Chemistry of Heterocyclic Compounds **2023**, *59*(4/5), 283–288

Unexpected transformation of 1,5-benzodiazepine derivatives under imidazo-annulation reaction conditions

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[2] *Vilnius University, Institute of Theoretical Physics and Astronomy, 3 Saulėtekio St., Vilnius LT-10257, Lithuania; e-mail: ausra.vektariene@tfai.vu.lt*

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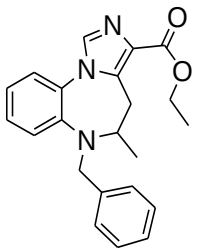
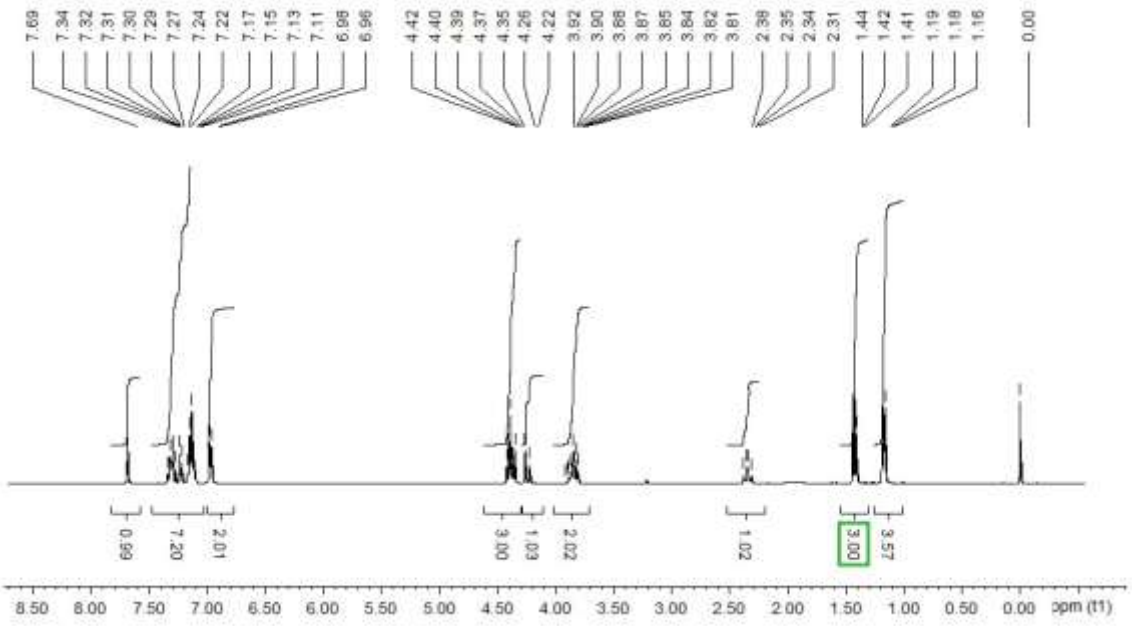
SUPPLEMENTARY INFORMATION

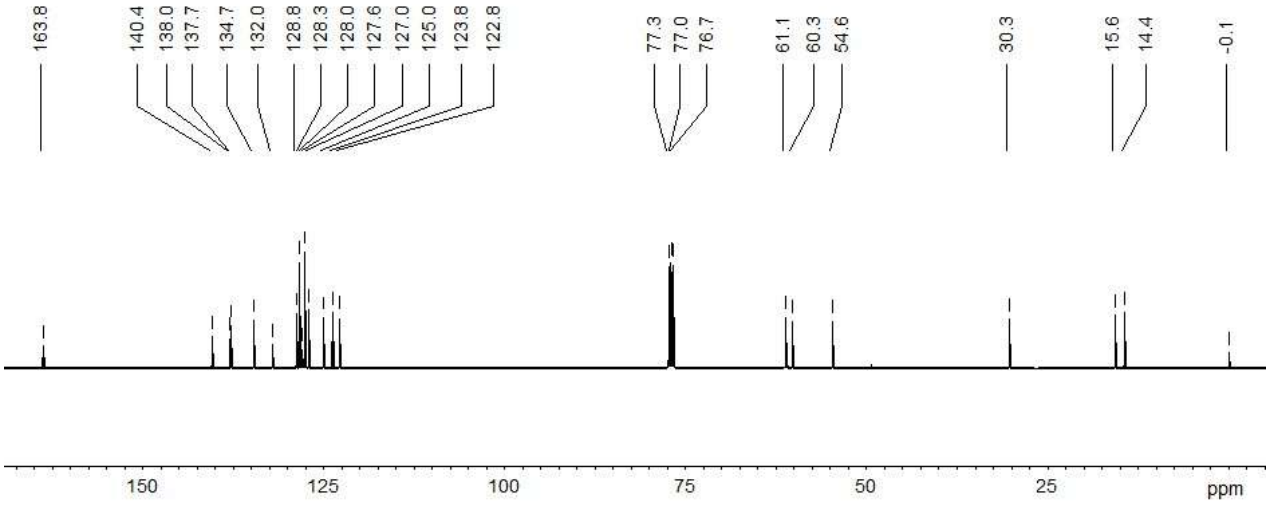
Ethyl 6-benzyl-5-methyl-5,6-dihydro-4*H*-imidazo[1,5-a][1,5]benzodiazepine-3-carboxylate (3b).



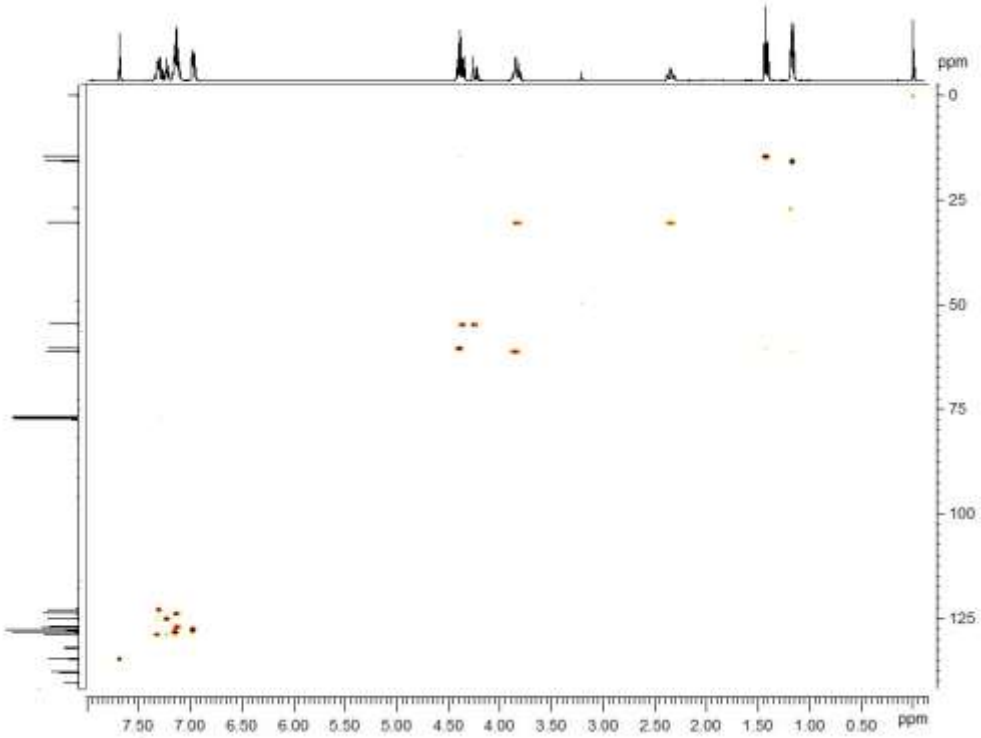
^{1}H NMR spectrum of compound **3b** in $CDCl_3$ solution



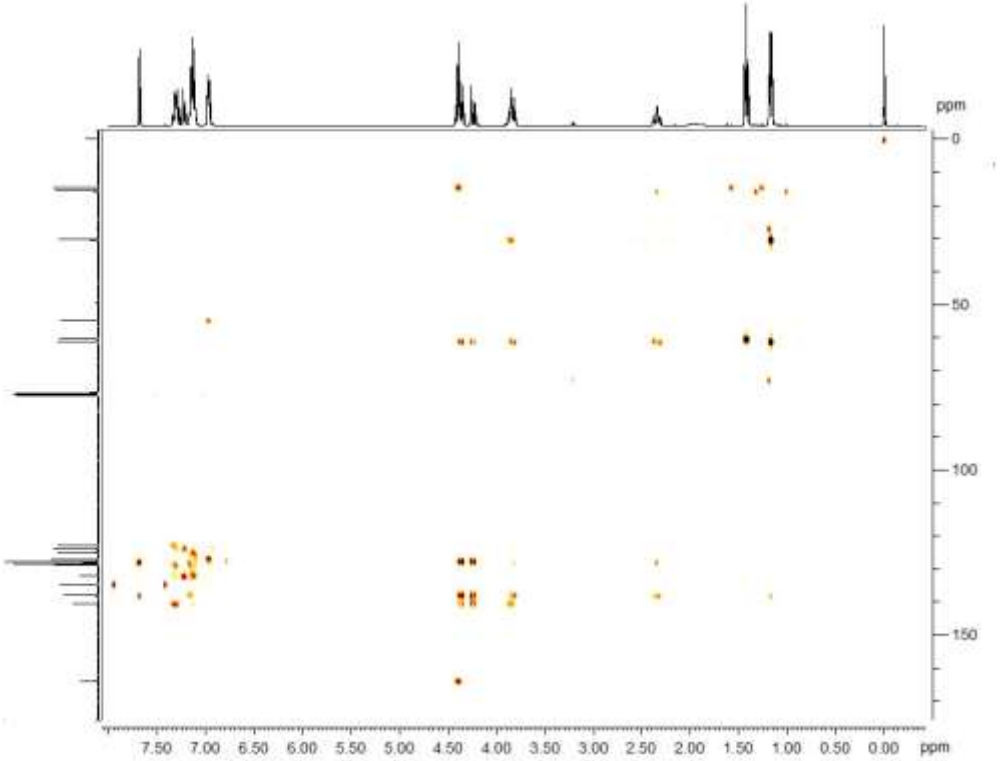
^{13}C NMR spectrum of compound **3b** in $CDCl_3$ solution



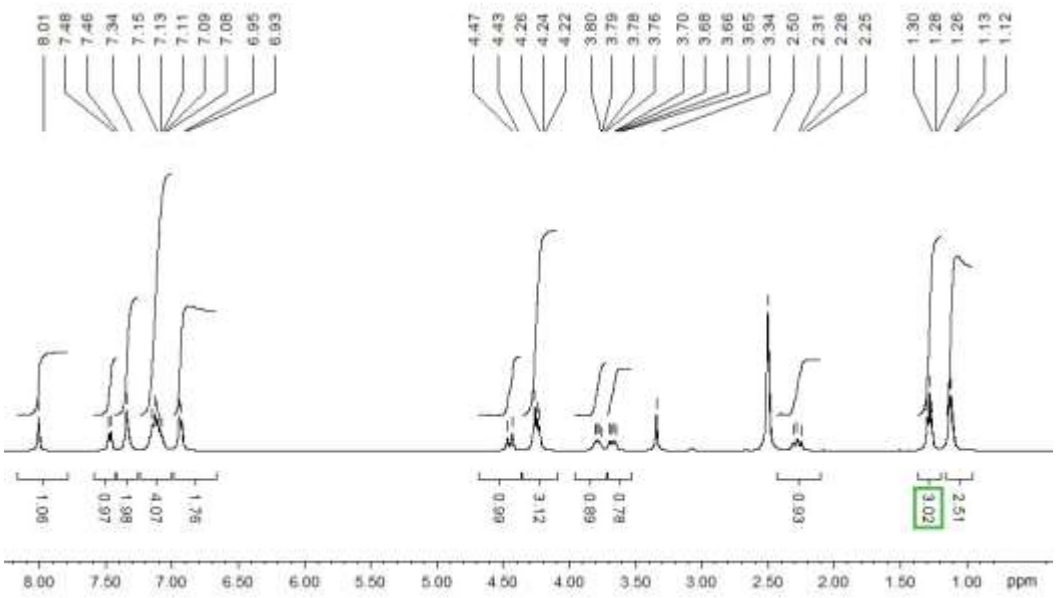
HSQC NMR spectrum of compound **3b** in $CDCl_3$ solution



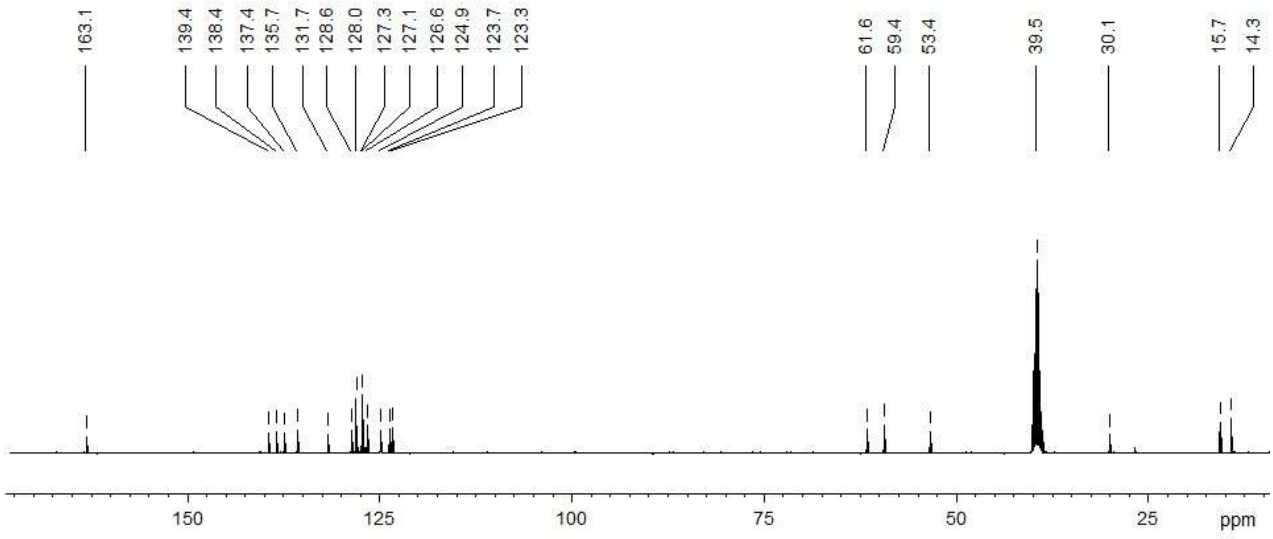
HMBC NMR spectrum of compound **3b** in $CDCl_3$ solution



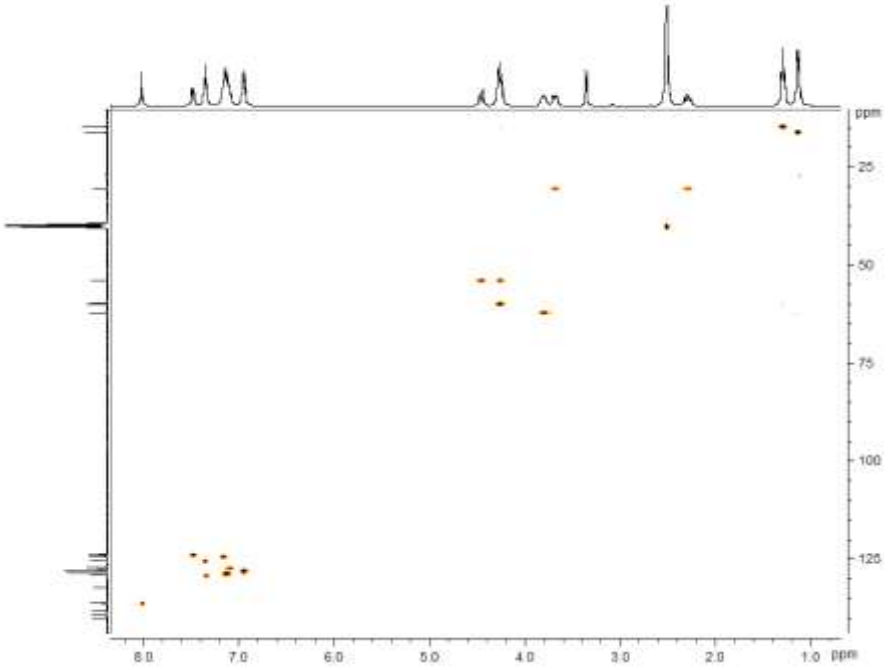
^{1}H spectrum of compound **3b** in DMSO-d_6 solution



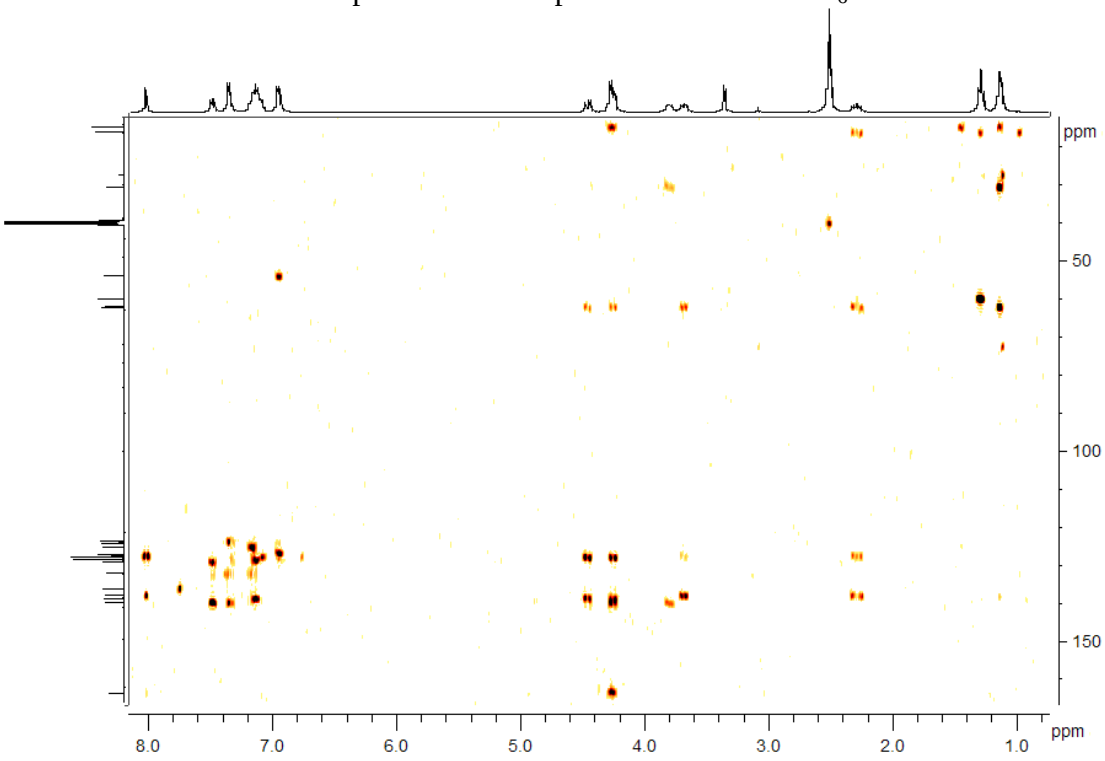
^{13}C NMR spectrum of compound **3b** in DMSO-d_6 solution



