflection collected	12028
Independent reflection	3364[R(int) = 0.0465]
Refinement method	Full-matrix least square on F^2
Data/restraints/parameter	3364/1/172
Goodness of fit on F^2	0.851
Final *R* indices [I>2σ (I)]	R_1 = 0.0617, wR_2 = 0.1470
R indices (all data)	R_1 = 0.0884, wR_2 = 0.1736
□□□(e Å^{-3}) min. and max.	0.317/-0.390

A suitable single crystal of compound **8a** (crystallized from acetone-*n*-hexane) was also analysed using similar method (**CCDC 1419467**). **Table 3** contains the data obtained.

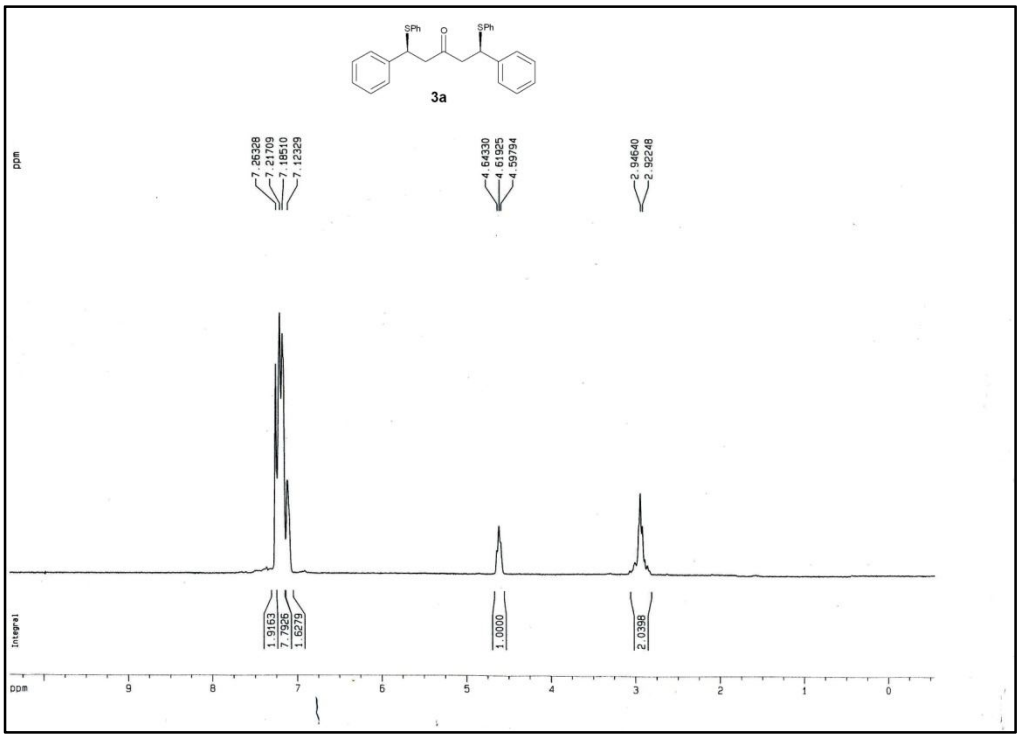
Table 3. Crystallographic data for compound 8a



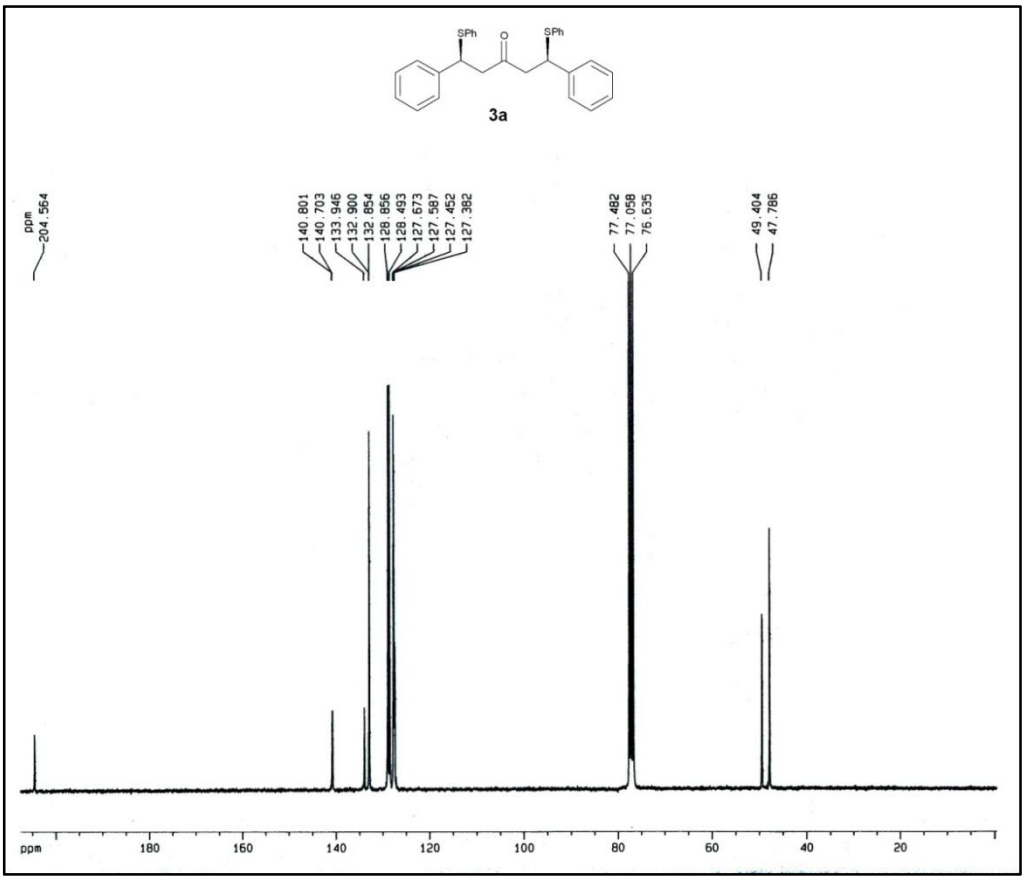
Molecular formula	$C_{33}H_{32}OS_2$
Formula weight	512.74
Temperature (K)	293.0
Wavelength (Mo-Kα)	0.71073 Å

Crystal system	Orthorhombic
Space group	Pnma
Cell axes (Å)	17.3688(11), 26.3114(16), 5.6621(3)
Cell angles (deg)	90.00, 90.00, 90.00
Volume ($Å^3$)	2587.6(3)
Z	4
Density (mg/mm^3)	1.316
Absorption coefficient (mm^{-1})	0.232
F (000)	1096
Theta range for data collection	1.55 to 19.13°
Index ranges	$-16 \leq h \leq 16, -24 \leq k \leq 24, -5 \leq l \leq 5$
Reflection collected	12309[R(int) = 0.0982]
Independent reflection	1093
Refinement method	Full-matrix least square on F^2
Data/restraints/parameter	1093/0/170
Goodness of fit on F^2	0.954
Final *R* indices [$I>2\sigma(I)$]	$R_1 = 0.0350$, $wR_2 = 0.0763$
R indices (all data)	$R_1 = 0.0500$, $wR_2 = 0.0822$
$\Delta\rho$ ($e\ Å^{-3}$) min. and max.	0.182/-0.245