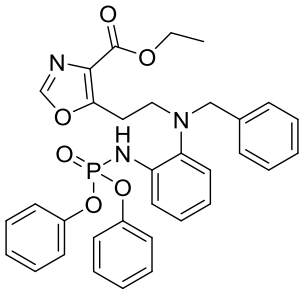
HSQC NMR spectrum of compound **3b** in DMSO-d_6 solution



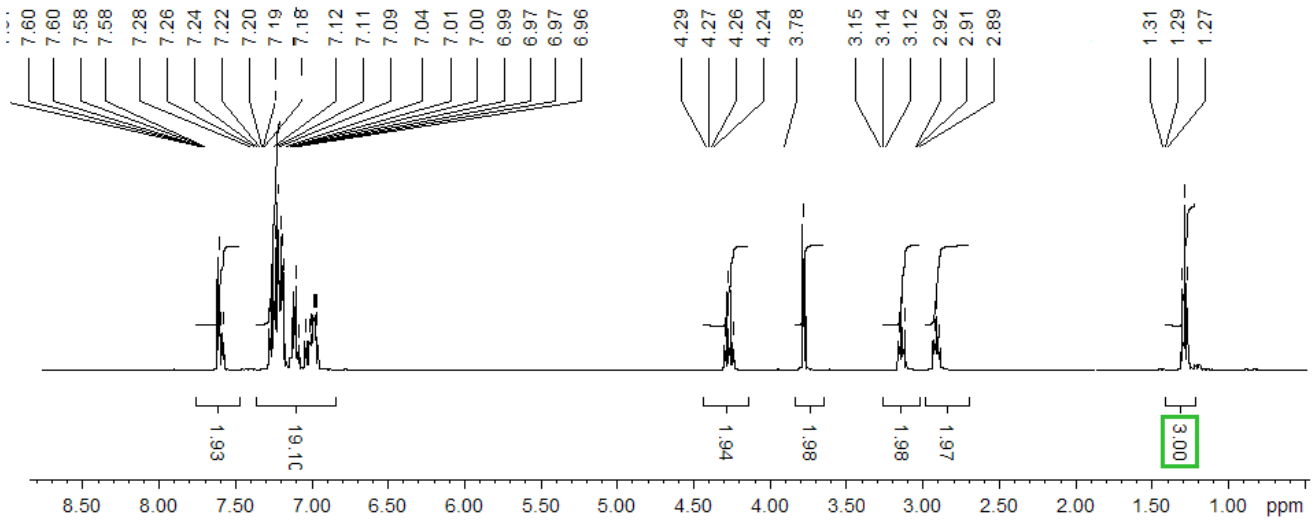
HMBC NMR spectrum of compound **3b** in DMSO-d_6 solution



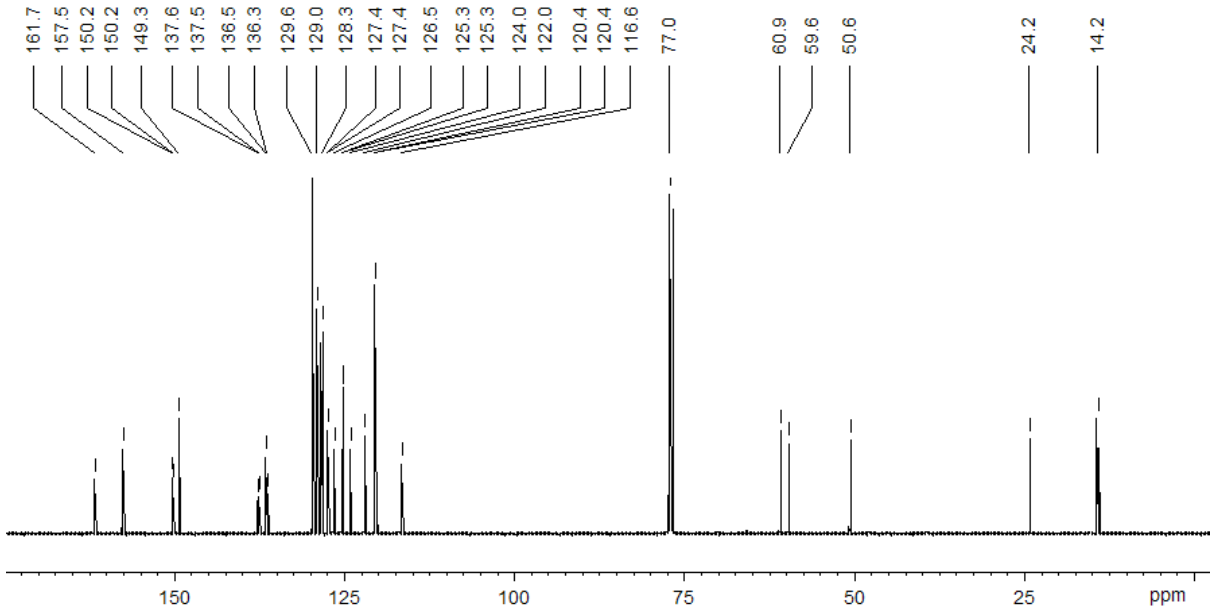
Ethyl 5-[2-(benzyl{2-[(diphenoxyphosphoryl)amino]phenyl}amino)ethyl]-1,3-oxazole-4-carboxylate (2a).



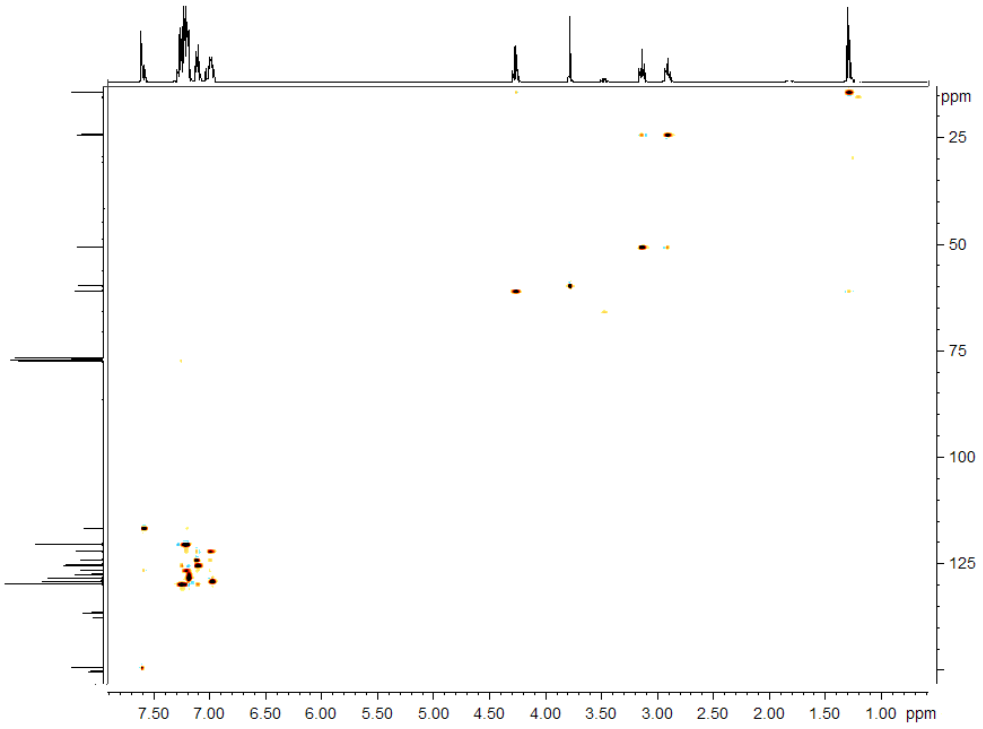
^{1}H NMR spectrum of compound **2a** in $CDCl_3$ solution



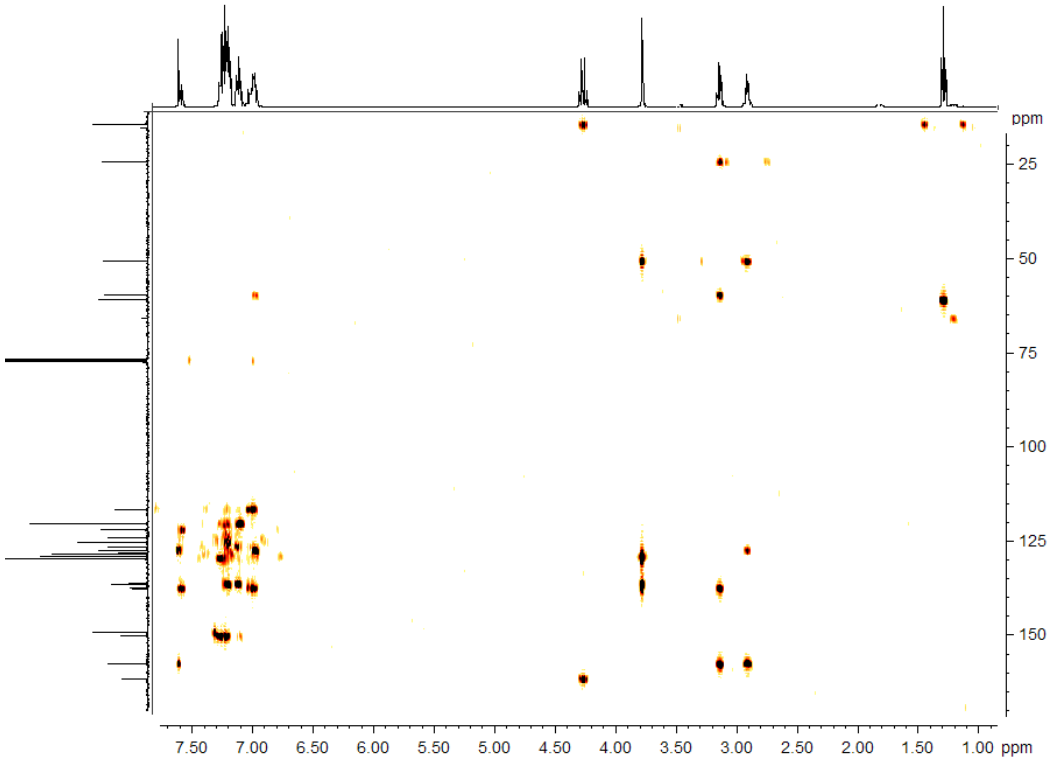
^{13}C NMR spectrum of compound **2a** in $CDCl_3$ solution



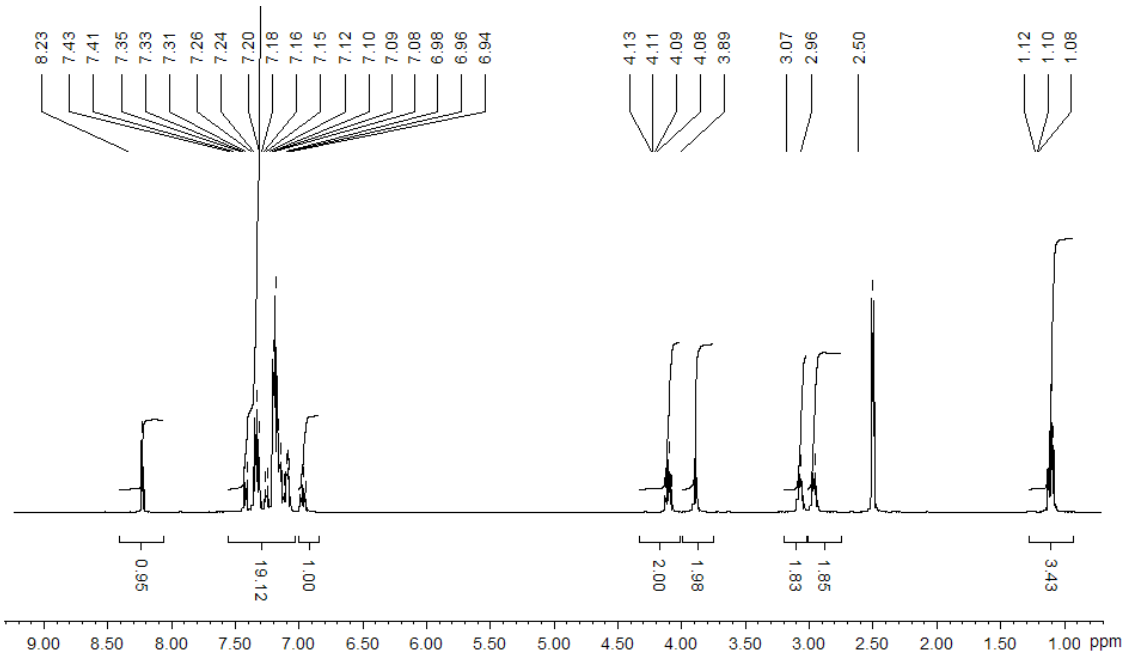
HSQC NMR spectrum of compound **2a** in $CDCl_3$ solution



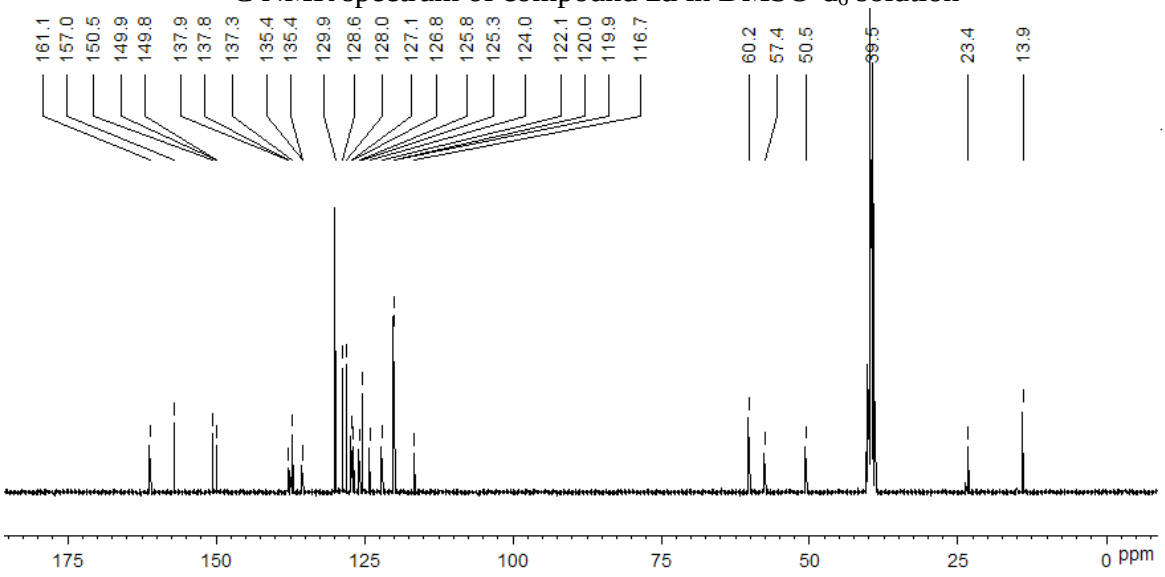
HMBC NMR spectrum of compound **2a** in $CDCl_3$ solution



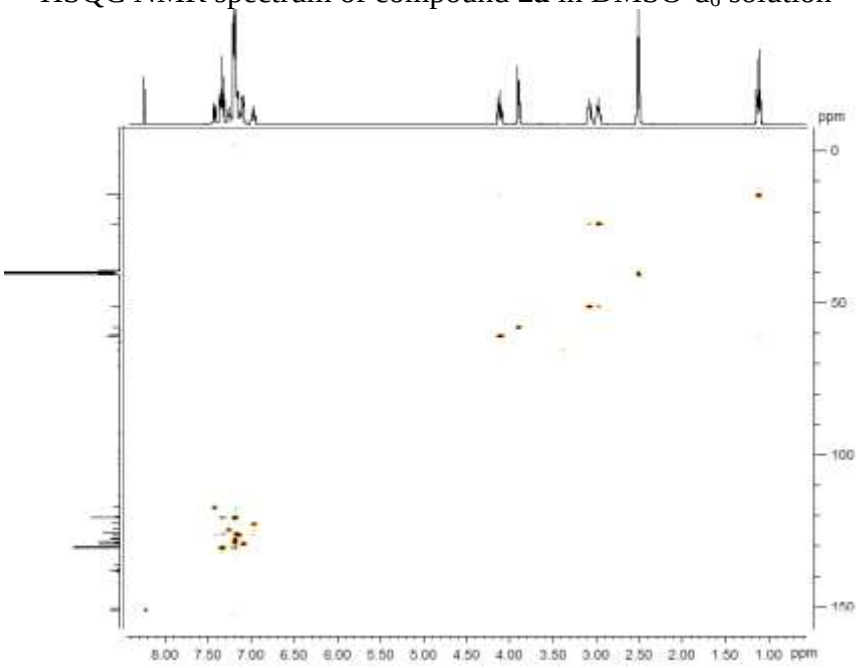
^{1}H NMR spectrum of compound **2a** in DMSO-d_6 solution



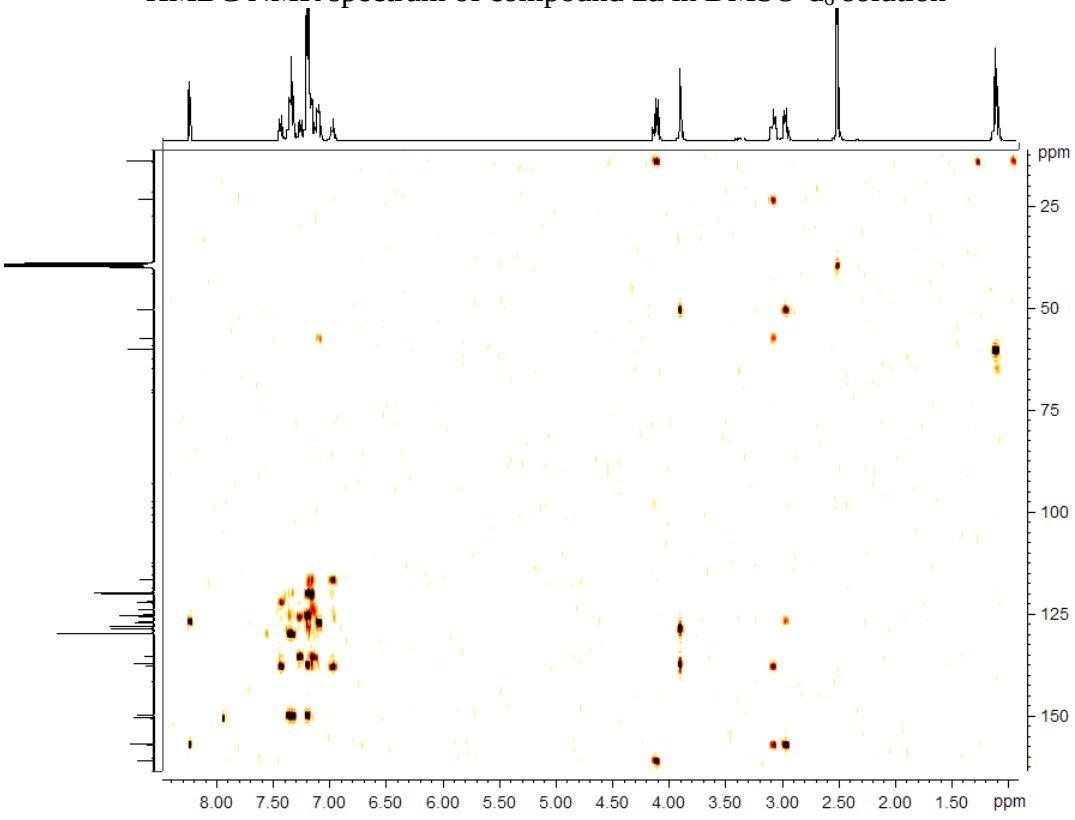
^{13}C NMR spectrum of compound **2a** in DMSO-d_6 solution



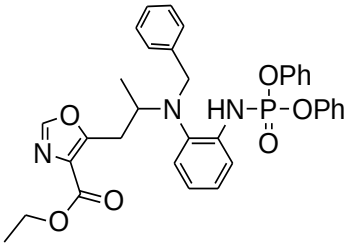
HSQC NMR spectrum of compound **2a** in DMSO-d_6 solution



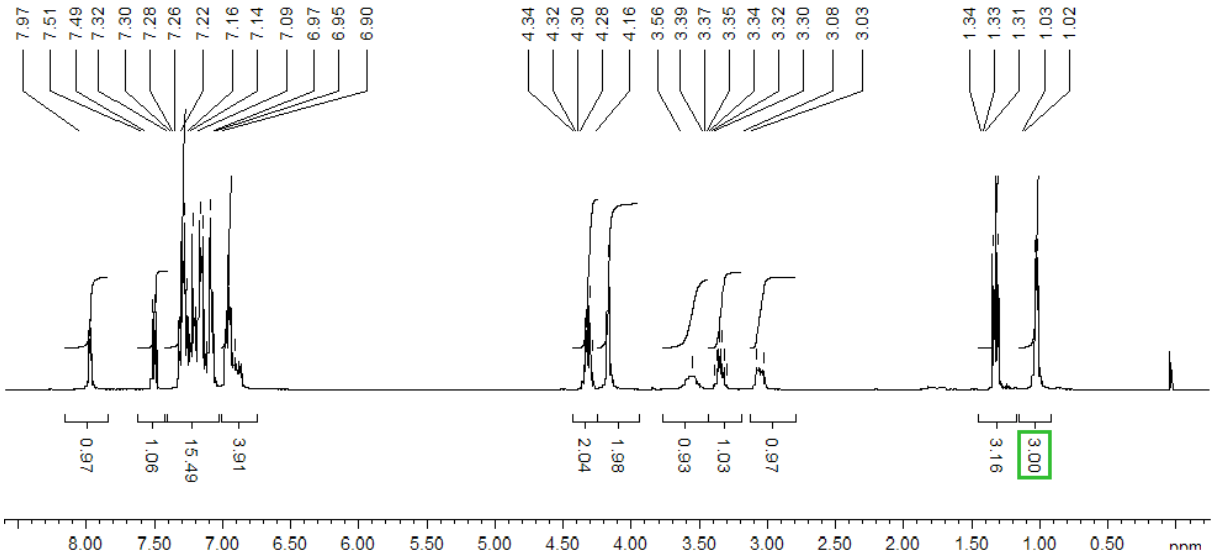
HMBC NMR spectrum of compound **2a** in DMSO-d_6 solution



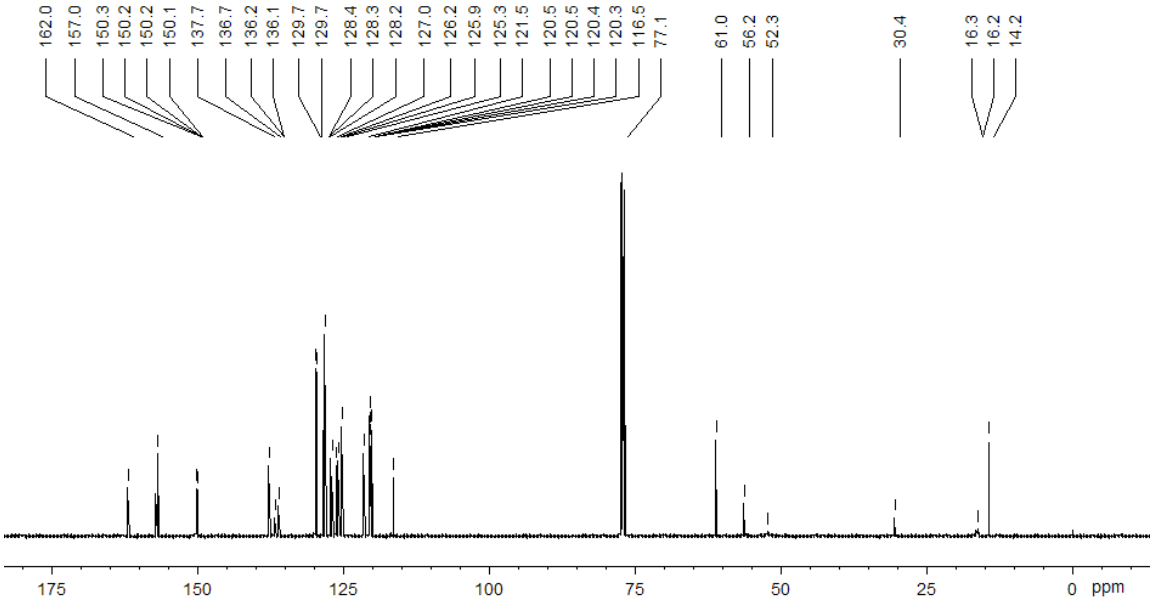
Ethyl 5-[2-(benzyl{2-[(diphenoxyphosphoryl)amino]phenyl}amino)propyl]-1,3-oxazole-4-carboxylate (2b).



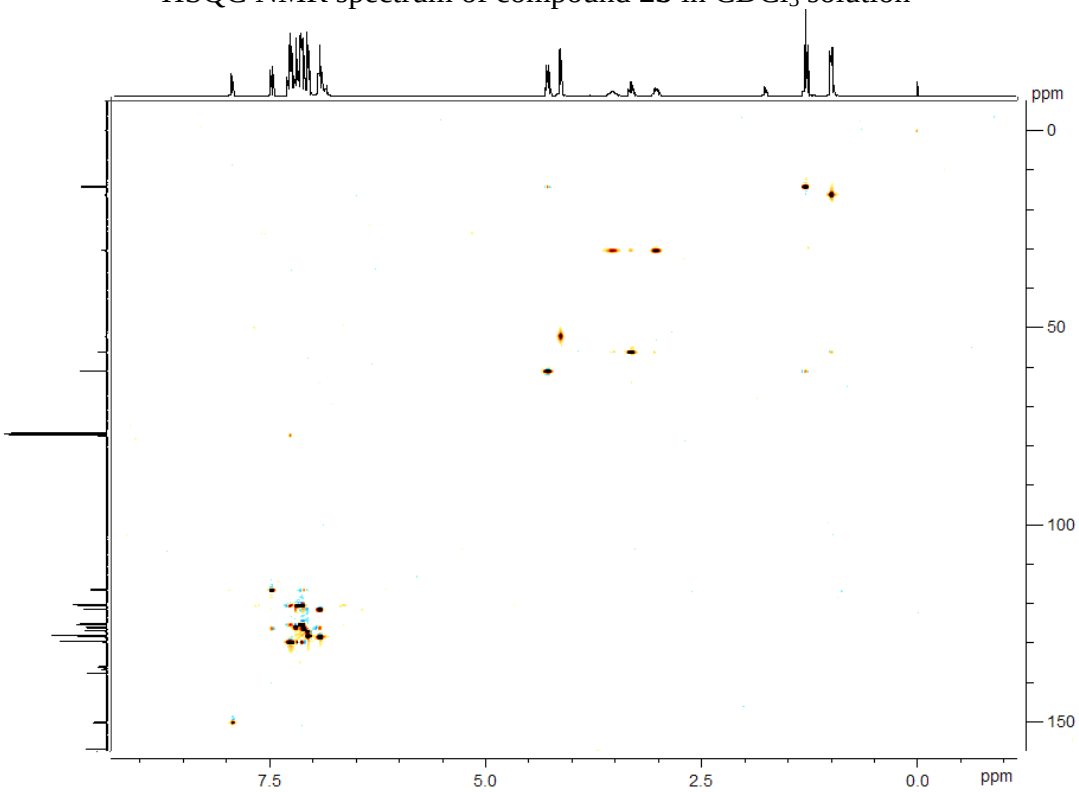
^{1}H NMR spectrum of compound **2b** in $CDCl_3$ solution



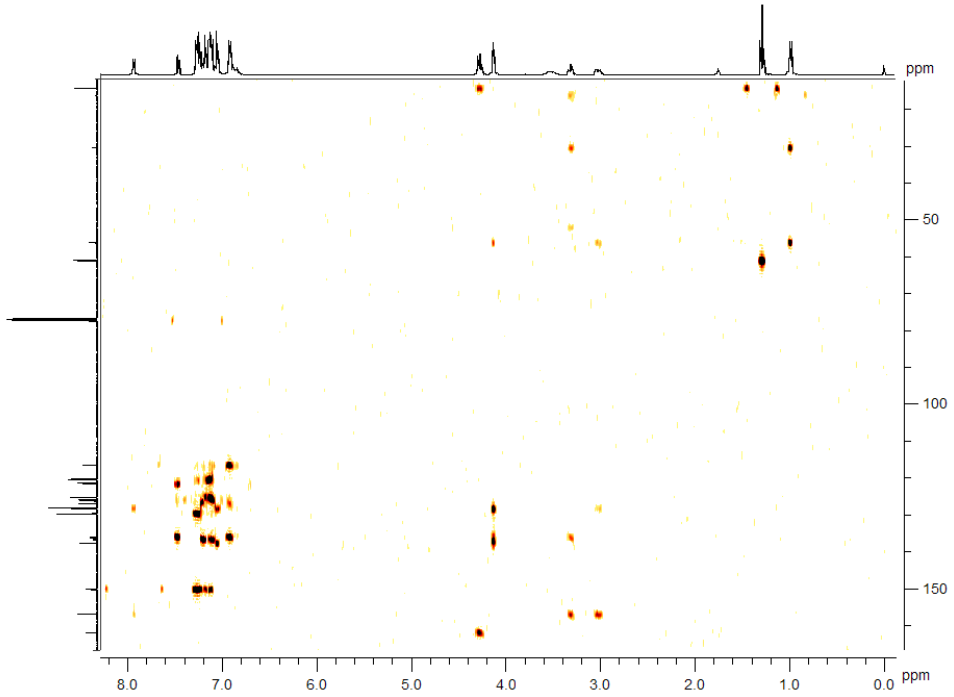
^{13}C NMR spectrum of compound **2b** in $CDCl_3$ solution



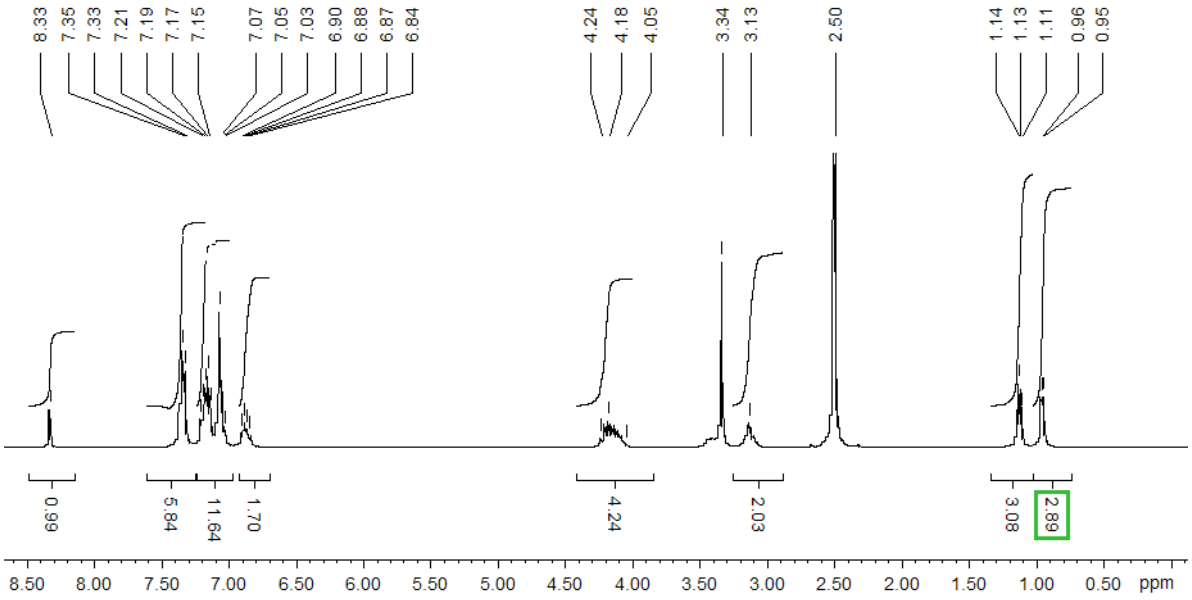
HSQC NMR spectrum of compound **2b** in $CDCl_3$ solution



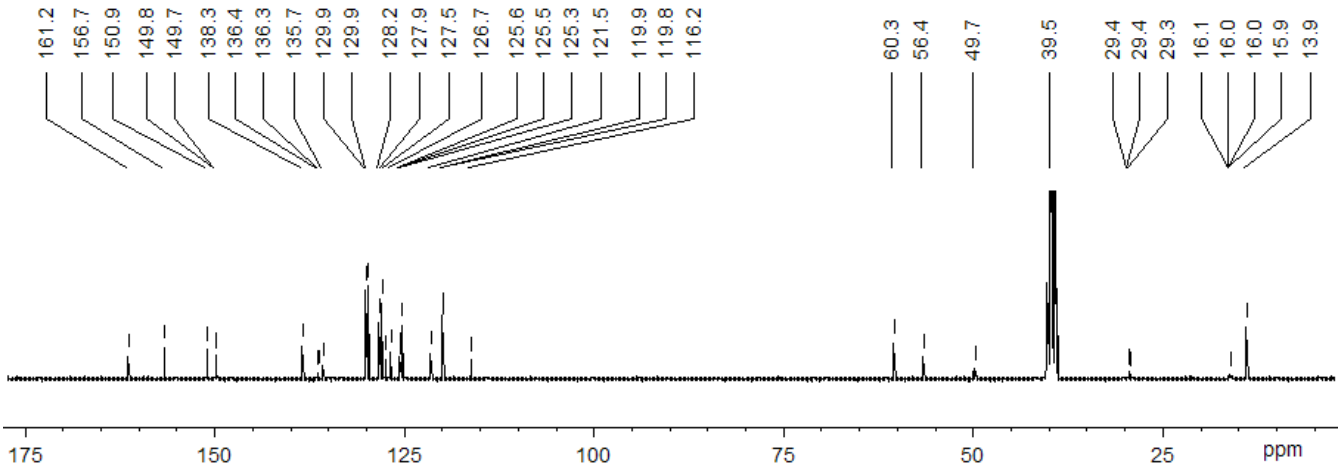
HMBC NMR spectrum of compound **2b** in $CDCl_3$ solution



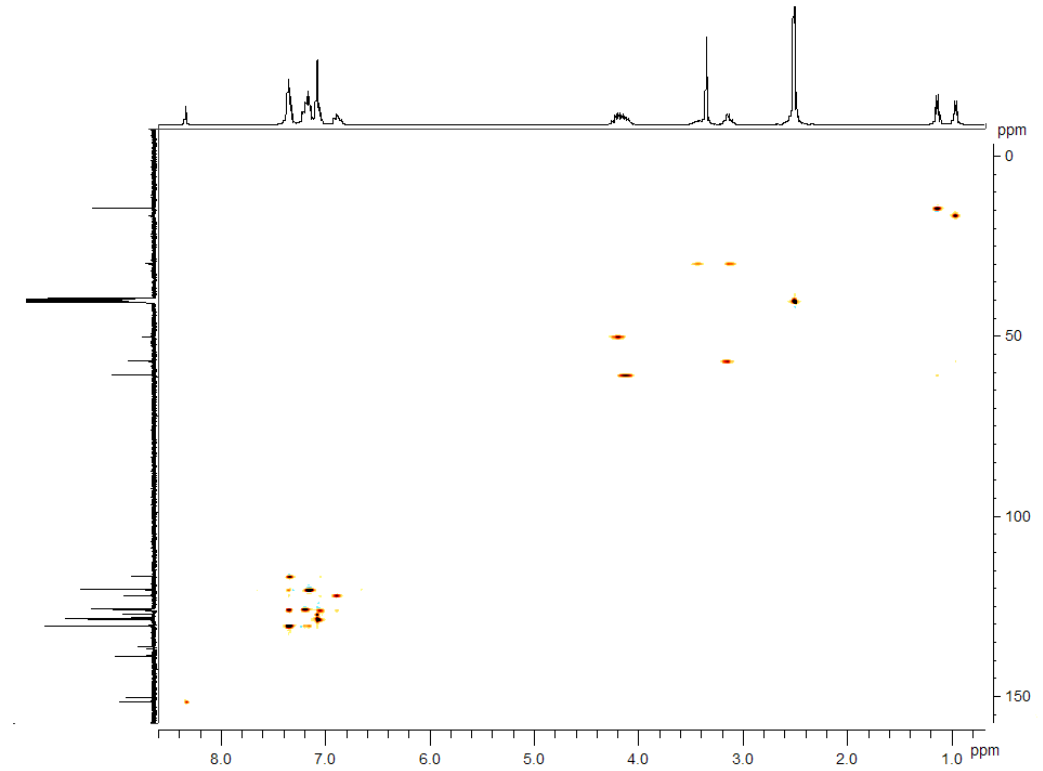
^{1}H NMR spectrum of compound **2b** in DMSO-d_6 solution