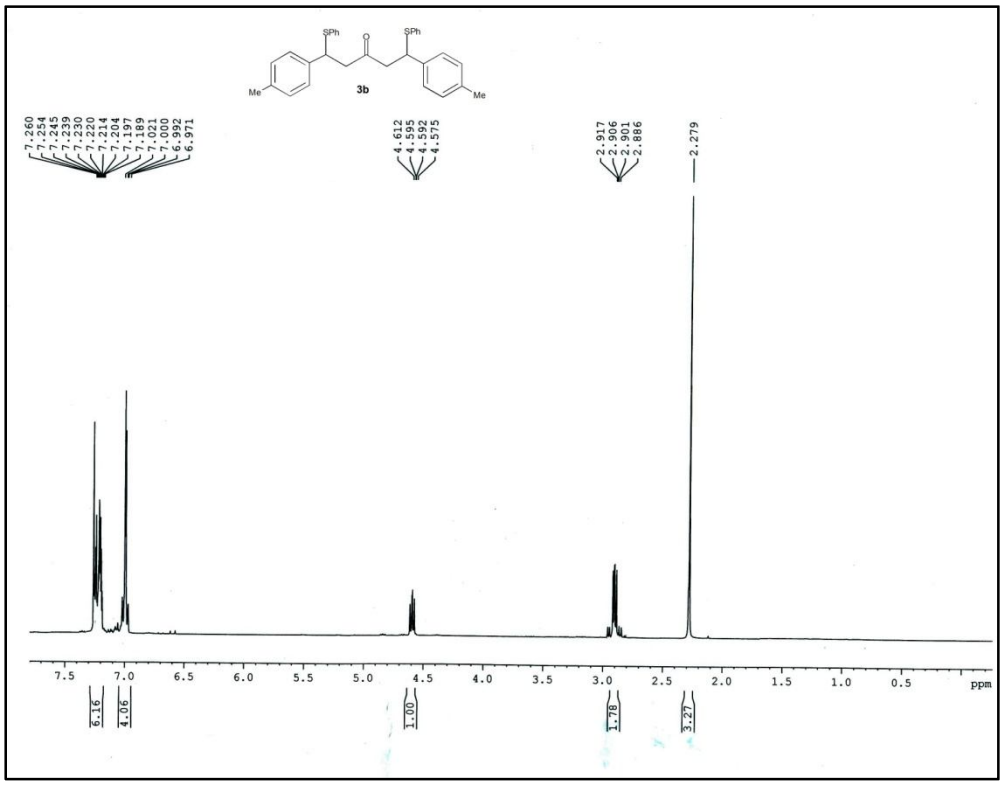
^{1}H NMR spectrum of **3a**



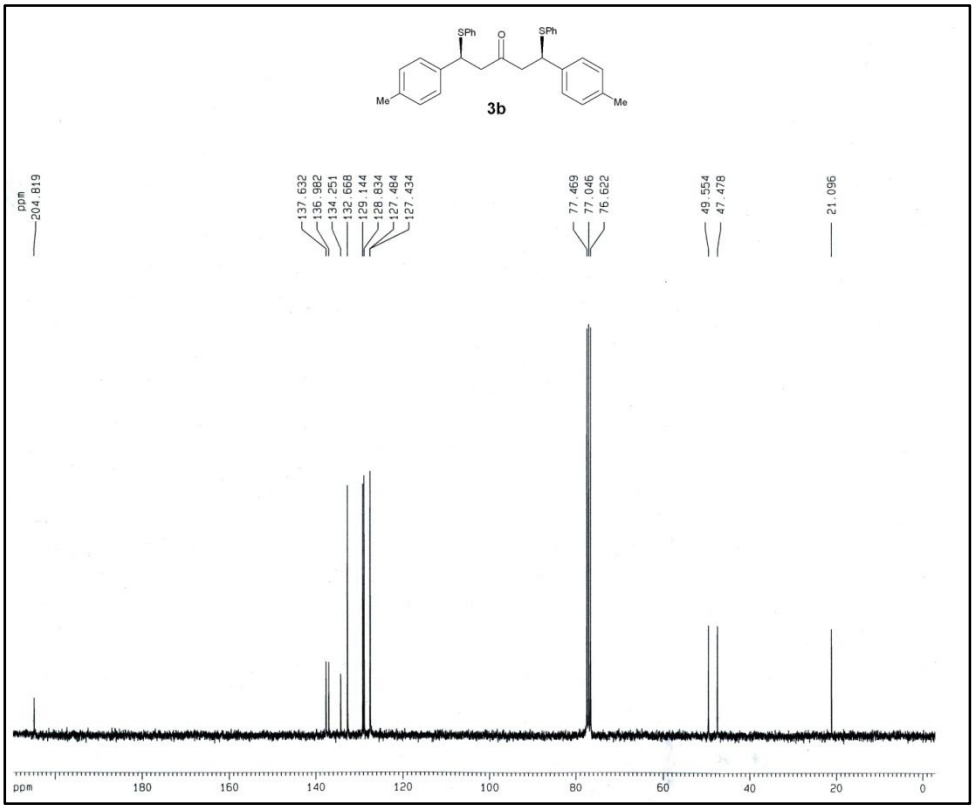
^{13}C NMR spectrum of **3a**



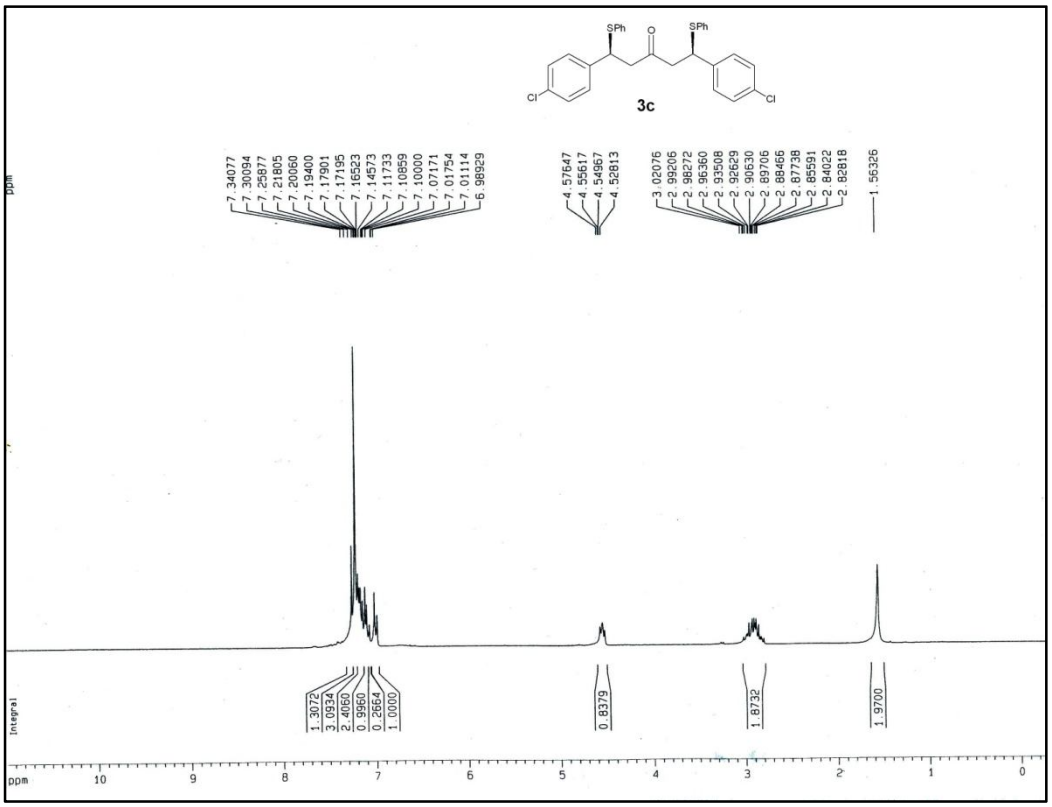
^{1}H NMR spectrum of **3b**



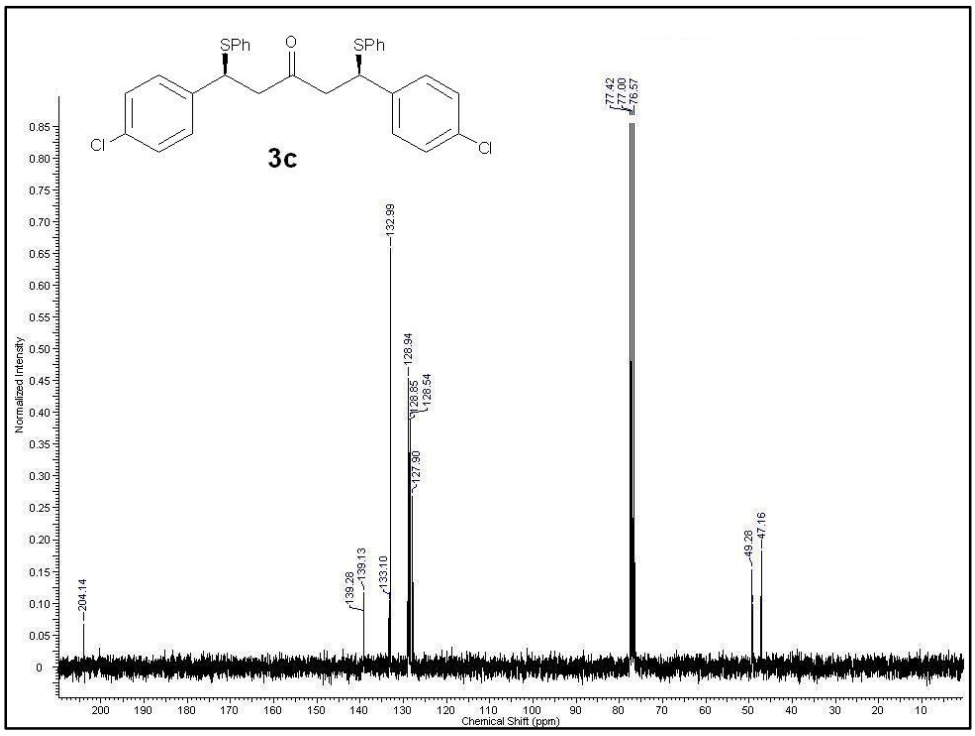