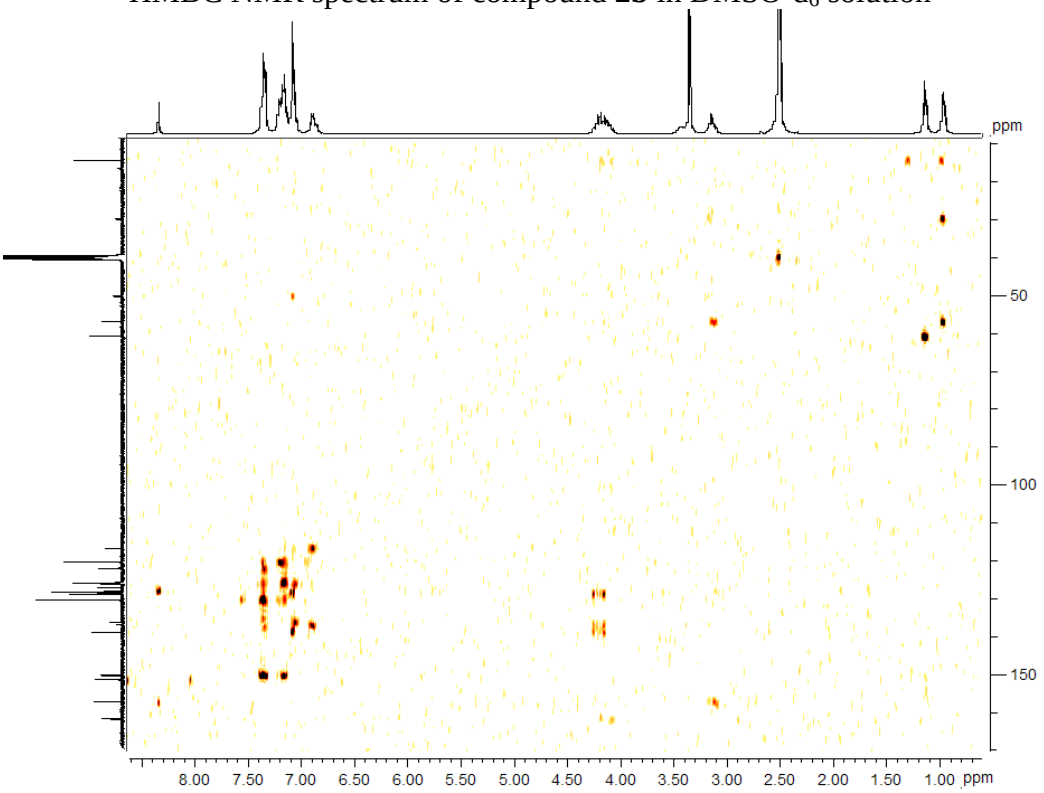
^{13}C NMR spectrum of compound **2b** in DMSO-d_6 solution



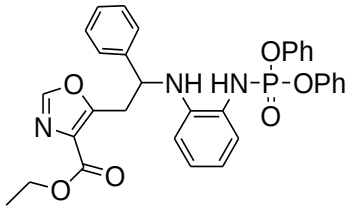
HSQC NMR spectrum of compound **2b** in DMSO-d_6 solution



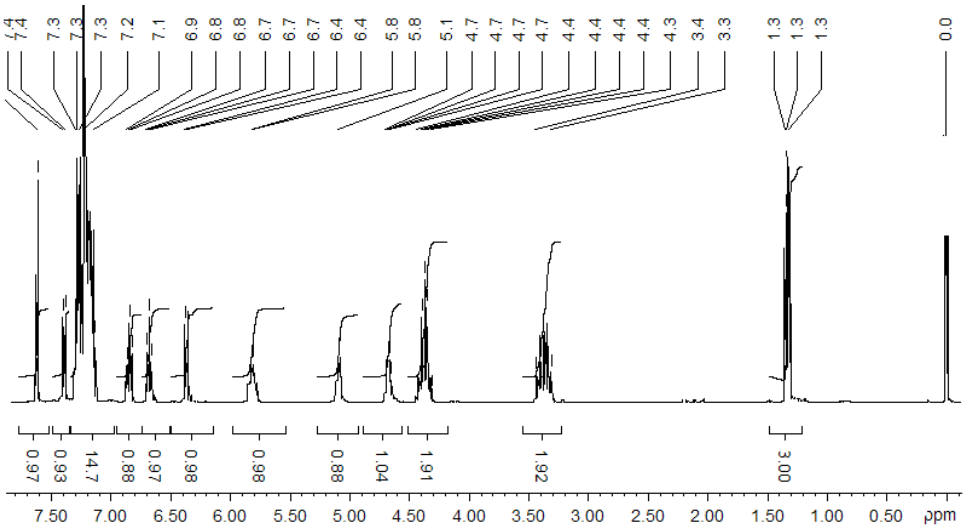
HMBC NMR spectrum of compound **2b** in DMSO-d_6 solution



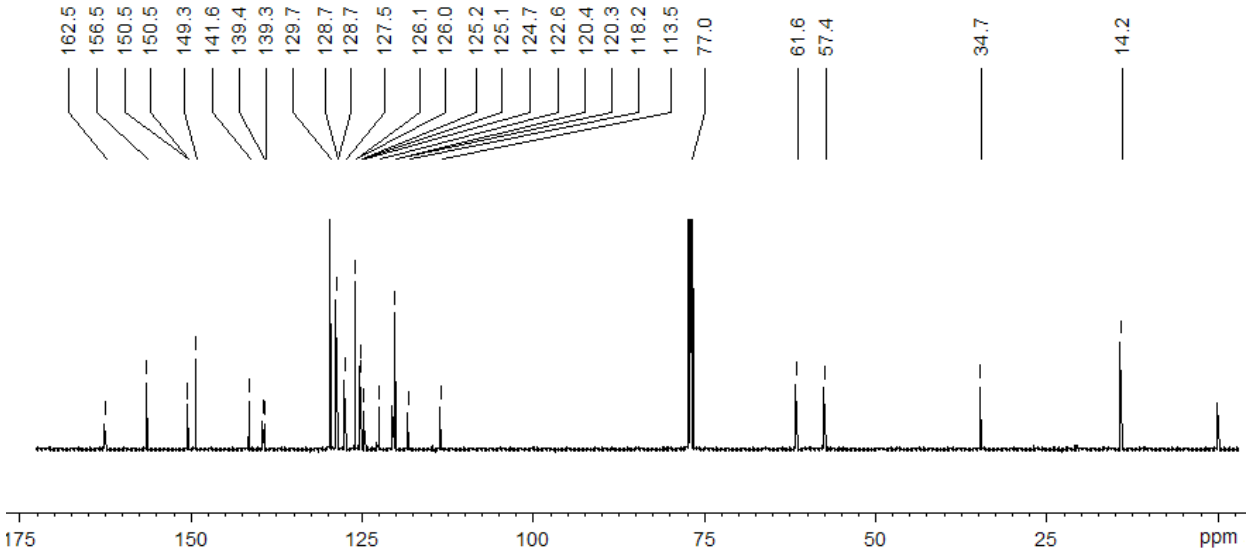
Ethyl 5-[2-({2-[(diphenoxyphosphoryl)amino]phenyl}amino)-2-phenylethyl]-1,3-oxazole-4-carboxylate (2c).



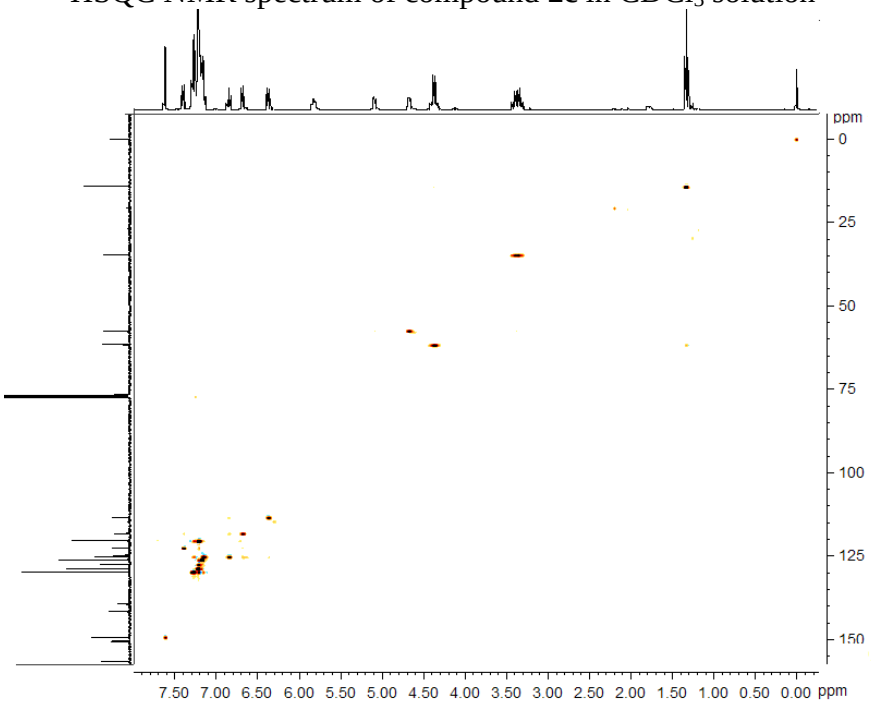
^{1}H NMR spectrum of compound **2c** in $CDCl_3$ solution



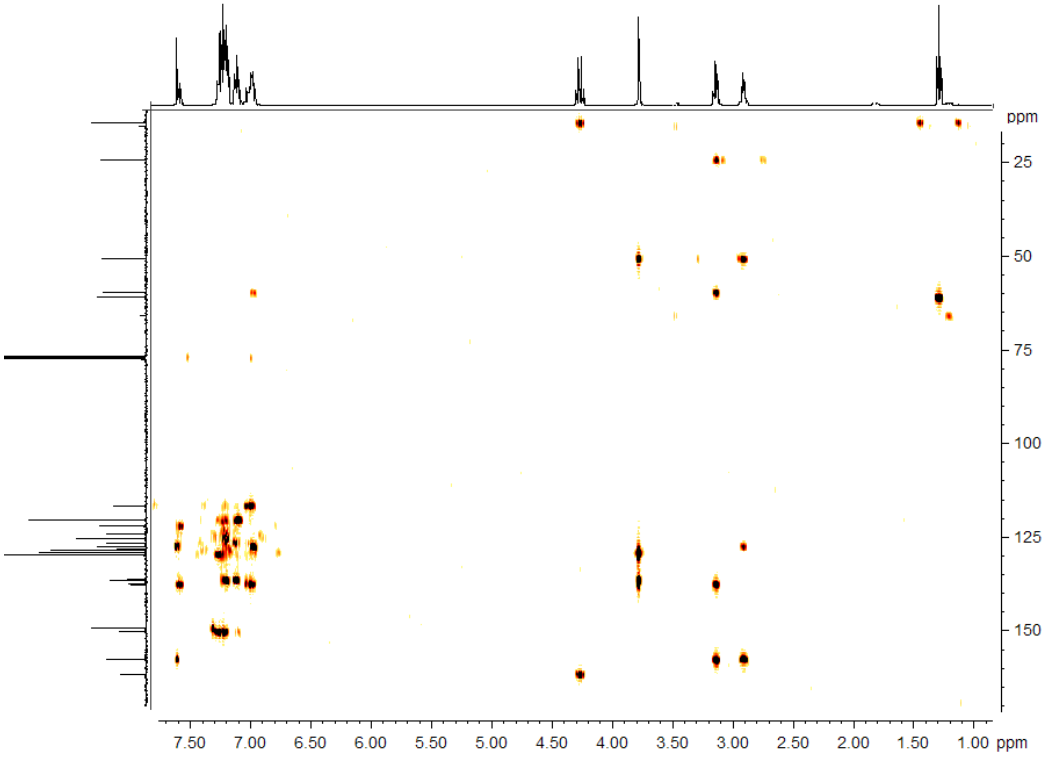
^{13}C NMR spectrum of compound **2c** in $CDCl_3$ solution



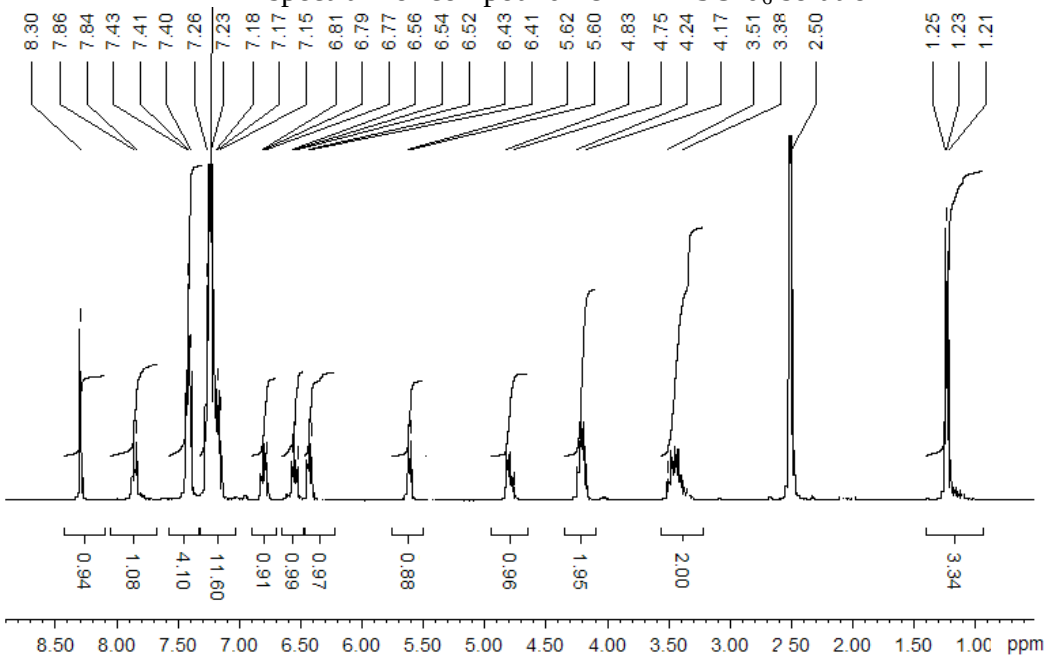
HSQC NMR spectrum of compound **2c** in $CDCl_3$ solution



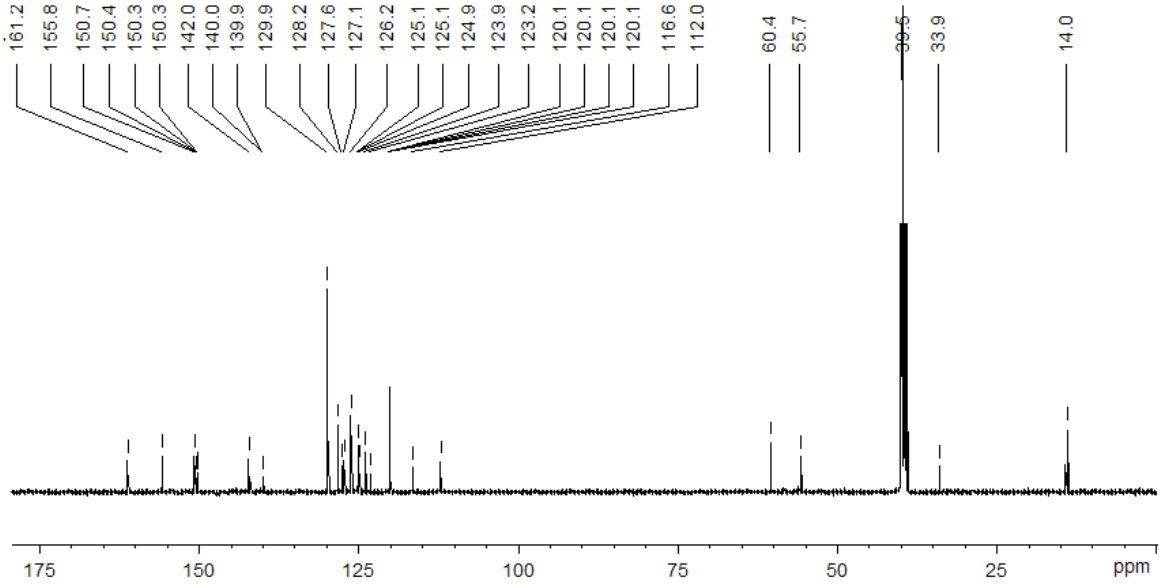
HMBC NMR spectrum of compound **2c** in $CDCl_3$ solution



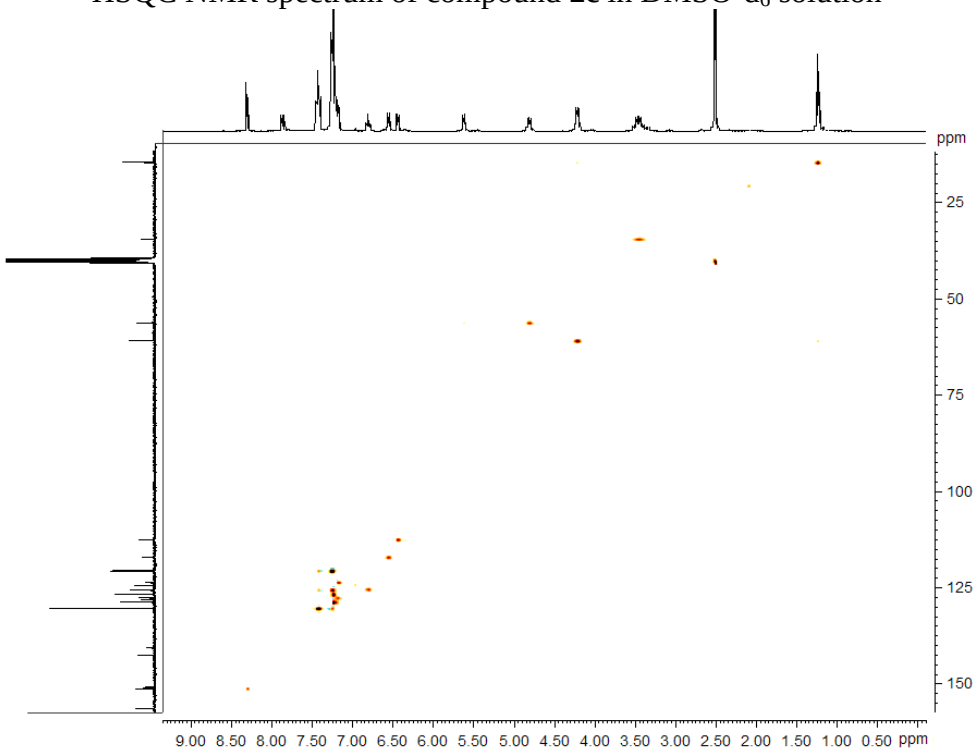
^{1}H NMR spectrum of compound **2c** in DMSO-d_6 solution