^{13}C NMR spectrum of **3b**



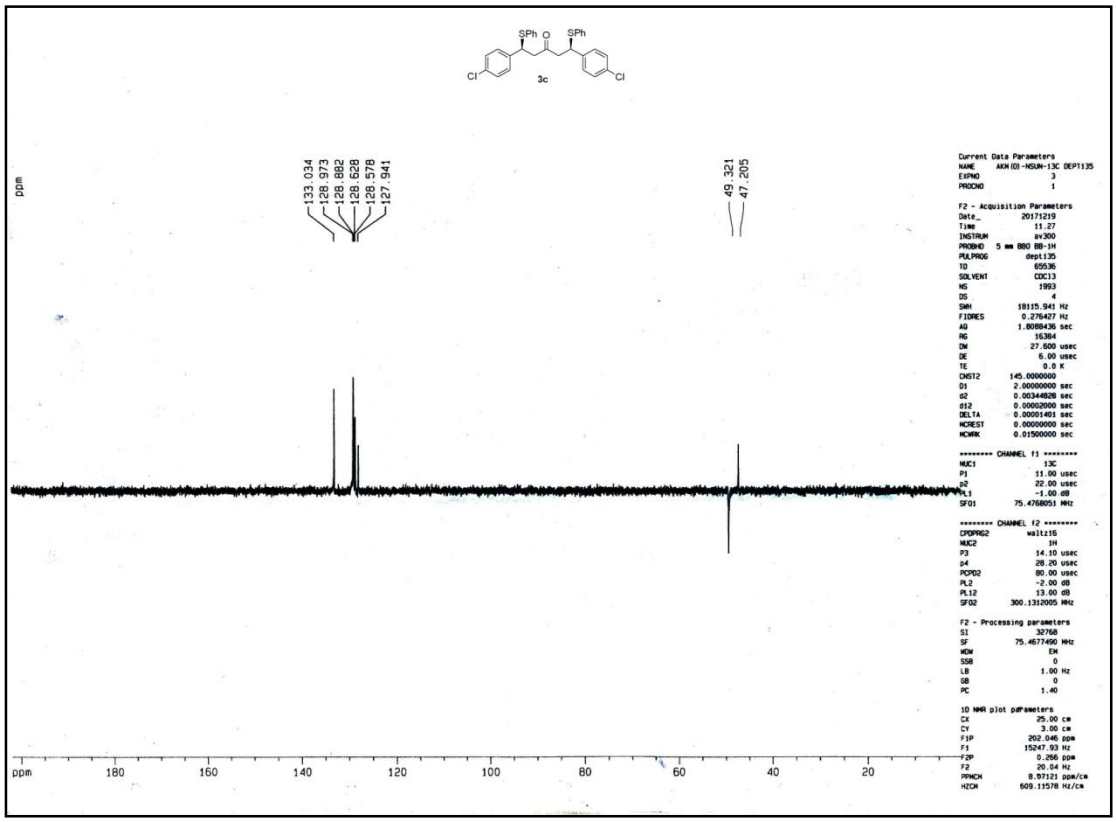
^{1}H NMR spectrum of **3c**



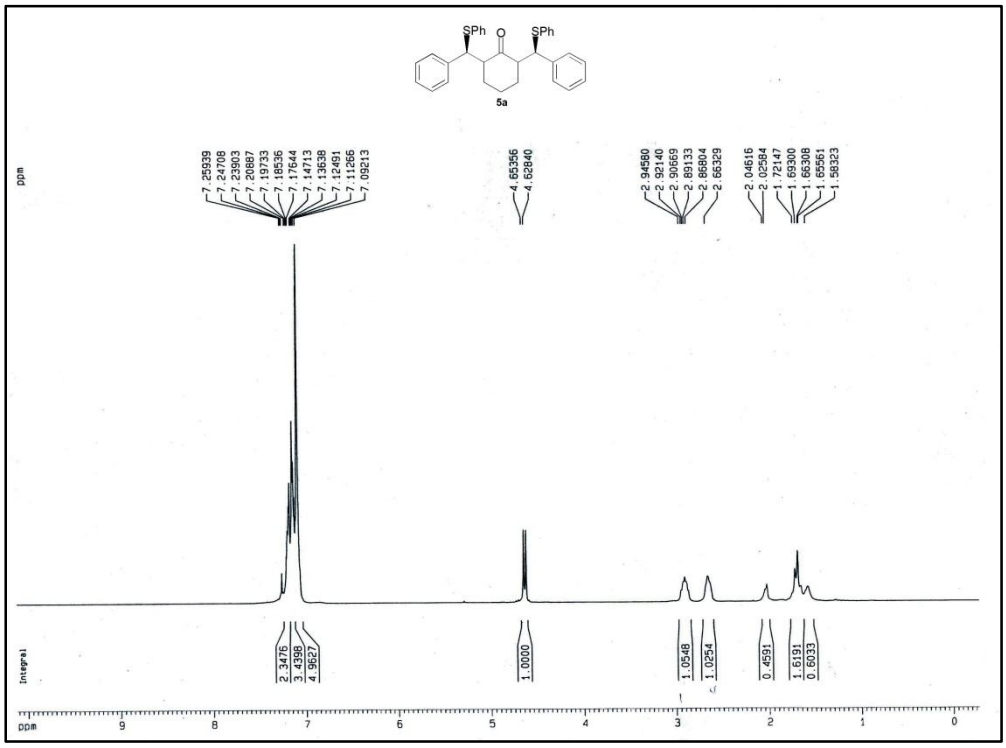
^{13}C NMR spectrum of **3c**



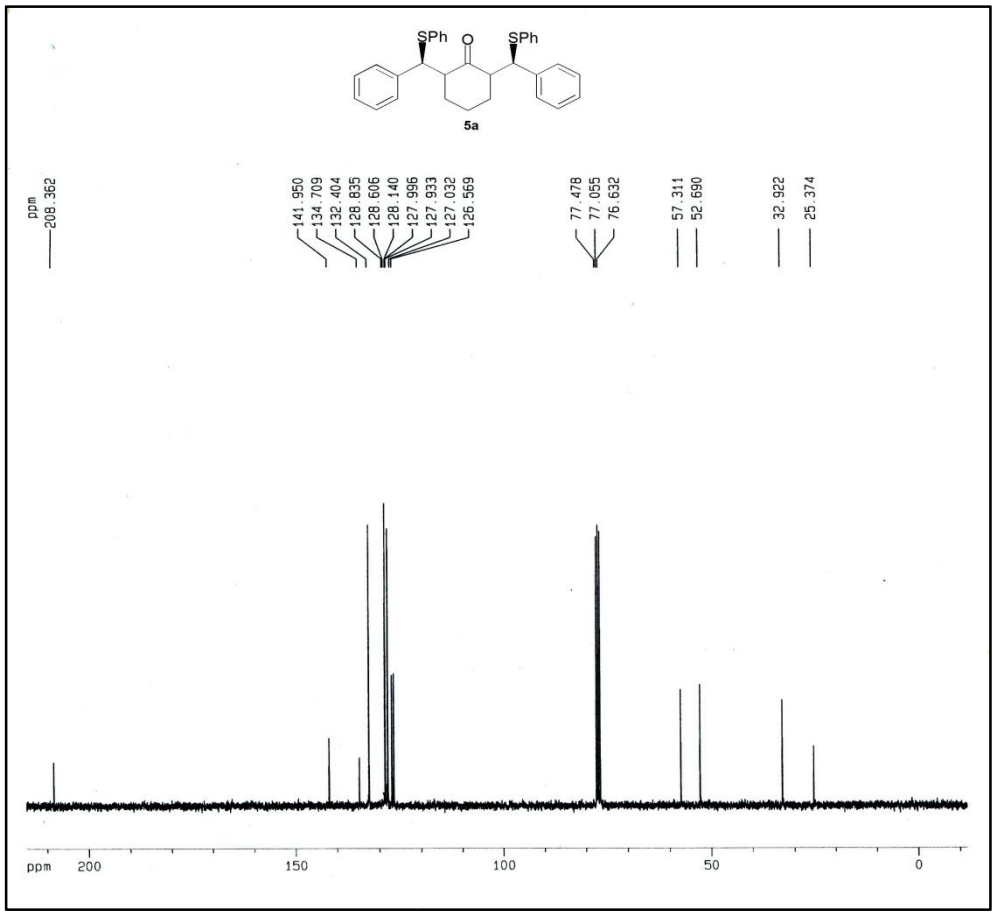
DEPT 135 spectrum of **3c**



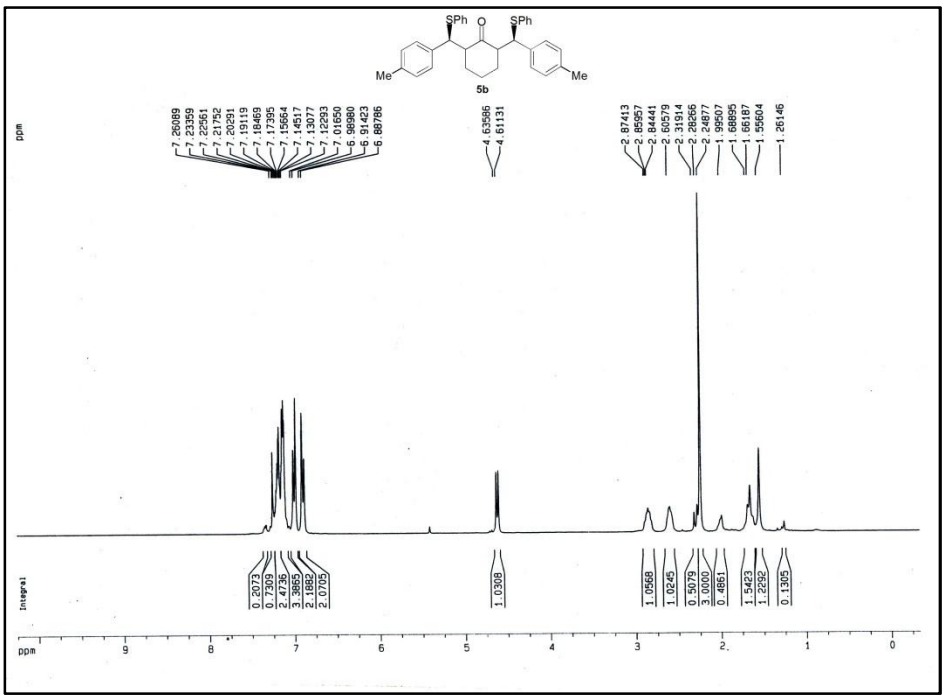
^{1}H NMR spectrum of **5a**



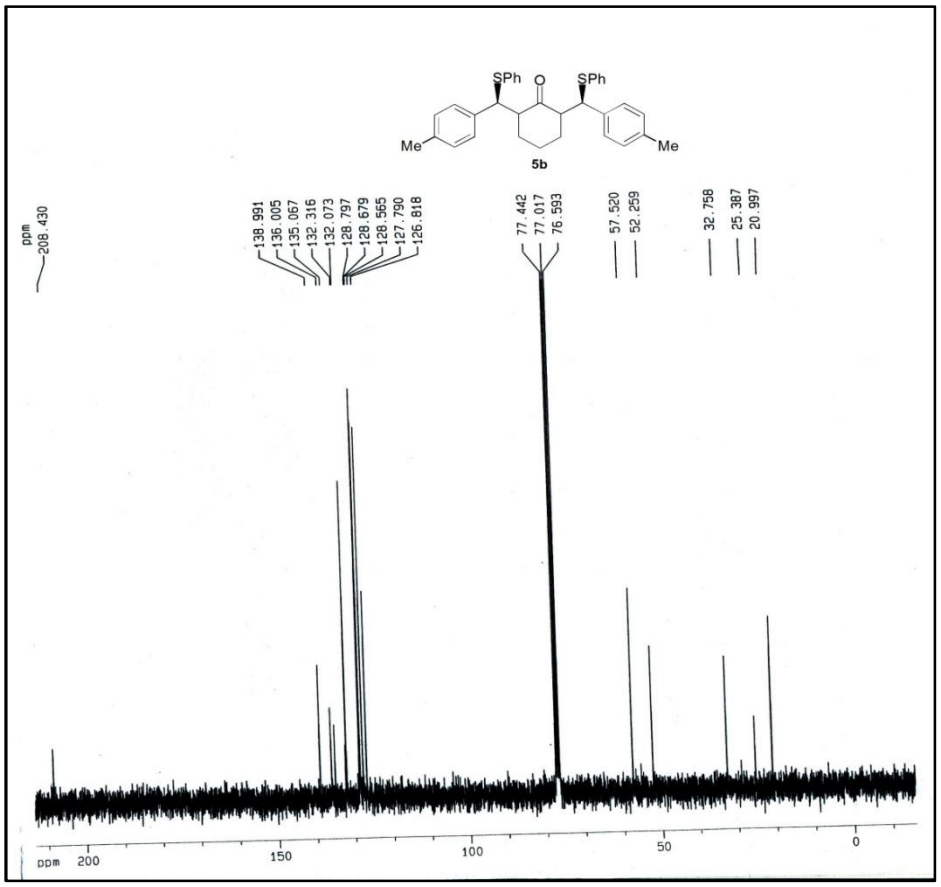
^{13}C NMR spectrum of **5a**



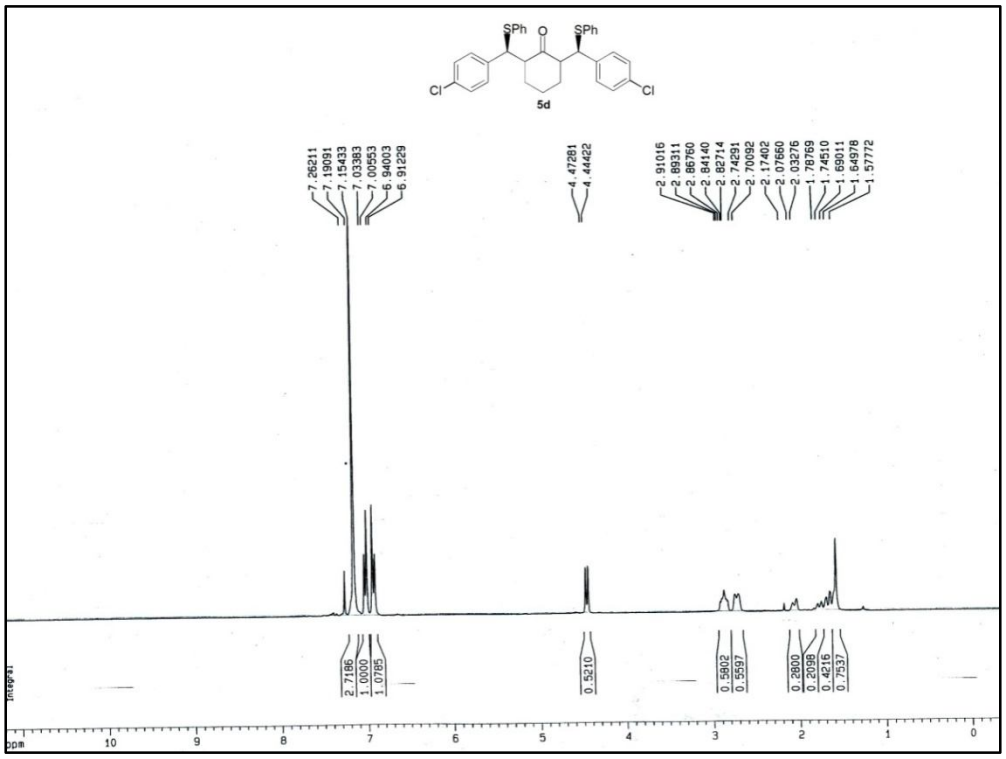
^{1}H NMR spectrum of **5b**



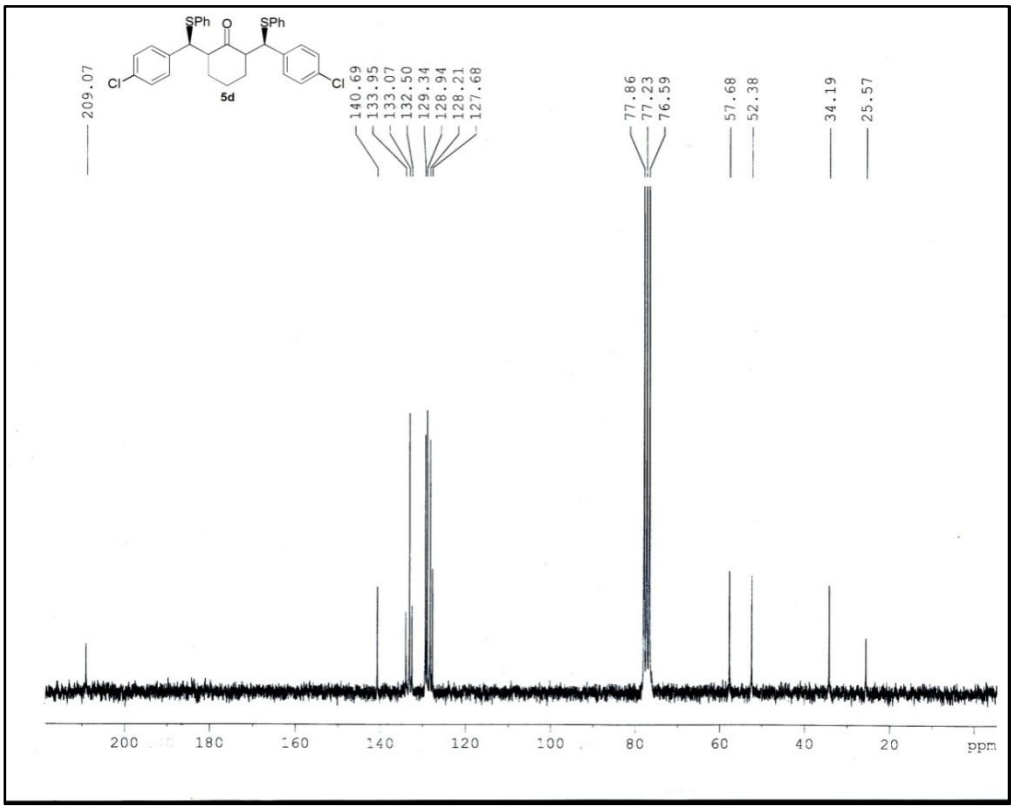