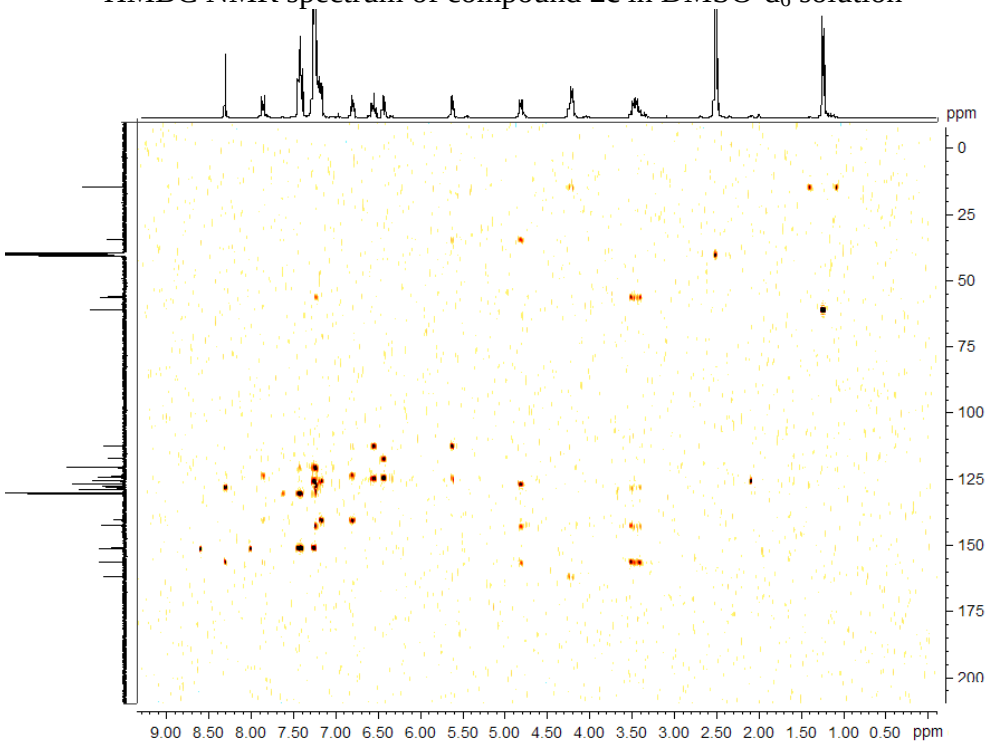
^{13}C NMR spectrum of compound **2c** in DMSO-d_6 solution



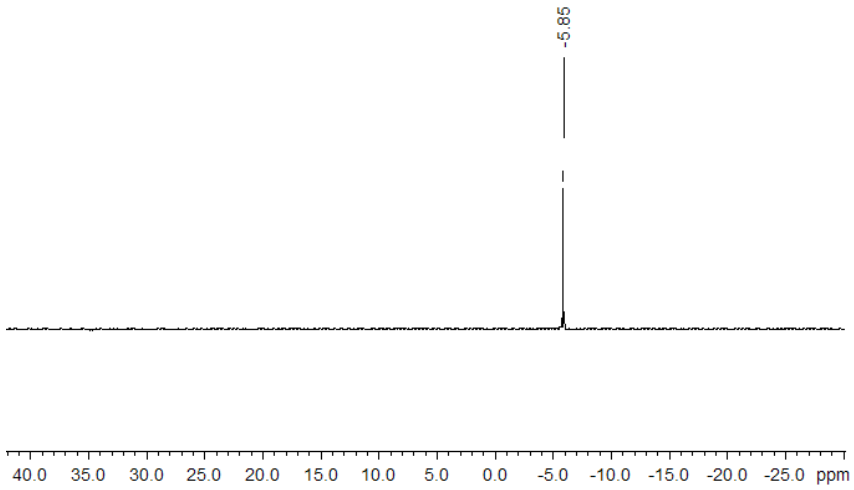
HSQC NMR spectrum of compound **2c** in DMSO-d_6 solution



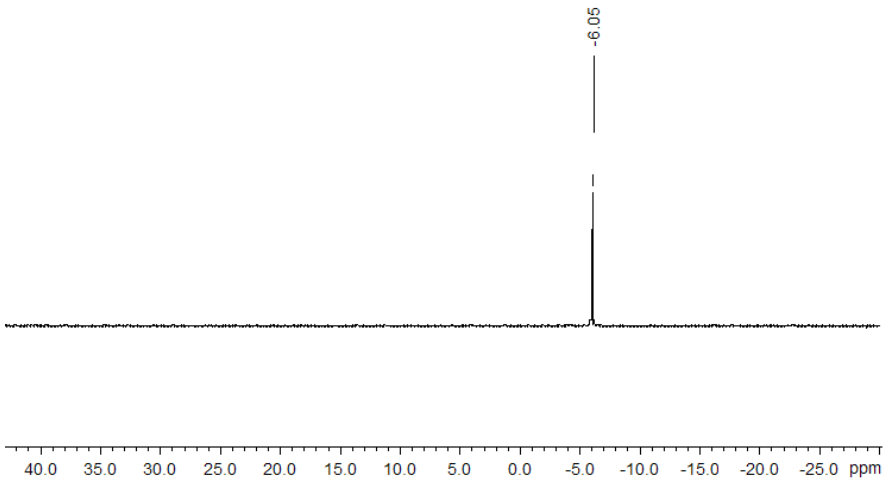
HMBC NMR spectrum of compound **2c** in DMSO-d_6 solution



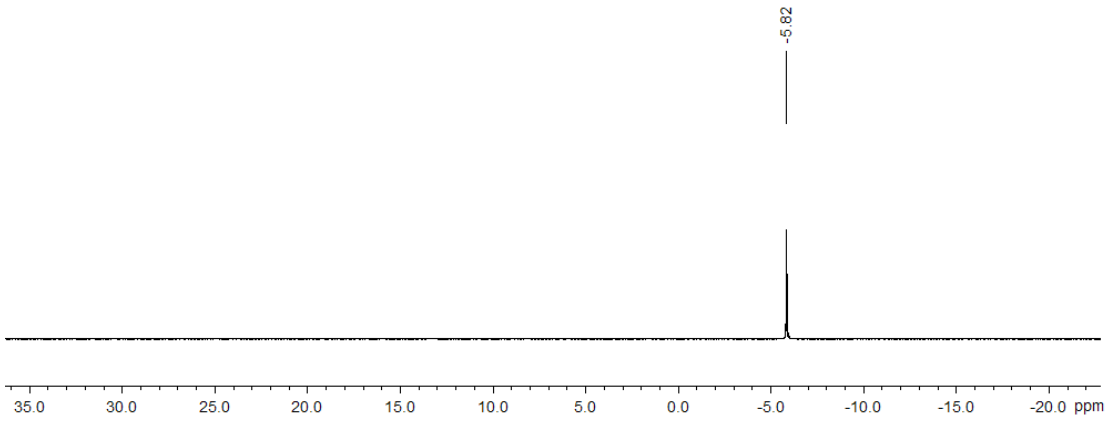
2a ^{31}P NMR



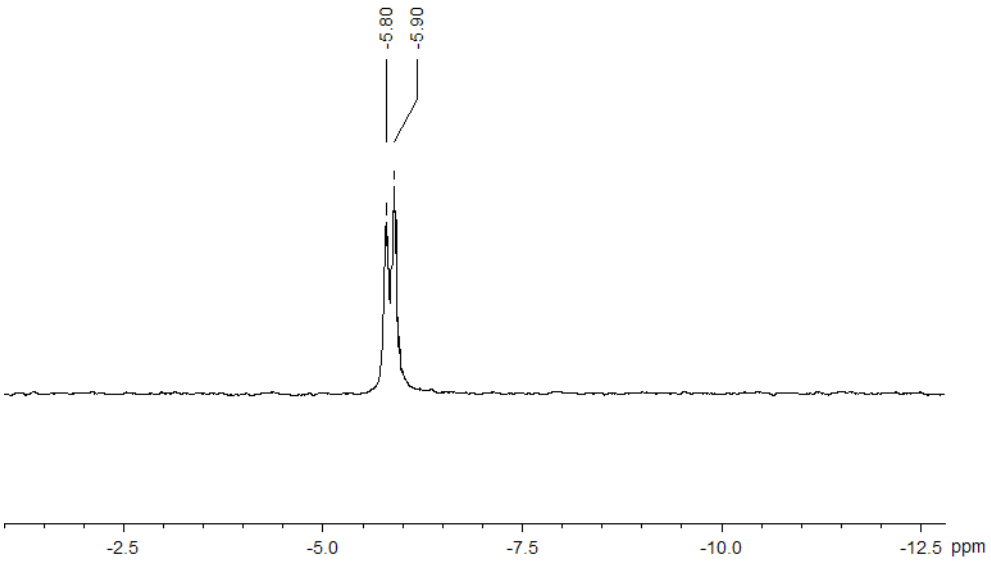
2b ^{31}P NMR



2c ^{31}P NMR



2b ^{31}P NMR (^{31}P coupling with ^{1}H)



2c IR spectrum.

10 Feb 2022

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Spectral Region	NIR-IR	***X Axis***	Wavenumber (cm-1)
Y Axis	%Transmittance	***Spectrum Range***	550.0000 - 4500.0000
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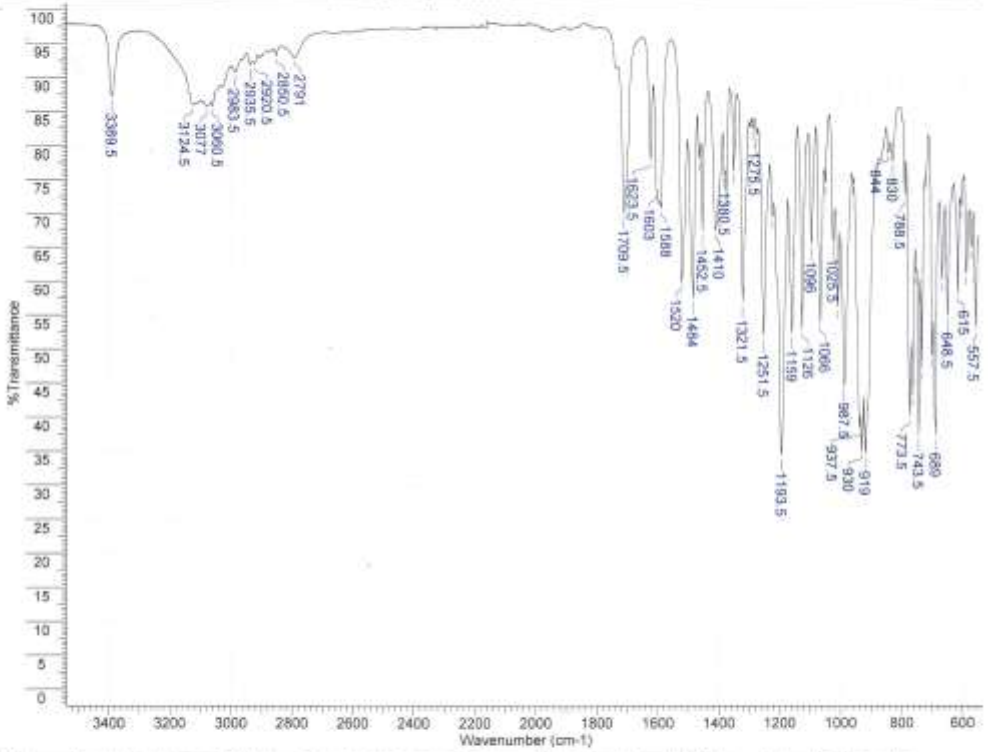

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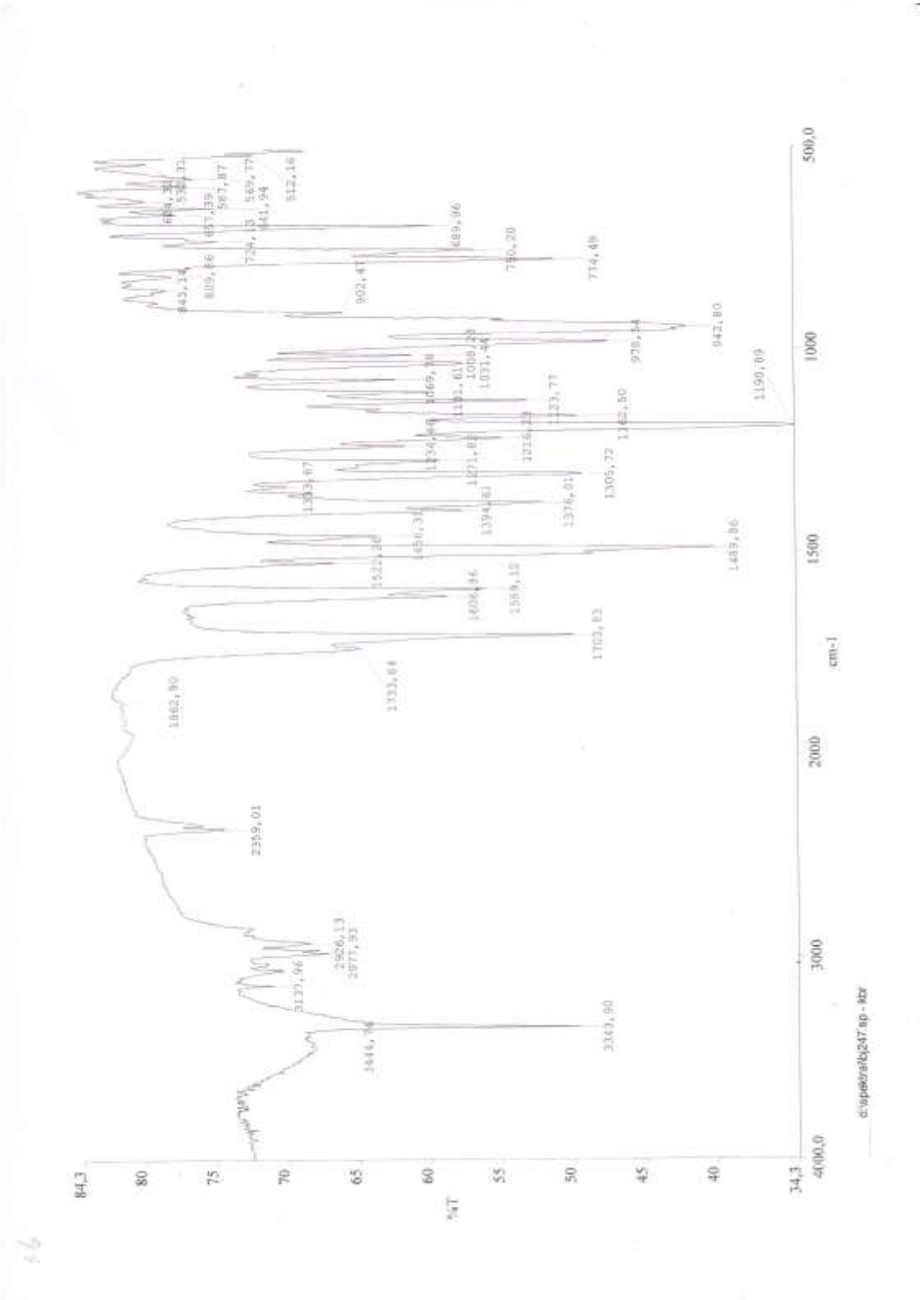
2	571.50	64.900	M
3	587.00	61.134	M
4	605.50	70.945	M
5	615.00	58.100	S
6	648.50	54.938	S
7	667.00	60.072	M
8	689.00	37.199	VS
9	699.50	49.024	S
10	720.00	75.568	M
11	733.00	47.216	S
12	743.50	37.281	VS
13	751.50	61.171	M
14	763.00	43.238	S
15	773.50	40.076	VS

No	cm-1	%T	Intensity
16	788.50	72.502	M
17	830.00	77.764	M
18	844.00	78.929	M
19	919.00	34.528	VS
20	930.00	34.991	VS
21	937.50	38.323	VS
22	959.50	74.551	M
23	987.50	44.632	S
24	1006.50	56.240	S
25	1025.50	65.864	M
26	1050.50	74.549	M
27	1066.00	53.835	S
28	1096.00	65.494	M
29	1126.00	52.913	S
30	1153.00	65.418	M

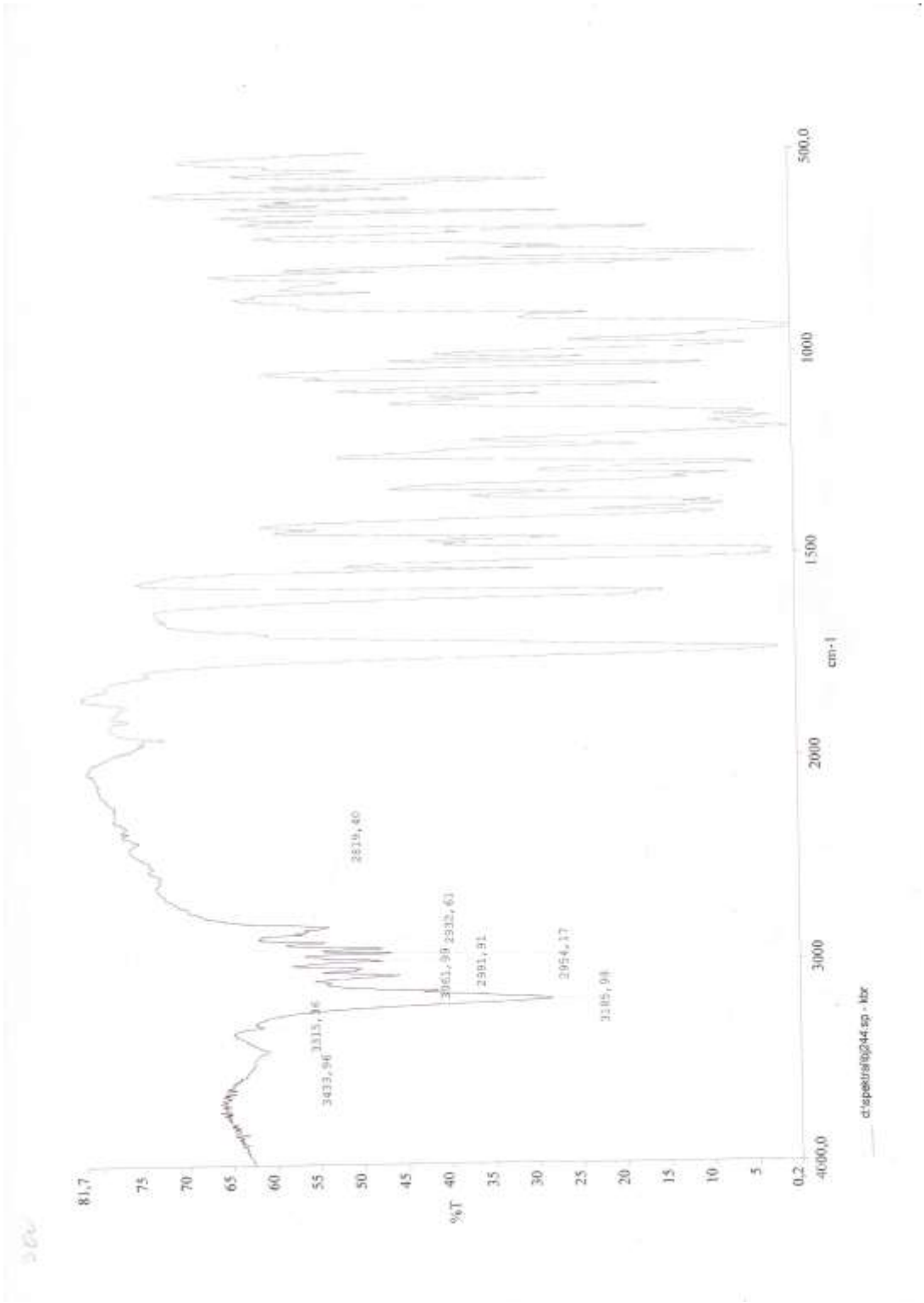
No	cm-1	%T	Intensity
31	1159.00	52.395	S
32	1193.50	34.437	VS
33	1223.00	69.494	M
34	1251.50	51.974	S
35	1275.50	81.624	W
36	1288.00	82.543	W
37	1321.50	56.934	S
38	1350.00	76.177	M
39	1374.50	73.053	M
40	1380.50	75.725	M
41	1410.00	67.520	M
42	1452.50	67.428	M
43	1463.50	78.024	M
44	1484.00	57.549	S
45	1520.00	59.936	S