^{13}C NMR spectrum of **5b**



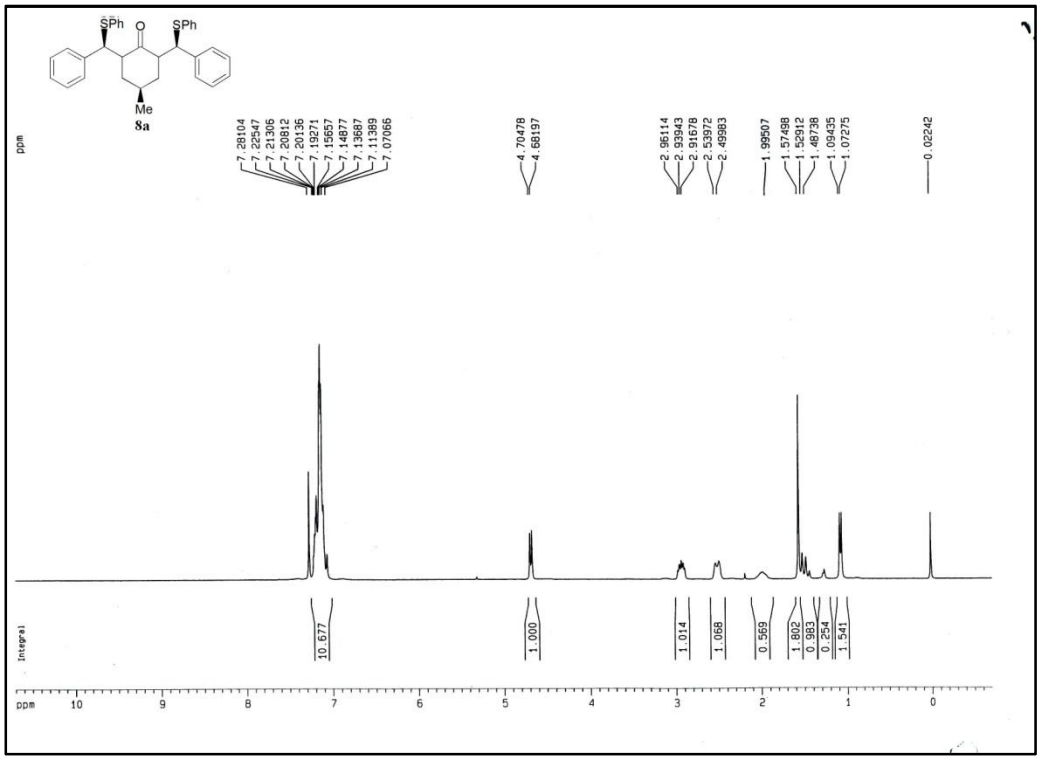
^{1}H NMR spectrum of **5d**



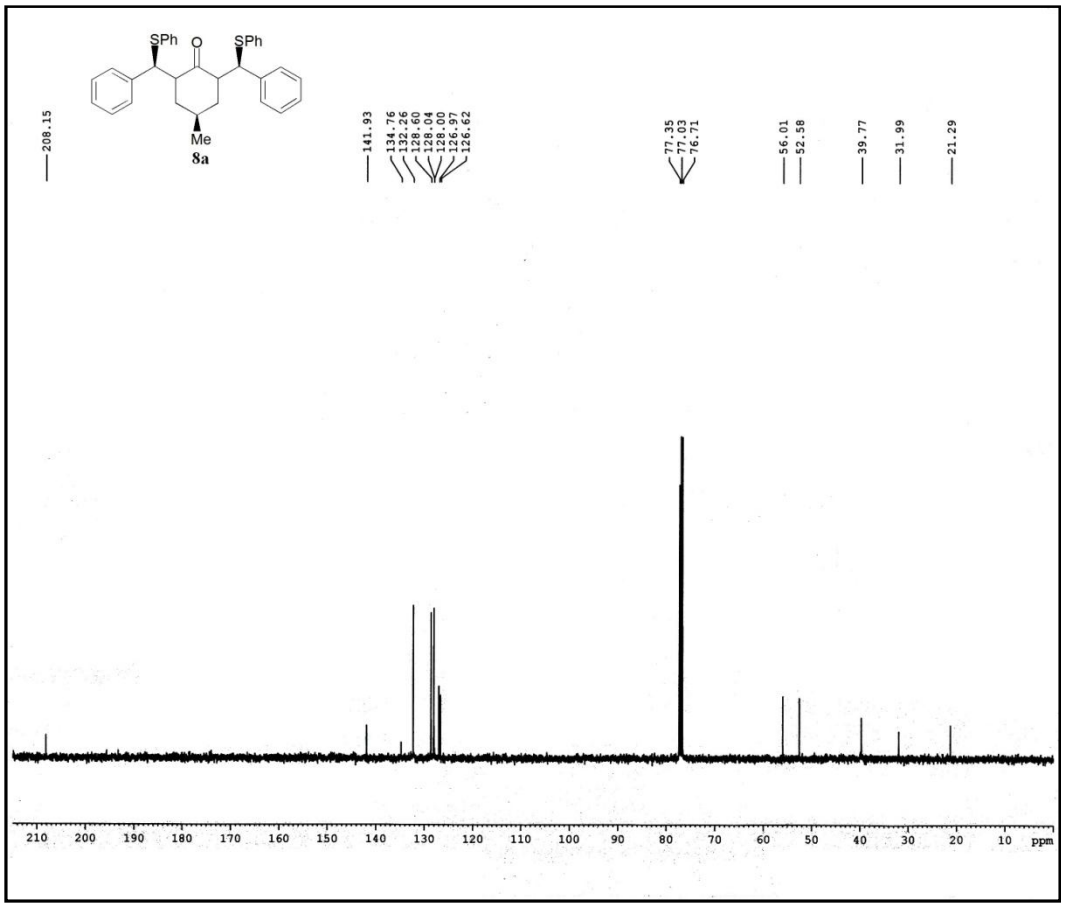
^{13}C NMR spectrum of **5d**



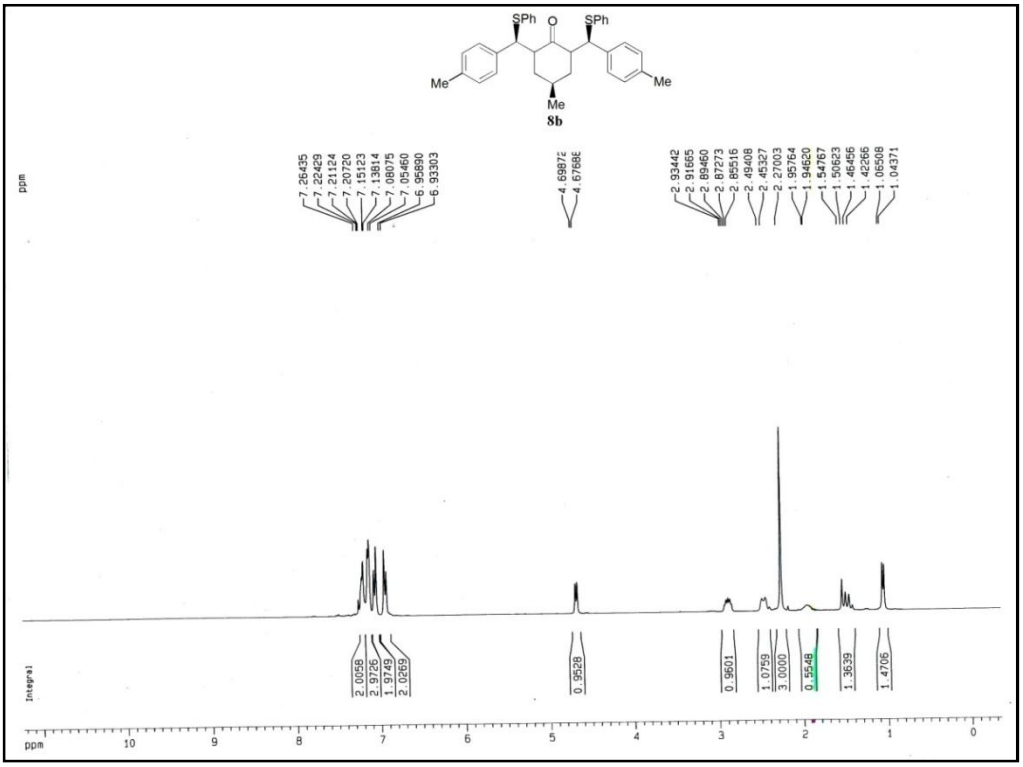
^{1}H NMR spectrum of **8a**