No	cm-1	%T	Intensity
46	1588.00	70.728	M
47	1603.00	73.312	M
48	1623.50	78.010	M
49	1709.50	70.245	M
50	2791.00	92.931	VW
51	2850.50	93.234	VW
52	2920.50	92.042	VW
53	2935.50	91.859	W
54	2983.50	90.794	W
55	3060.50	85.758	W
56	3077.00	85.668	W
57	3124.50	85.957	W
58	3389.50	87.202	W

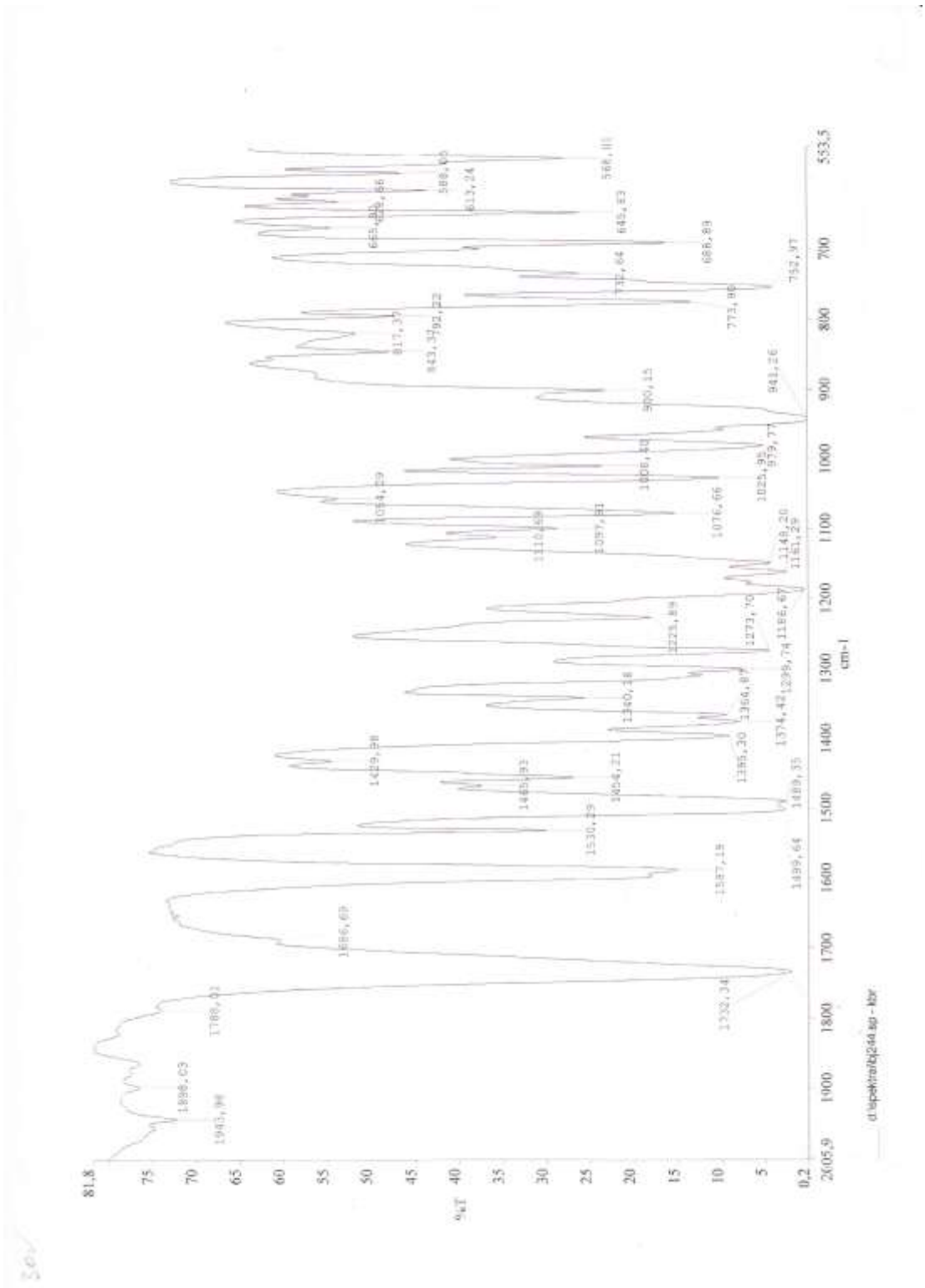
2b IR spectrum.



2a IR spectrum.



2a IR spectrum.



3b IR spectrum.

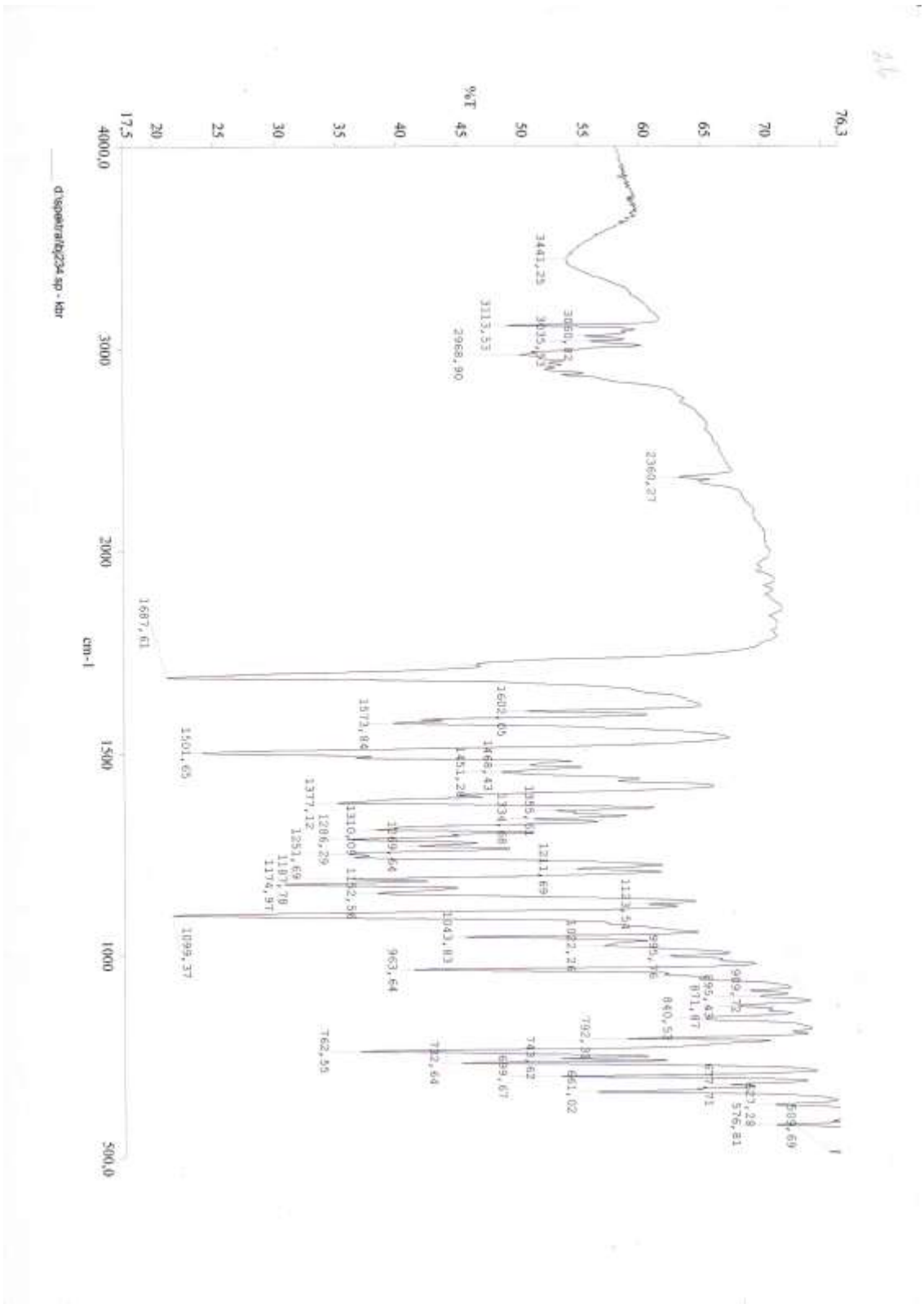
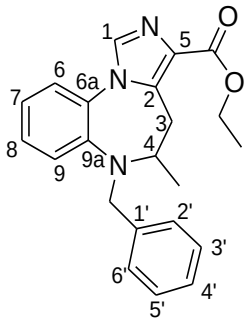


Table S1

3b

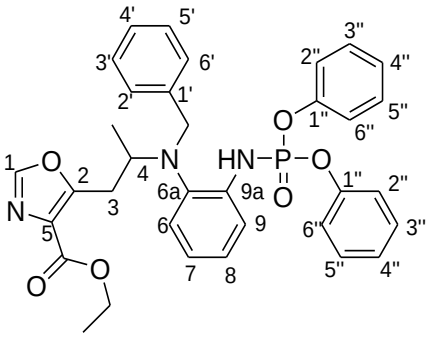


^{13}C NMR chemical shifts of compound **3b:**
calculated for S and R isomers,
experimental in $CDCl_3$, DMSO-d_6 solutions,
and their comparison

atoms or fragments	δ_{calc}, ppm			δ_{exp}, ppm		$\Delta\delta$, (δ_{exp} - δ_{calc})	
	S isomer	R isomer	average	$CDCl_3$	DMSO-d_6	$CDCl_3$	DMSO-d_6
HC(1)	138.386	138.203	138.3	134.7	135.7	-3.6	-2.6
C(2)	143.996	143.645	143.8	137.7	137.4	-6.1	-6.4
3-CH_2	31.194	29.149	30.2	30.3	30.1	0.1	-0.1
4-CH-$\underline{CH_3}$	15.237	16.328	15.8	15.6	15.7	-0.2	-0.1
4-$\underline{C}$*$\underline{H}$-CH_3	59.653	60.969	60.3	61.1	61.7	0.8	1.4
C=O	169.669	169.828	169.7	163.8	163.1	-5.9	-6.7
$OCH_2\underline{CH_3}$	14.929	15.386	15.2	14.4	14.3	-0.8	-0.9
$O\underline{CH_2}CH_3$	61.071	62.163	61.6	60.3	59.4	-1.3	-2.2
CH_2Ph	52.606	58.761	55.7	54.6	53.4	-1.1	-2.3
C(5)	138.239	139.109	138.7	128.0	127.2	-10.7	-11.5
HC(6)	138.720	141.408	140.1	125.0	124.9	-15.6	-15.2
C(6a)	150.862	144.807	147.8	140.4	139.4	-7.4	-8.4
HC(7)	130.518	129.902	130.2	128.8	128.6	-1.4	-1.6
HC(8)	130.797	130.887	130.8	123.8	123.7	-7.0	-7.1
HC(9)	125.982	124.894	125.4	122.8	123.3	2.6	-2.1
C(9a)	144.183	145.408	144.8	132.0	131.7	-12.8	-13.1
C(1□)	146.497	145.618	146.1	138.0	138.4	-8.1	-7.7
HC(2□,6□)	134.487 / 133.789	135.114 / 134.278	134.8 134.1	127.6	127.3	-7.2 -6.4	-7.5 -6.7
HC(3□,5□)	132.277 / 132.070	132.200 / 132.200	132.2 132.1	128.4	128.1	-3.8 -3.7	-4.1 -4.0
HC(4□)	131.078	131.426	131.3	127.0	126.6	-4.3	-4.7

Table S2

2b



^{13}C NMR chemical shifts of compound **2b:**
calculated for S and R isomers,
experimental in $CDCl_3$, DMSO-d_6 solutions,
and their comparison

atoms or fragments	δ_{calc}			δ_{exp}		$\nabla\ \delta$, (δ_{exp} -δ_{calc})	
	S isomer	R isomer	average	$CDCl_3$	DMSO-d6	$CDCl_3$	DMSO-d6
1	2	3	4	5	6	7	8
HC(1)	156.770	152.271	154.5	150.1	150.9	-4.4	-3.6
C(2)	162.728	165.332	164.0	157.0	156.7	-7.0	-7.3
3-CH_2	32.931	30.561	31.7	30.4	29.4	-1.3	-2.3
4-CH-$\underline{CH_3}$	13.571	17.723	15.6	16.2	16.0	0.6	0.4
4-$\underline{C*H}$-CH_3	59.967	61.987	60.9	56.2	56.4	-4.8	-4.6
C=O	165.913	165.850	165.9	161.9	161.3	-4.0	-4.6
$OCH_2\underline{CH_3}$	14.385	13.941	14.2	14.2	13.9	0.0	-0.3
$O\underline{CH_2}CH_3$	62.098	61.770	61.9	61.0	61.6	-0.9	-0.3
CH_2Ph	54.452	55.537	55.0	52.3	49.7	-2.7	-5.3
C(5)	136.048	135.643	135.8	128.3	127.5	-7.5	-8.3
HC(6)	130.364	129.842	130.1	125.9, or 126.2	125.6	-4.2 or -3.9	-4.5
C(6a)	141.065	142.112	141.6	136.1	136.3	-5.5	-5.3
HC(7)	122.871	123.118	123.0	121.5	121.5	-1.5	-1.5
HC(8)	129.245	129.069	129.2	125.9, or 126.2	125.5	-3.3 or -3.0	-3.7
HC(9)	120.555	120.526	120.5	116.5	116.2	-4.0	-4.3
C(9a)	143.208	142.966	143.1	136.7	135.7	-6.4	-7.4
C(1′)	144.167	144.940	144.5	137.6	138.3	-7.0	-6.3
HC(2′,6′)	132.740 132.739	131.486 134.038	132.1 133.4	128.2	127.9	-3.9 -5.2	-4.2 -5.5
HC(3′,5′)	131.145 132.826	132.087 131.477	131.6 132.7	128.4	128.2	-3.2 -4.3	-3.4 -4.5
HC(4′)	130.436	130.869	130.7	127.0	126.7	-3.7	-4.0
P-O-C(1″)	157.066	157.186	157.7	150.2	149.8	-7.5	-7.9
P-O-C(1″)	157.541	157.872	157.7	150.3	149.8	-7.4	-7.9

P-O-C(3″)	133.334 133.334	132.557 132.953	132.9 133.1	120.3, 120.5	119.8 or 119.9	-12.6 -12.6	-13.1 -13.2
P-O-C(2″)	127.090 128.900	127.077 128.2041	127.1 128.6	120.3, 120.5	119.8 or 119.9	-6.8 -8.1	-7.3 -8.7
P-O-C(6″)	125.770 126.014	125.582 125.811	125.7 125.9	120.3, 120.5	119.8, 119.9	-5.4 -5.4	-5,9 -6.0
P-O-C(5″)	132.826 133.741	132.181 132.476	132.5 133.1	129.7	129.9	-2.8 -3.4	-2.6 -3.2
P-O-C(4″)	128.684 129.593	128.123 128.631	128.4 129.1	125.3	125.3	-3.1 -3.8	-3.1 -3.8

Table S3

B3LYP /6-311+g(2d,p) calculated optimal geometry, energy (in a.u.), GIAO nuclear magnetic shielding tensors of **3b** compound S optical isomer

E =-1167.23500463 a. u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.925072	3.250711	-0.613530
2	6	0	-2.913160	1.708620	0.531435
3	6	0	-0.617755	1.973828	-0.134978
4	6	0	-2.223926	3.733954	-0.553810
5	6	0	-3.228971	2.953520	0.004551
6	6	0	-1.614881	1.201096	0.483035
7	7	0	0.708199	1.481377	-0.341058
8	6	0	1.503808	0.635343	0.414520
9	7	0	-1.337109	-0.038216	1.134875
10	6	0	-0.306775	0.094172	2.185726
11	6	0	1.140122	-0.053237	1.692982
12	6	0	1.455121	1.816426	-1.461257
13	7	0	2.631871	1.271996	-1.459926
14	6	0	2.688113	0.535532	-0.296412
15	6	0	3.856484	-0.256106	0.107491
16	8	0	4.866816	-0.168666	-0.775094
17	6	0	6.065093	-0.918403	-0.472357
18	1	0	1.048510	2.435948	-2.243241
19	6	0	-1.258311	-1.218374	0.259026
20	6	0	-2.599698	-1.624000	-0.317006
21	6	0	-5.062802	-2.429782	-1.383922
22	6	0	-3.661208	-1.968025	0.523327
23	6	0	-2.790650	-1.689445	-1.695181
24	6	0	-4.013857	-2.089712	-2.228626
25	6	0	-4.882295	-2.368297	-0.003441
26	6	0	-0.572522	-0.867820	3.345770
27	1	0	6.862774	-0.347782	-0.947546
28	1	0	6.217023	-0.925330	0.606512
29	1	0	1.382248	-1.111888	1.565539
30	1	0	1.821775	0.281336	2.480590
31	1	0	-0.437707	1.107240	2.574100
32	1	0	-0.139838	3.871923	-1.023242
33	1	0	-2.442858	4.724690	-0.932637
34	1	0	-4.246113	3.321990	0.055199
35	1	0	-3.669990	1.099595	1.007773
36	1	0	-0.546193	-1.081065	-0.566272
37	1	0	-0.874424	-2.041839	0.865298

38	1	0	0.162774	-0.717677	4.139746
39	1	0	-0.502634	-1.911993	3.031500
40	1	0	-1.568144	-0.699716	3.758056
41	1	0	-3.525816	-1.913486	1.597592
42	1	0	-5.695186	-2.636190	0.661636
43	1	0	-6.015598	-2.741432	-1.795244
44	1	0	-4.145250	-2.131491	-3.303523
45	1	0	-1.975788	-1.423006	-2.359748
46	8	0	3.904376	-0.913913	1.129938
47	6	0	5.990045	-2.328650	-1.028818
48	1	0	6.938240	-2.844080	-0.854174
49	1	0	5.802420	-2.311185	-2.104019
50	1	0	5.198087	-2.898126	-0.541041