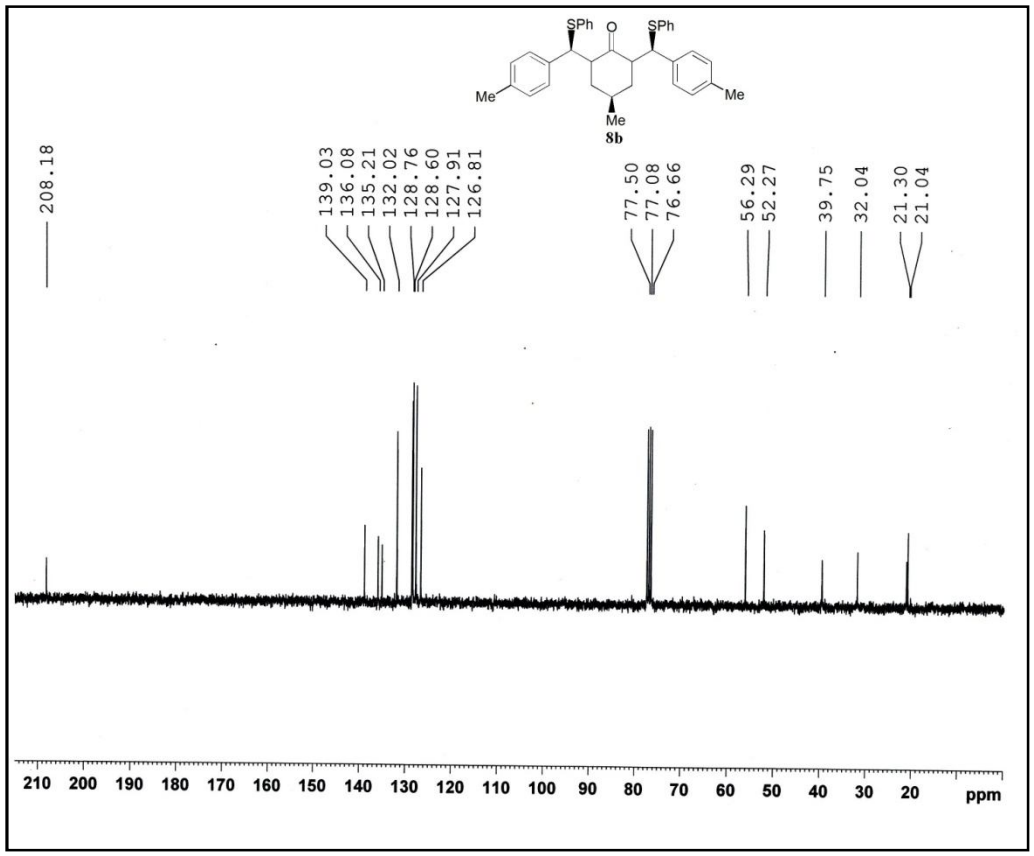
^{13}C NMR spectrum of **8a**



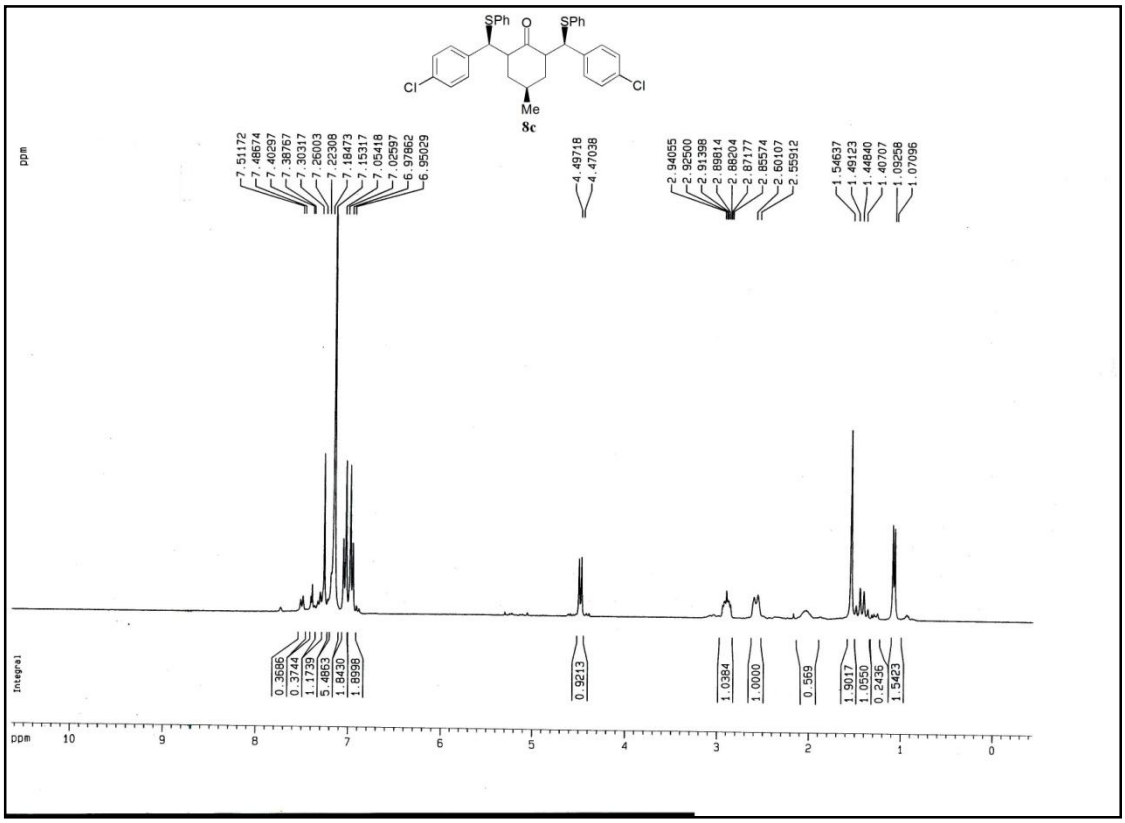
^{1}H NMR spectrum of **8b**



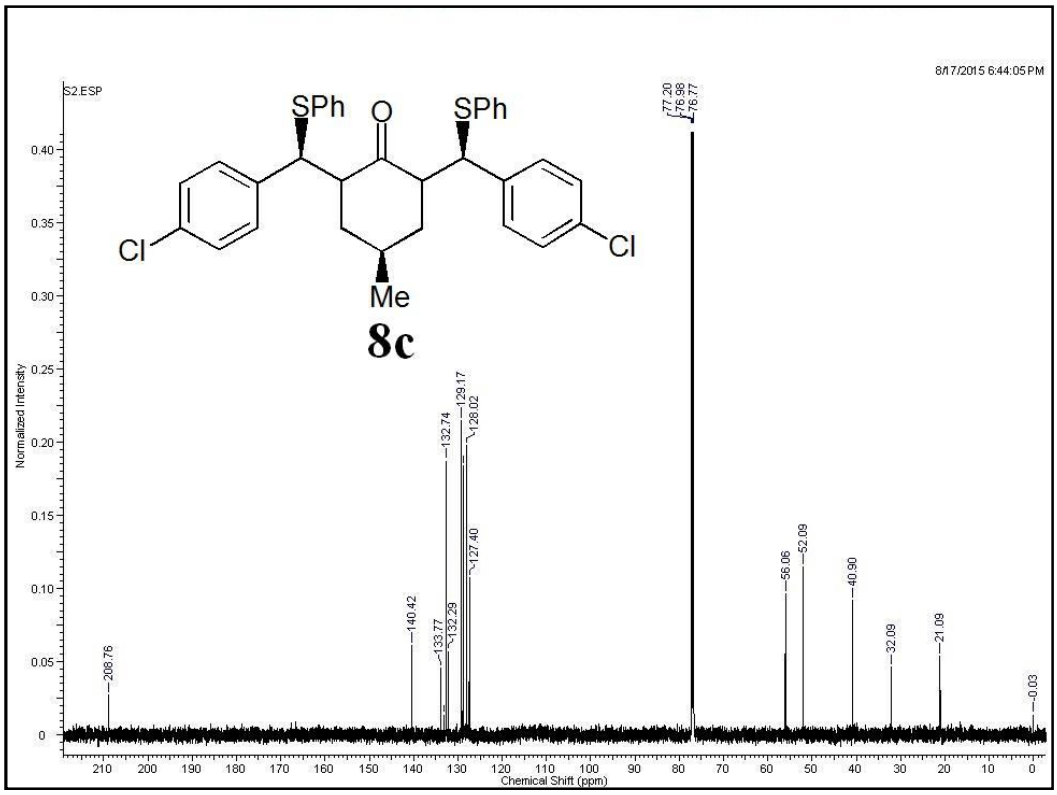
^{13}C NMR spectrum of **8b**