Calculated GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 56.4833 Anisotropy = 155.6956
XX= 14.6704 YX= -36.5134 ZX= 42.1934
XY= -18.8457 YY= 24.5156 ZY= 60.0336
XZ= 52.0059 YZ= 45.7146 ZZ= 130.2638
Eigenvalues: -37.9210 47.0904 160.2804
2 C Isotropic = 43.7452 Anisotropy = 163.5807
XX= -4.9871 YX= -21.3685 ZX= 42.7541
XY= -22.0090 YY= 31.2810 ZY= 67.8142
XZ= 63.7931 YZ= 65.8397 ZZ= 104.9418
Eigenvalues: -55.4177 33.8544 152.7990
3 C Isotropic = 38.2823 Anisotropy = 132.1390
XX= -34.4784 YX= 35.0053 ZX= 32.4559
XY= 45.3290 YY= 40.5573 ZY= 22.9390
XZ= 18.7890 YZ= 28.2979 ZZ= 108.7679
Eigenvalues: -53.0899 41.5618 126.3749
4 C Isotropic = 51.6684 Anisotropy = 180.7800
XX= 39.6839 YX= 27.9356 ZX= 14.8922
XY= 28.8852 YY= -22.0099 ZY= 78.1298
XZ= 14.1347 YZ= 73.8597 ZZ= 137.3311
Eigenvalues: -57.1128 39.9295 172.1884
5 C Isotropic = 51.9478 Anisotropy = 179.3235
XX= -42.0174 YX= 42.0817 ZX= 26.3411
XY= 42.4025 YY= 54.4179 ZY= 44.8233
XZ= 23.8492 YZ= 49.7341 ZZ= 143.4428
Eigenvalues: -58.1648 42.5113 171.4967
6 C Isotropic = 31.6041 Anisotropy = 151.7073
XX= 11.0530 YX= 18.3682 ZX= 20.8666
XY= 14.9733 YY= -13.5645 ZY= 74.1311
XZ= 24.9352 YZ= 53.4655 ZZ= 97.3238
Eigenvalues: -43.2899 5.3599 132.7423

```
  7  N    Isotropic =    40.4932   Anisotropy =   139.1357
XX=   -22.9072   YX=    70.8175   ZX=    13.3944
XY=    41.8935   YY=    88.1277   ZY=    37.1384
XZ=    24.2864   YZ=    35.3295   ZZ=    56.2592
Eigenvalues:   -46.6223    34.8516   133.2504
  8  C    Isotropic =    38.4695   Anisotropy =   132.4037
XX=    36.6129   YX=    45.2028   ZX=    -3.5964
XY=    47.4798   YY=    61.8362   ZY=    66.8115
XZ=     5.9735   YZ=    66.2567   ZZ=    16.9594
Eigenvalues:   -40.8531    29.5230   126.7387
  9  N    Isotropic =   166.1845   Anisotropy =    35.2491
XX=   157.3609   YX=   -19.1614   ZX=    14.6885
XY=    11.9778   YY=   161.8289   ZY=    10.2493
XZ=    21.5797   YZ=    -2.2078   ZZ=   179.3637
Eigenvalues:   145.5464   163.3233   189.6840
  10  C    Isotropic =   122.8122   Anisotropy =    52.7141
XX=   128.2324   YX=    10.1278   ZX=    27.2830
XY=     9.9844   YY=   105.3297   ZY=    -4.1037
XZ=    23.5385   YZ=     3.2485   ZZ=   134.8744
Eigenvalues:    97.4297   113.0519   157.9549
  11  C    Isotropic =   151.2716   Anisotropy =    32.6288
XX=   155.3046   YX=     5.3680   ZX=   -16.1342
XY=     4.6969   YY=   134.6313   ZY=    -5.3430
XZ=   -11.0122   YZ=    -8.6136   ZZ=   145.8790
Eigenvalues:   131.1554   137.6354   167.0242
  12  C    Isotropic =    44.0793   Anisotropy =    77.8941
XX=    74.2295   YX=     9.0562   ZX=     0.1274
XY=    11.1285   YY=    63.5789   ZY=    48.0576
XZ=    22.6978   YZ=    44.3829   ZZ=    -5.5706
Eigenvalues:   -29.0353    65.2645    96.0087
  13  N    Isotropic =   -44.4364   Anisotropy =   416.5511
XX=   -93.2956   YX=   150.1844   ZX=    -0.0274
XY=   155.2013   YY=    56.6858   ZY=   177.4738
XZ=    21.6515   YZ=   184.8059   ZZ=   -96.6996
Eigenvalues:  -261.2456  -105.3280   233.2643
  14  C    Isotropic =    44.2264   Anisotropy =    88.9943
XX=    28.2581   YX=    35.2869   ZX=    -2.5464
XY=    40.5629   YY=    59.6677   ZY=    42.6872
XZ=   -11.9613   YZ=    40.5197   ZZ=    44.7535
Eigenvalues:   -14.2242    43.3475   103.5559
  15  C    Isotropic =    12.7968   Anisotropy =    84.8064
XX=   -56.7339   YX=    44.7116   ZX=    20.9576
XY=    32.9002   YY=    47.6162   ZY=    10.4520
XZ=    44.4567   YZ=    -7.7507   ZZ=    47.5079
Eigenvalues:   -77.1647    46.2206    69.3344
  16  O    Isotropic =   110.9227   Anisotropy =   159.0478
```

XX= 105.8259 YX= 39.6891 ZX= -15.8227
XY= 102.1067 YY= 123.6026 ZY= 74.8817
XZ= -112.0374 YZ= 128.3037 ZZ= 103.3397
Eigenvalues: -47.5669 163.3806 216.9546
17 C Isotropic = 121.3948 Anisotropy = 65.4209
XX= 148.7700 YX= -21.8389 ZX= 17.0802
XY= -22.8411 YY= 126.7072 ZY= 2.8662
XZ= 13.6658 YZ= 8.3988 ZZ= 85.7070
Eigenvalues: 79.4928 117.6828 164.0087
18 H Isotropic = 24.2528 Anisotropy = 6.3101
XX= 25.0524 YX= -2.2890 ZX= -0.9115
XY= -1.9191 YY= 22.3142 ZY= -1.7876
XZ= -5.5468 YZ= -2.5749 ZZ= 25.3919
Eigenvalues: 19.1184 25.1806 28.4596
19 C Isotropic = 129.8601 Anisotropy = 27.7250
XX= 140.1084 YX= 12.1431 ZX= -3.9321
XY= 7.9706 YY= 128.8265 ZY= 14.5711
XZ= 1.3280 YZ= 19.5090 ZZ= 123.6455
Eigenvalues: 107.2021 136.0348 149.3435
20 C Isotropic = 35.9684 Anisotropy = 199.0791
XX= -30.6470 YX= -62.4970 ZX= -31.5353
XY= -69.6357 YY= 146.0759 ZY= 5.2710
XZ= -22.6680 YZ= -1.0184 ZZ= -7.5236
Eigenvalues: -63.8483 3.0657 168.6878
21 C Isotropic = 51.3876 Anisotropy = 183.3218
XX= -22.0805 YX= -63.2152 ZX= -34.6595
XY= -64.6465 YY= 152.7129 ZY= -13.0407
XZ= -33.1147 YZ= -10.3161 ZZ= 23.5302
Eigenvalues: -58.6051 39.1657 173.6021
22 C Isotropic = 47.9778 Anisotropy = 184.9693
XX= 46.1381 YX= -41.1118 ZX= -9.9757
XY= -37.3872 YY= 158.9613 ZY= -2.8164
XZ= -14.4426 YZ= -9.1657 ZZ= -61.1661
Eigenvalues: -63.0495 35.6921 171.2907
23 C Isotropic = 48.6763 Anisotropy = 165.6027
XX= -2.9653 YX= -51.7999 ZX= 46.3823
XY= -48.7041 YY= 143.2405 ZY= 23.6364
XZ= 51.0819 YZ= 18.4517 ZZ= 5.7537
Eigenvalues: -60.6293 47.5801 159.0781
24 C Isotropic = 50.3954 Anisotropy = 181.6487
XX= 51.0266 YX= -38.5530 ZX= -14.1935
XY= -38.3759 YY= 159.2001 ZY= -2.1137
XZ= -13.4896 YZ= -3.2716 ZZ= -59.0406
Eigenvalues: -61.0182 40.7098 171.4945
25 C Isotropic = 50.1881 Anisotropy = 183.5307
XX= -2.9674 YX= -57.2682 ZX= 46.8573

XY= -58.1088 YY= 153.5678 ZY= 18.1285
XZ= 48.3932 YZ= 15.9820 ZZ= -0.0361
Eigenvalues: -62.7270 40.7495 172.5419
26 C Isotropic = 167.2289 Anisotropy = 38.2888
XX= 163.7802 YX= 4.8795 ZX= -5.3465
XY= 3.4588 YY= 149.4293 ZY= -23.5093
XZ= -11.2046 YZ= -17.5891 ZZ= 170.4773
Eigenvalues: 136.8430 160.0890 186.7548
27 H Isotropic = 28.1281 Anisotropy = 7.4949
XX= 32.2687 YX= 1.8761 ZX= -2.0730
XY= 1.4286 YY= 28.8974 ZY= -1.0644
XZ= -0.2049 YZ= -0.4417 ZZ= 23.2184
Eigenvalues: 23.0239 28.2357 33.1248
28 H Isotropic = 26.7656 Anisotropy = 4.9749
XX= 28.8048 YX= -1.9842 ZX= 2.7942
XY= -0.7741 YY= 24.2500 ZY= 1.2194
XZ= 0.9404 YZ= 1.4270 ZZ= 27.2420
Eigenvalues: 23.0465 27.1680 30.0822
29 H Isotropic = 28.0037 Anisotropy = 6.7768
XX= 31.2025 YX= -1.9910 ZX= -3.3539
XY= -1.9275 YY= 27.9261 ZY= -2.7882
XZ= -2.0695 YZ= -1.5362 ZZ= 24.8826
Eigenvalues: 22.4969 28.9926 32.5216
30 H Isotropic = 28.3772 Anisotropy = 7.5315
XX= 32.3307 YX= 1.1528 ZX= 1.5279
XY= 1.2487 YY= 22.6194 ZY= 0.8365
XZ= 1.9884 YZ= -1.3134 ZZ= 30.1814
Eigenvalues: 22.4460 29.2873 33.3981
31 H Isotropic = 28.3577 Anisotropy = 4.3794
XX= 26.4319 YX= -0.6608 ZX= 1.2980
XY= -0.6689 YY= 27.8483 ZY= 1.7225
XZ= 1.6186 YZ= -0.5421 ZZ= 30.7929
Eigenvalues: 25.6843 28.1115 31.2773
32 H Isotropic = 24.2961 Anisotropy = 8.3667
XX= 24.8476 YX= -2.5640 ZX= -0.8312
XY= -3.9857 YY= 27.6682 ZY= -2.7642
XZ= -1.1625 YZ= -0.1716 ZZ= 20.3724
Eigenvalues: 19.4887 23.5256 29.8739
33 H Isotropic = 24.5879 Anisotropy = 4.3077
XX= 27.1420 YX= -0.4638 ZX= -1.3632
XY= -0.2606 YY= 24.6008 ZY= -1.4129
XZ= -1.2626 YZ= -1.2044 ZZ= 22.0210
Eigenvalues: 21.1676 25.1365 27.4597
34 H Isotropic = 24.8390 Anisotropy = 5.7822
XX= 24.2776 YX= -0.2928 ZX= -0.9783
XY= 0.2230 YY= 27.7645 ZY= -2.2375

XZ= -0.8046 YZ= -2.5138 ZZ= 22.4750
Eigenvalues: 21.3222 24.5011 28.6938
35 H Isotropic = 24.9093 Anisotropy = 9.1808
XX= 25.5410 YX= -3.8739 ZX= -0.4841
XY= -3.3079 YY= 28.6206 ZY= 1.7084
XZ= 0.2009 YZ= -0.3103 ZZ= 20.5663
Eigenvalues: 20.4980 23.2001 31.0298
36 H Isotropic = 28.5800 Anisotropy = 5.5758
XX= 30.1308 YX= 3.6369 ZX= -2.6663
XY= 2.8279 YY= 26.7134 ZY= 2.2868
XZ= -0.8987 YZ= 5.4589 ZZ= 28.8959
Eigenvalues: 22.1109 31.3319 32.2972
37 H Isotropic = 27.6805 Anisotropy = 2.6286
XX= 27.7637 YX= 1.1863 ZX= 2.5707
XY= -0.9157 YY= 29.3583 ZY= -2.3947
XZ= 2.0064 YZ= 1.7141 ZZ= 25.9197
Eigenvalues: 24.3488 29.2598 29.4330
38 H Isotropic = 30.6601 Anisotropy = 9.9938
XX= 30.3440 YX= 0.6301 ZX= 3.1603
XY= 0.0664 YY= 25.9926 ZY= -1.8219
XZ= 3.1335 YZ= -1.9210 ZZ= 35.6438
Eigenvalues: 25.4325 29.2253 37.3227
39 H Isotropic = 30.4017 Anisotropy = 5.3198
XX= 28.2825 YX= 0.4271 ZX= 0.2368
XY= -0.1734 YY= 32.8406 ZY= -1.6186
XZ= 0.1640 YZ= -2.5201 ZZ= 30.0821
Eigenvalues: 28.2093 29.0476 33.9483
40 H Isotropic = 30.4023 Anisotropy = 9.7520
XX= 32.8107 YX= -1.0210 ZX= -3.5939
XY= 0.8560 YY= 26.1107 ZY= -0.7780
XZ= -4.9872 YZ= -1.6739 ZZ= 32.2855
Eigenvalues: 25.7022 28.6011 36.9036
41 H Isotropic = 23.8827 Anisotropy = 10.6472
XX= 29.3209 YX= 3.7634 ZX= -1.1139
XY= 3.9024 YY= 21.9107 ZY= -0.8737
XZ= 0.3095 YZ= -0.3015 ZZ= 20.4165
Eigenvalues: 19.9472 20.7200 30.9808
42 H Isotropic = 24.2848 Anisotropy = 5.7785
XX= 25.6588 YX= 1.8626 ZX= 1.8715
XY= 1.8817 YY= 21.7731 ZY= 0.4803
XZ= 2.2907 YZ= 0.7509 ZZ= 25.4226
Eigenvalues: 21.0057 23.7116 28.1371
43 H Isotropic = 24.4888 Anisotropy = 4.1040
XX= 24.6613 YX= 1.3660 ZX= -1.0134
XY= 1.5162 YY= 21.9380 ZY= -0.3468
XZ= -0.6608 YZ= 0.0592 ZZ= 26.8671

Eigenvalues: 21.3096 24.9320 27.2248
44 H Isotropic = 24.6504 Anisotropy = 5.7412
XX= 27.3885 YX= 2.3532 ZX= 0.0754
XY= 2.6675 YY= 22.2722 ZY= 0.4935
XZ= 0.4861 YZ= 0.8448 ZZ= 24.2906
Eigenvalues: 21.1611 24.3123 28.4779
45 H Isotropic = 24.9916 Anisotropy = 9.3804
XX= 24.9280 YX= 2.0385 ZX= 3.6903
XY= 2.1155 YY= 22.6271 ZY= 1.8825
XZ= 3.4215 YZ= 3.3877 ZZ= 27.4198
Eigenvalues: 21.3014 22.4282 31.2452
46 O Isotropic = -56.7582 Anisotropy = 560.9304
XX= -122.2646 YX= 135.0804 ZX= 113.7953
XY= 127.7225 YY= 105.5816 ZY= 242.7572
XZ= 107.3204 YZ= 243.7031 ZZ= -153.5914
Eigenvalues: -305.2191 -182.2508 317.1955
47 C Isotropic = 167.5364 Anisotropy = 25.4691
XX= 165.4835 YX= -2.3271 ZX= 7.3798
XY= -7.9625 YY= 179.9375 ZY= 9.8368
XZ= 5.0520 YZ= 10.2933 ZZ= 155.6883
Eigenvalues: 148.5969 168.4966 184.0159
48 H Isotropic = 30.9634 Anisotropy = 10.2624
XX= 33.3609 YX= -4.5468 ZX= 0.2714
XY= -5.6506 YY= 31.9545 ZY= -0.0354
XZ= -0.2263 YZ= 0.2744 ZZ= 27.5749
Eigenvalues: 27.4330 27.6523 37.8050
49 H Isotropic = 30.6404 Anisotropy = 7.5301
XX= 27.7937 YX= -0.7337 ZX= 0.5599
XY= -0.9081 YY= 29.1194 ZY= 2.8258
XZ= -0.4463 YZ= 1.2890 ZZ= 35.0081
Eigenvalues: 27.2607 29.0000 35.6605
50 H Isotropic = 30.3614 Anisotropy = 5.7906
XX= 30.2808 YX= 2.1029 ZX= -3.1254
XY= 1.2820 YY= 32.8337 ZY= -1.1261
XZ= -2.7948 YZ= 0.4039 ZZ= 27.9699
Eigenvalues: 25.8819 30.9806 34.2218

B3LYP /6-311+g(2d,p) calculated optimal geometry, energy (in a.u.), GIAO nuclear magnetic shielding tensors of **3b** compound R optical isomer

E(RB3LYP) = -1167.23249857

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.919696	2.963668	-1.063254

2	6	0	-2.892406	1.628830	0.328942
3	6	0	-0.605983	1.771829	-0.400086
4	6	0	-2.215783	3.455380	-1.066233
5	6	0	-3.215857	2.774505	-0.382721
6	6	0	-1.596205	1.110571	0.345286
7	7	0	0.722507	1.263433	-0.539700
8	6	0	1.526849	0.531188	0.320218
9	7	0	-1.336247	-0.019765	1.176311
10	6	0	-0.268487	0.161195	2.176889
11	6	0	1.157766	-0.064728	1.643783
12	6	0	1.483851	1.491412	-1.678308
13	7	0	2.674796	0.987069	-1.595057
14	6	0	2.728248	0.388847	-0.355007
15	6	0	3.908289	-0.322182	0.150747
16	8	0	4.938357	-0.289516	-0.712932
17	6	0	6.149318	-0.967055	-0.308389
18	1	0	1.078120	2.004381	-2.533798
19	6	0	-1.350394	-1.332819	0.511615
20	6	0	-2.712560	-1.724385	-0.019936
21	6	0	-5.226592	-2.490725	-0.991761
22	6	0	-3.775383	-1.954199	0.857214
23	6	0	-2.927498	-1.885894	-1.386567
24	6	0	-4.176353	-2.266256	-1.872870
25	6	0	-5.022147	-2.334350	0.377886
26	1	0	-0.436209	-0.630746	2.914771
27	1	0	6.941291	-0.427646	-0.827522
28	1	0	6.277818	-0.853023	0.767556
29	1	0	1.341664	-1.138857	1.556520
30	1	0	1.883826	0.264363	2.391447
31	6	0	-0.416640	1.490279	2.920563
32	1	0	-0.139463	3.517618	-1.566937
33	1	0	-2.435561	4.377028	-1.590951
34	1	0	-4.231884	3.149334	-0.376679
35	1	0	-3.642161	1.108776	0.909982
36	1	0	-0.617341	-1.399153	-0.304852
37	1	0	-1.043462	-2.062331	1.266892
38	1	0	-0.169718	2.350687	2.296219
39	1	0	0.256317	1.501106	3.780018
40	1	0	-1.438409	1.616300	3.282445
41	1	0	-3.620480	-1.829390	1.923357
42	1	0	-5.835575	-2.514066	1.071317
43	1	0	-6.198835	-2.788225	-1.366463
44	1	0	-4.326287	-2.384766	-2.939569
45	1	0	-2.110855	-1.712262	-2.078982
46	8	0	3.949960	-0.876649	1.233154
47	6	0	6.125793	-2.431048	-0.709072