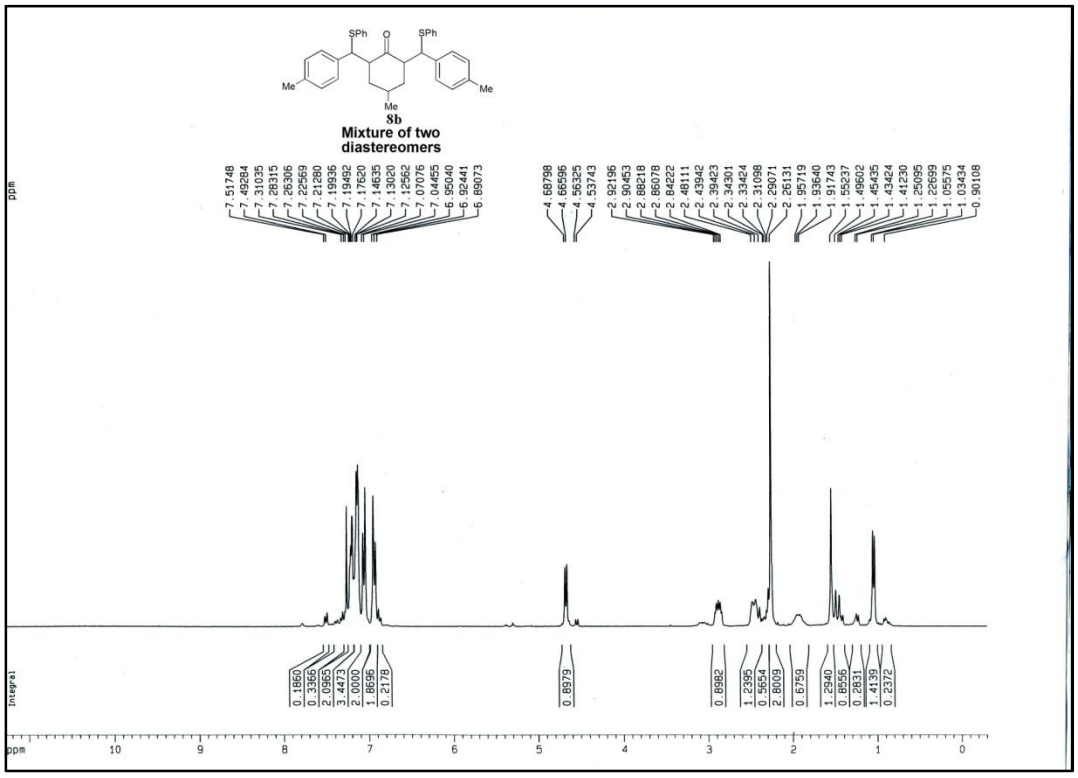
^{1}H NMR spectrum of **8c**



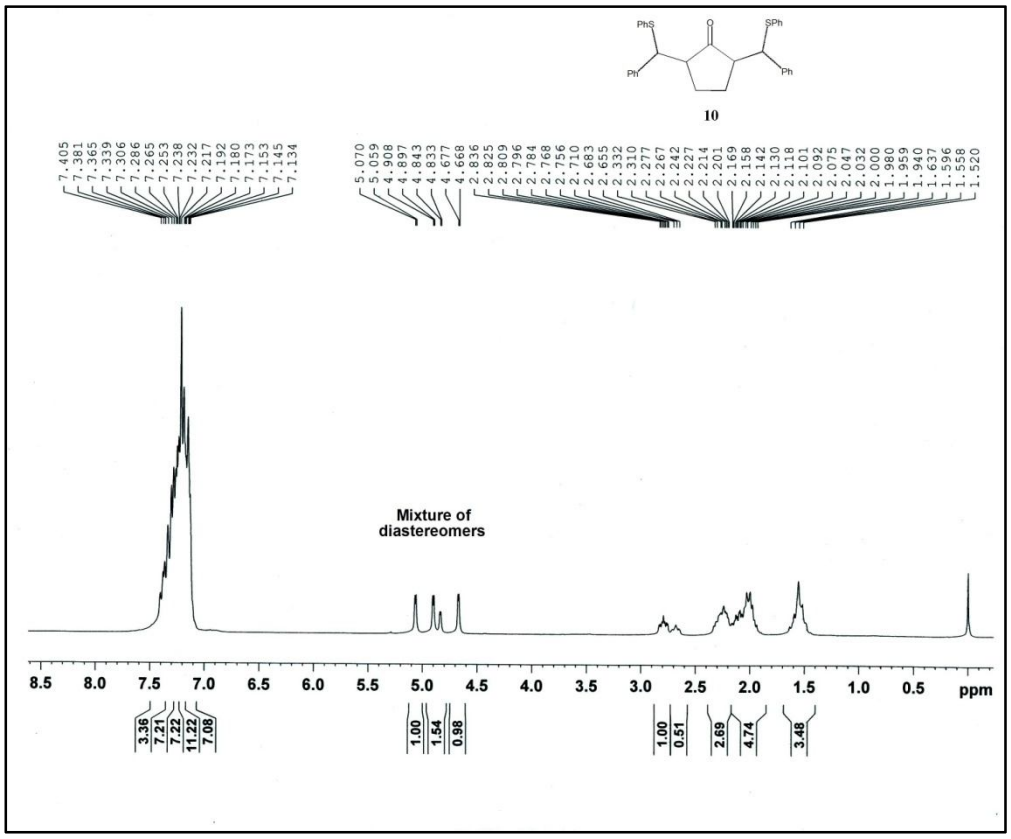
^{13}C NMR spectrum of **8c**



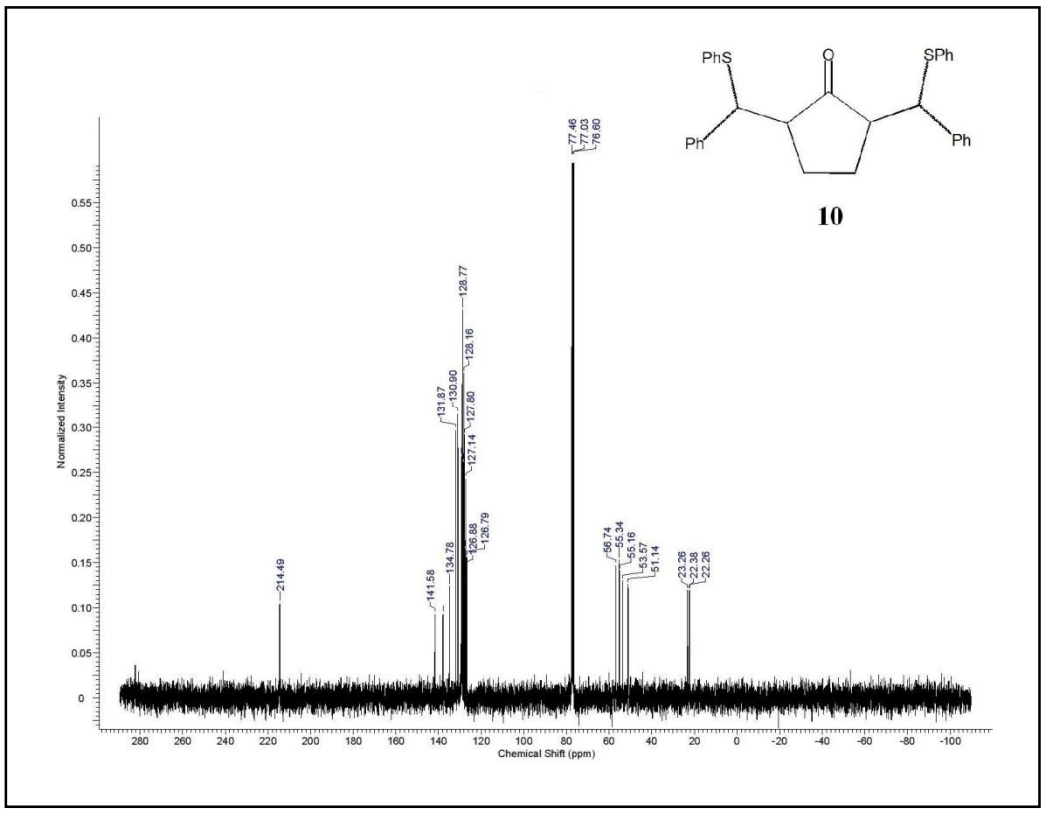
^{1}H NMR spectrum of impure **8b** (when reaction done at higher temperature)



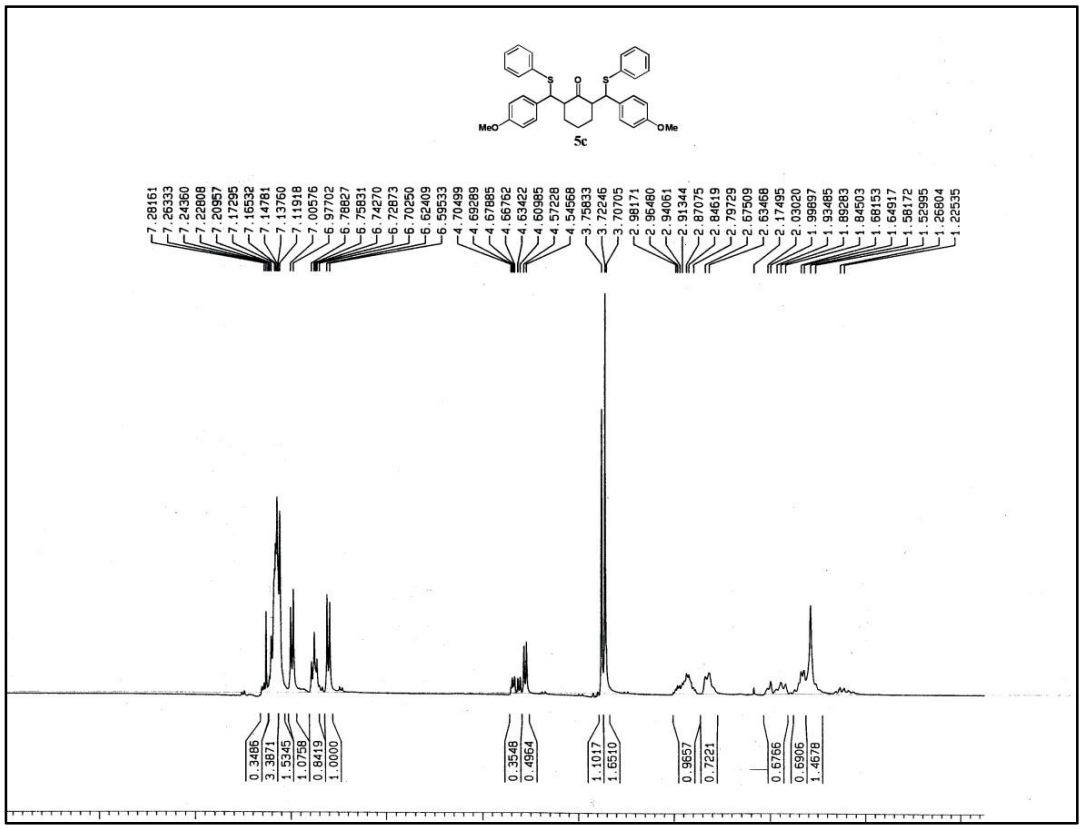
^{1}H NMR spectrum of impure**10**



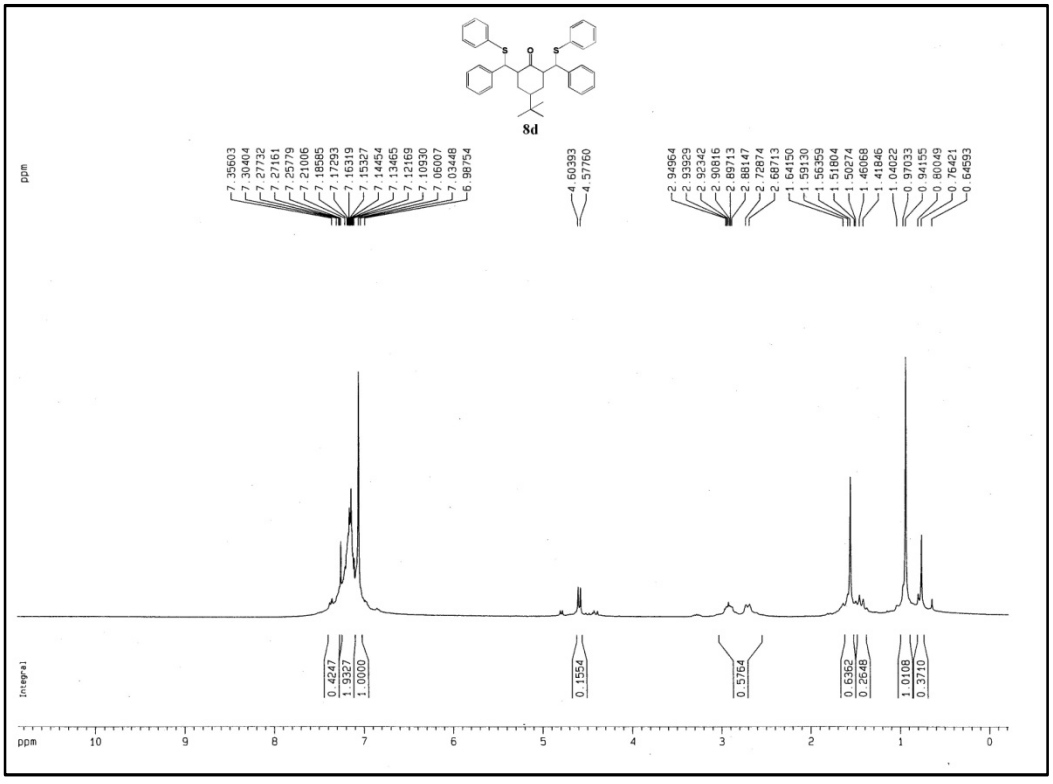
^{13}C NMR spectrum of impure **10**



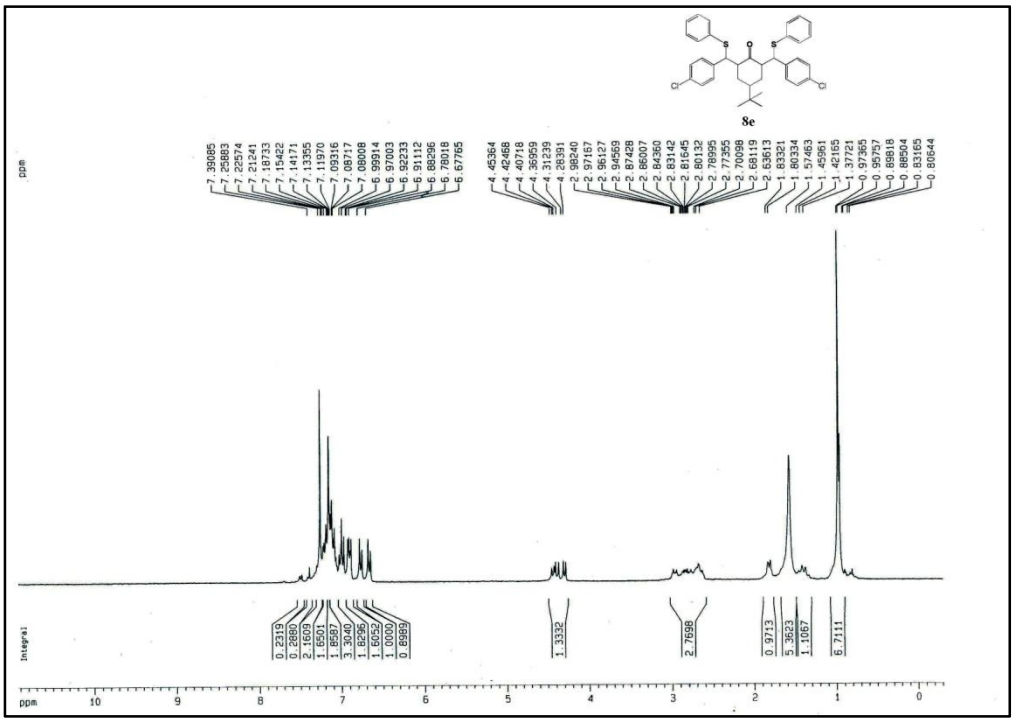
^{1}H NMR spectrum of impure 5c



^{1}H NMR spectrum of impure 8d

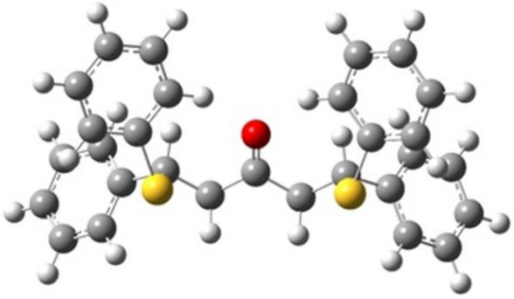


^{1}H NMR spectrum of impure 8e



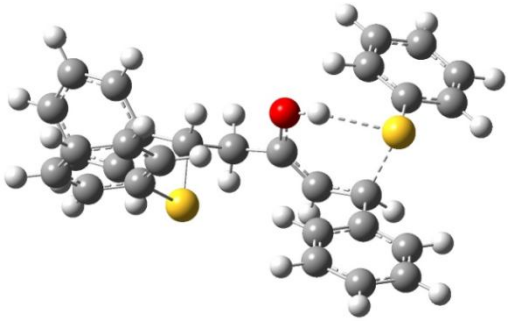
Results obtained from DFT Calculations

DFT calculations were done to optimise the structure of **3a**, the *dl* isomer of **3a** and the corresponding transition states leading to them. The structure of **5a**, **5′a** and the corresponding intermediates (**11a**, **11′a**) were also subjected to similar calculations. All the structures were optimised under B3lyp/3-21g basis set using Gaussian 09W software[2]. The optimised structures and corresponding free energies obtained from the calculations are given below.



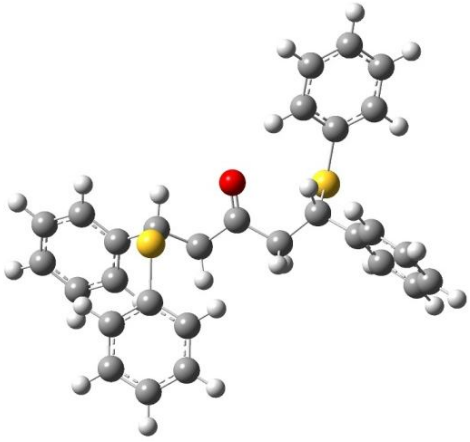
Optimised structure for **3a**

Electronic and thermal free energy: -5202365.282478 kJ mol^{-1}



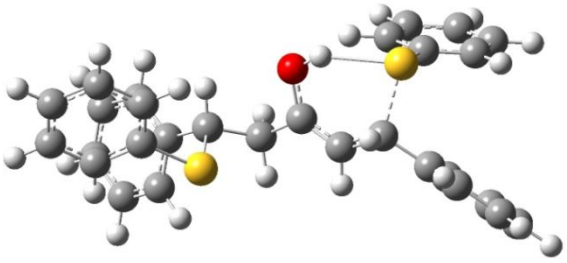
Optimised structure for the transition state leading to **3a**

Electronic and thermal free energy: -5202323.702432 kJ mol^{-1}



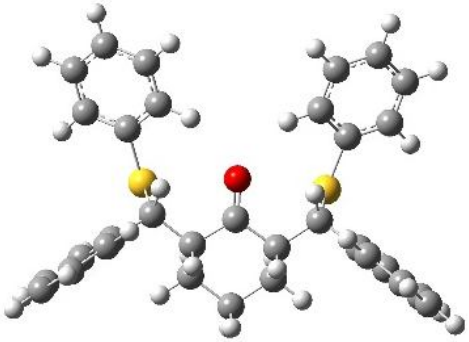
Optimised structure for the *dl*-isomer of **3a**

Electronic and thermal free energy: -5202361.124925 kJ mol^{-1}



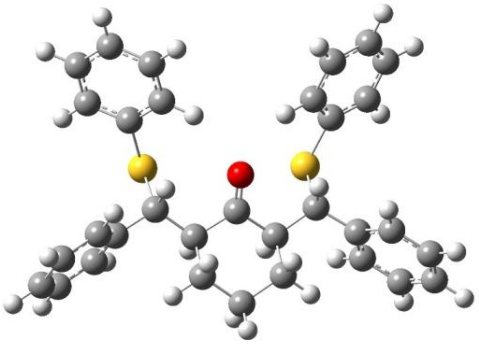
Optimised structure for the transition state leading to the *dl*-isomer of **3a**

Electronic and thermal free energy: -5202314.106228 kJ mol^{-1}



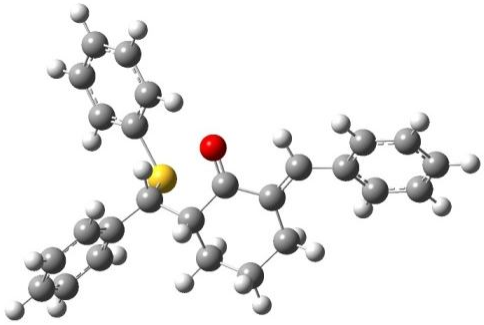
Optimised structure for **5a**

Electronic and thermal free energy: -5507031.439529 kJ mol^{-1}



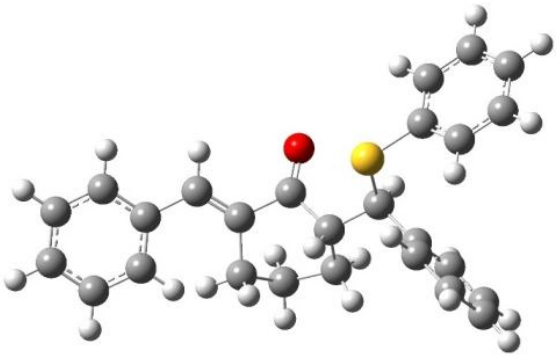
Optimised structure for **5′a**

Electronic and thermal free energy: -5507037.598953 kJ mol^{-1}



Optimised structure for **11a**

Electronic and thermal free energy: -3860486.743792 kJ mol^{-1}



Optimised structure for **11′a**

Electronic and thermal free energy: -380483.107475 kJ mol^{-1}

References

1. Konduru NK, Dey S, Sajid M, Owais M, Ahmed N. Eur. J. Med. Chem. 2013;30:5923

2. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.