48	1	0	7.082776	-2.896474	-0.458601
49	1	0	5.964203	-2.536216	-1.783507
50	1	0	5.337523	-2.966662	-0.178941

Calculated GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 57.5712 Anisotropy = 154.2650
XX= 19.0400 YX= -29.4624 ZX= 47.4718
XY= -8.8834 YY= 41.9134 ZY= 73.3254
XZ= 55.5000 YZ= 58.3838 ZZ= 111.7600
Eigenvalues: -35.7525 48.0515 160.4145
2 C Isotropic = 41.0575 Anisotropy = 167.3171
XX= -5.0528 YX= -15.0286 ZX= 49.4343
XY= -7.4744 YY= 50.5661 ZY= 77.4377
XZ= 71.3912 YZ= 76.0048 ZZ= 77.6594
Eigenvalues: -60.6378 31.2081 152.6023
3 C Isotropic = 37.0574 Anisotropy = 132.9740
XX= -36.3169 YX= 43.3807 ZX= 26.1787
XY= 49.9913 YY= 48.2568 ZY= 30.1607
XZ= 13.7865 YZ= 36.7219 ZZ= 99.2324
Eigenvalues: -57.1737 42.6393 125.7067
4 C Isotropic = 51.5788 Anisotropy = 181.0730
XX= 40.2607 YX= 31.3185 ZX= 11.3805
XY= 31.0030 YY= 4.0502 ZY= 98.7840
XZ= 11.1266 YZ= 93.8913 ZZ= 110.4253
Eigenvalues: -57.5070 39.9492 172.2941
5 C Isotropic = 52.5635 Anisotropy = 178.8853
XX= -40.7238 YX= 46.5294 ZX= 22.3064
XY= 48.0297 YY= 72.0937 ZY= 54.6730
XZ= 18.8708 YZ= 60.7642 ZZ= 126.3206
Eigenvalues: -57.9183 43.7884 171.8203
6 C Isotropic = 37.6586 Anisotropy = 147.2293
XX= 25.3713 YX= 22.3761 ZX= 12.6732
XY= 18.4227 YY= 9.2032 ZY= 91.6123
XZ= 13.5142 YZ= 69.2200 ZZ= 78.4014
Eigenvalues: -45.1695 22.3339 135.8115
7 N Isotropic = 40.7412 Anisotropy = 139.4278
XX= -24.4745 YX= 70.6553 ZX= 4.6765
XY= 36.0742 YY= 97.4457 ZY= 36.9892
XZ= 16.5276 YZ= 34.0215 ZZ= 49.2525
Eigenvalues: -44.6097 33.1403 133.6931
8 C Isotropic = 38.8211 Anisotropy = 134.8671
XX= 35.9295 YX= 40.9939 ZX= -9.4432
XY= 51.8612 YY= 75.9413 ZY= 63.4494
XZ= 2.9823 YZ= 60.8911 ZZ= 4.5925
Eigenvalues: -41.4472 29.1780 128.7325
9 N Isotropic = 162.9148 Anisotropy = 46.2285

XX= 149.8417 YX= -3.2954 ZX= 15.8423
XY= 19.9274 YY= 167.6403 ZY= 16.5262
XZ= 19.5278 YZ= 15.5665 ZZ= 171.2625
Eigenvalues: 139.8566 155.1541 193.7339
10 C Isotropic = 121.4963 Anisotropy = 43.9717
XX= 126.4558 YX= 3.2222 ZX= 24.4776
XY= 4.2684 YY= 107.2610 ZY= 2.6502
XZ= 18.3367 YZ= 5.2625 ZZ= 130.7721
Eigenvalues: 106.5519 107.1262 150.8108
11 C Isotropic = 153.3159 Anisotropy = 24.9034
XX= 157.2613 YX= -2.8400 ZX= -9.6374
XY= 2.1336 YY= 134.7694 ZY= 1.6498
XZ= -9.6369 YZ= -0.2675 ZZ= 149.9170
Eigenvalues: 134.7375 143.2920 163.9182
12 C Isotropic = 44.2625 Anisotropy = 77.4129
XX= 72.7746 YX= 8.3587 ZX= -0.9027
XY= 12.2989 YY= 74.2517 ZY= 39.2267
XZ= 21.8759 YZ= 36.0334 ZZ= -14.2388
Eigenvalues: -28.4719 65.3884 95.8711
13 N Isotropic = -44.6287 Anisotropy = 419.7856
XX= -104.0199 YX= 141.7337 ZX= -22.0206
XY= 146.9117 YY= 107.3161 ZY= 157.7719
XZ= -1.8729 YZ= 166.9895 ZZ= -137.1824
Eigenvalues: -263.2315 -105.8830 235.2283
14 C Isotropic = 43.3569 Anisotropy = 88.7085
XX= 26.6664 YX= 33.1495 ZX= -10.1476
XY= 39.7513 YY= 68.2835 ZY= 41.6016
XZ= -16.6479 YZ= 37.1591 ZZ= 35.1208
Eigenvalues: -16.5398 44.1147 102.4959
15 C Isotropic = 12.6379 Anisotropy = 85.3759
XX= -60.6601 YX= 42.7093 ZX= 14.2162
XY= 33.3332 YY= 50.5150 ZY= 12.1003
XZ= 39.2034 YZ= -5.1456 ZZ= 48.0589
Eigenvalues: -77.2405 45.5991 69.5552
16 O Isotropic = 111.0928 Anisotropy = 157.7705
XX= 106.3568 YX= 33.3596 ZX= -21.1345
XY= 89.5951 YY= 146.1701 ZY= 72.2072
XZ= -123.5383 YZ= 120.7852 ZZ= 80.7517
Eigenvalues: -46.9159 163.9212 216.2732
17 C Isotropic = 120.3031 Anisotropy = 65.4332
XX= 149.1193 YX= -19.4144 ZX= 20.6048
XY= -20.6044 YY= 126.2247 ZY= -1.3321
XZ= 17.1529 YZ= 4.2496 ZZ= 85.5653
Eigenvalues: 79.3133 117.6708 163.9253
18 H Isotropic = 24.1701 Anisotropy = 6.5903
XX= 25.2542 YX= -2.4066 ZX= -0.8577

XY= -2.6188 YY= 21.4648 ZY= -1.4538
XZ= -5.1658 YZ= -2.3114 ZZ= 25.7914
Eigenvalues: 18.8091 25.1376 28.5637
19 C Isotropic = 123.7046 Anisotropy = 34.0930
XX= 120.8329 YX= 9.3957 ZX= 2.2346
XY= 9.7766 YY= 133.0207 ZY= 10.0869
XZ= 8.8291 YZ= 16.3819 ZZ= 111.2601
Eigenvalues: 104.9411 115.7394 144.4332
20 C Isotropic = 36.8472 Anisotropy = 199.3715
XX= -37.1074 YX= -56.5072 ZX= -27.2737
XY= -62.0959 YY= 152.7537 ZY= -3.7481
XZ= -18.3142 YZ= -11.7234 ZZ= -5.1045
Eigenvalues: -63.9347 4.7148 169.7616
21 C Isotropic = 51.0392 Anisotropy = 184.3707
XX= -29.9857 YX= -57.9251 ZX= -30.2144
XY= -56.7919 YY= 156.9951 ZY= -20.2076
XZ= -28.5818 YZ= -18.1071 ZZ= 26.1083
Eigenvalues: -59.3770 38.5417 173.9530
22 C Isotropic = 47.3516 Anisotropy = 182.3452
XX= 45.3743 YX= -35.2434 ZX= -11.0340
XY= -39.3602 YY= 156.4893 ZY= -16.2882
XZ= -14.3380 YZ= -23.8980 ZZ= -59.8088
Eigenvalues: -64.1448 37.2845 168.9151
23 C Isotropic = 48.1880 Anisotropy = 167.0769
XX= -5.2310 YX= -40.5196 ZX= 51.4894
XY= -40.0821 YY= 149.3654 ZY= 6.5002
XZ= 54.3779 YZ= 5.2388 ZZ= 0.4298
Eigenvalues: -60.8085 45.7999 159.5727
24 C Isotropic = 50.2824 Anisotropy = 182.2662
XX= 46.9860 YX= -34.5550 ZX= -13.2220
XY= -34.2910 YY= 161.2744 ZY= -18.6093
XZ= -12.6335 YZ= -19.0809 ZZ= -57.4132
Eigenvalues: -61.4414 40.4954 171.7931
25 C Isotropic = 50.2479 Anisotropy = 183.8545
XX= -6.5813 YX= -45.9761 ZX= 51.4283
XY= -46.3056 YY= 160.2932 ZY= 3.7646
XZ= 52.2399 YZ= 2.3408 ZZ= -2.9683
Eigenvalues: -62.4503 40.3764 172.8175
26 H Isotropic = 27.9323 Anisotropy = 6.5525
XX= 27.3800 YX= 0.1004 ZX= 0.0986
XY= 1.4889 YY= 26.3106 ZY= -2.6089
XZ= -0.4192 YZ= -4.5036 ZZ= 30.1063
Eigenvalues: 24.0679 27.4284 32.3006
27 H Isotropic = 28.1492 Anisotropy = 7.3893
XX= 32.1931 YX= 1.7216 ZX= -2.0535
XY= 1.4652 YY= 28.8609 ZY= -1.7223

XZ= -0.1369 YZ= -0.9921 ZZ= 23.3935
Eigenvalues: 23.0181 28.3541 33.0754
28 H Isotropic = 26.8020 Anisotropy = 4.9160
XX= 28.7780 YX= -1.6147 ZX= 2.9946
XY= -0.5850 YY= 24.6284 ZY= 1.5293
XZ= 1.0089 YZ= 1.7512 ZZ= 26.9997
Eigenvalues: 23.1175 27.2093 30.0794
29 H Isotropic = 27.7262 Anisotropy = 6.9092
XX= 30.4759 YX= -2.8488 ZX= -2.8713
XY= -2.0606 YY= 28.9776 ZY= -2.8133
XZ= -1.3017 YZ= -1.0525 ZZ= 23.7251
Eigenvalues: 22.1412 28.7050 32.3323
30 H Isotropic = 28.2928 Anisotropy = 8.2546
XX= 33.0365 YX= -1.2752 ZX= 1.6498
XY= -1.4804 YY= 22.1554 ZY= 2.0104
XZ= 1.6586 YZ= -0.3075 ZZ= 29.6863
Eigenvalues: 21.8395 29.2430 33.7959
31 C Isotropic = 166.1369 Anisotropy = 31.0185
XX= 160.1873 YX= -4.7811 ZX= -0.2033
XY= -9.0924 YY= 162.1439 ZY= 22.5802
XZ= 0.6433 YZ= 16.1144 ZZ= 158.0794
Eigenvalues: 139.5065 160.0882 180.8159
32 H Isotropic = 24.3512 Anisotropy = 8.2494
XX= 25.0806 YX= -2.7023 ZX= -0.6485
XY= -4.1739 YY= 26.9037 ZY= -3.9977
XZ= -0.7720 YZ= -1.0609 ZZ= 21.0692
Eigenvalues: 19.3771 23.8257 29.8508
33 H Isotropic = 24.5653 Anisotropy = 4.2962
XX= 27.1101 YX= -0.5975 ZX= -1.2721
XY= -0.4794 YY= 24.0706 ZY= -1.8293
XZ= -1.2178 YZ= -1.5979 ZZ= 22.5152
Eigenvalues: 21.1119 25.1546 27.4294
34 H Isotropic = 24.8641 Anisotropy = 5.7452
XX= 24.2956 YX= -0.3514 ZX= -0.7178
XY= 0.1527 YY= 27.0207 ZY= -2.9211
XZ= -0.8300 YZ= -3.0563 ZZ= 23.2761
Eigenvalues: 21.4370 24.4611 28.6943
35 H Isotropic = 25.0602 Anisotropy = 8.5263
XX= 25.8039 YX= -3.6342 ZX= 0.3462
XY= -2.8316 YY= 28.6274 ZY= 1.0591
XZ= 0.5072 YZ= -0.7482 ZZ= 20.7495
Eigenvalues: 20.6833 23.7530 30.7444
36 H Isotropic = 28.0756 Anisotropy = 5.4776
XX= 29.5856 YX= 2.6862 ZX= -2.0551
XY= 1.5144 YY= 27.9226 ZY= 2.6199
XZ= -0.7541 YZ= 5.4765 ZZ= 26.7187

Eigenvalues: 22.3971 30.1024 31.7273
37 H Isotropic = 27.6452 Anisotropy = 4.4702
XX= 28.5833 YX= 1.9805 ZX= 1.7555
XY= -0.0194 YY= 29.7612 ZY= -3.9478
XZ= 1.4271 YZ= -0.3266 ZZ= 24.5910
Eigenvalues: 23.1982 29.1120 30.6253
38 H Isotropic = 31.1628 Anisotropy = 4.2083
XX= 27.5974 YX= 0.6166 ZX= 0.7966
XY= 1.9165 YY= 32.6588 ZY= 1.7141
XZ= 1.8641 YZ= -0.8505 ZZ= 33.2323
Eigenvalues: 27.0631 32.4570 33.9684
39 H Isotropic = 30.8416 Anisotropy = 10.5928
XX= 29.5786 YX= -0.3482 ZX= 3.6099
XY= 0.7381 YY= 27.3590 ZY= 3.9811
XZ= 3.4752 YZ= 1.6918 ZZ= 35.5874
Eigenvalues: 26.1471 28.4744 37.9035
40 H Isotropic = 30.9259 Anisotropy = 9.0079
XX= 32.6182 YX= -1.7675 ZX= -2.5110
XY= -2.6944 YY= 27.2227 ZY= 4.4033
XZ= -3.2214 YZ= 1.0874 ZZ= 32.9370
Eigenvalues: 25.9251 29.9215 36.9312
41 H Isotropic = 23.9963 Anisotropy = 10.0370
XX= 29.0755 YX= 3.1615 ZX= -1.8599
XY= 3.5159 YY= 22.0876 ZY= -1.4795
XZ= -0.7503 YZ= -0.8204 ZZ= 20.8259
Eigenvalues: 20.0688 21.2325 30.6877
42 H Isotropic = 24.3189 Anisotropy = 5.5874
XX= 25.8201 YX= 1.8117 ZX= 1.6875
XY= 2.0037 YY= 21.8311 ZY= 0.5427
XZ= 2.0790 YZ= 0.8009 ZZ= 25.3056
Eigenvalues: 21.0639 23.8490 28.0439
43 H Isotropic = 24.4673 Anisotropy = 4.1487
XX= 24.6489 YX= 1.1140 ZX= -1.1395
XY= 1.4432 YY= 21.9101 ZY= 0.0452
XZ= -0.8327 YZ= 0.4205 ZZ= 26.8430
Eigenvalues: 21.3431 24.8258 27.2331
44 H Isotropic = 24.6274 Anisotropy = 5.7660
XX= 27.5557 YX= 2.1507 ZX= -0.1488
XY= 2.5332 YY= 22.2764 ZY= 0.6728
XZ= 0.2523 YZ= 0.9679 ZZ= 24.0500
Eigenvalues: 21.1902 24.2205 28.4714
45 H Isotropic = 25.0207 Anisotropy = 9.2790
XX= 25.1098 YX= 2.2057 ZX= 3.4655
XY= 2.3100 YY= 23.2324 ZY= 2.3541
XZ= 3.2544 YZ= 3.8314 ZZ= 26.7198
Eigenvalues: 21.3807 22.4746 31.2066

46 O Isotropic = -56.8271 Anisotropy = 562.5109
XX= -134.6559 YX= 127.9162 ZX= 98.0853
XY= 125.8471 YY= 153.5447 ZY= 229.9166
XZ= 89.8288 YZ= 219.4279 ZZ= -189.3702
Eigenvalues: -306.5586 -182.1030 318.1802
47 C Isotropic = 167.0795 Anisotropy = 25.5217
XX= 165.5461 YX= -2.1808 ZX= 7.6137
XY= -7.8453 YY= 181.6253 ZY= 7.1674
XZ= 6.2102 YZ= 7.6276 ZZ= 154.0671
Eigenvalues: 148.4660 168.6785 184.0940
48 H Isotropic = 30.9825 Anisotropy = 10.2346
XX= 33.5995 YX= -4.4470 ZX= 0.9088
XY= -5.5553 YY= 31.6913 ZY= -0.6318
XZ= 0.5279 YZ= -0.2537 ZZ= 27.6566
Eigenvalues: 27.4533 27.6885 37.8056
49 H Isotropic = 30.6541 Anisotropy = 7.5575
XX= 27.8045 YX= -0.7929 ZX= 0.3952
XY= -1.0940 YY= 29.6432 ZY= 3.4020
XZ= -0.4809 YZ= 1.8756 ZZ= 34.5147
Eigenvalues: 27.2186 29.0513 35.6925
50 H Isotropic = 30.3511 Anisotropy = 5.8374
XX= 30.2476 YX= 1.6298 ZX= -3.2723
XY= 0.9472 YY= 32.8612 ZY= -1.7656
XZ= -2.8894 YZ= -0.1400 ZZ= 27.9445

B3LYP /6-311+g(2d,p) calculated optimal geometry, energy (in a.u.), GIAO nuclear magnetic shielding tensors of **2b** compound S optical isomer

E= -2273.73233049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.693060	0.071218	-0.795751
2	8	0	3.457636	1.448234	-0.497929
3	8	0	2.306831	-0.182793	-2.190128
4	8	0	3.840940	-0.850923	-0.158872
5	7	0	1.375864	-0.027275	0.204297
6	6	0	1.254427	0.140458	1.592377
7	6	0	-0.714590	-0.815582	-2.945506
8	8	0	-0.587457	-1.515309	-1.776302
9	6	0	-0.005408	-0.103102	2.183859
10	6	0	-1.860889	-1.669149	-1.307726
11	6	0	2.997244	2.661895	-1.029011
12	7	0	-1.089491	-0.540696	1.344328
13	6	0	3.251751	2.972940	-2.357291

14	6	0	3.604784	-2.994172	-1.273650
15	6	0	2.324784	0.549527	2.392355
16	8	0	-4.739073	-1.436162	-1.115733
17	7	0	-1.926315	-0.531453	-3.249007
18	6	0	3.733329	-2.244501	-0.111193
19	6	0	2.155965	0.737132	3.757946
20	6	0	-1.091769	-2.012880	1.120573
21	6	0	-2.017049	-2.437220	-0.045136
22	6	0	1.960388	4.790727	-0.683447
23	6	0	-0.147082	0.103469	3.554917
24	6	0	-2.690404	-1.066749	-2.211674
25	6	0	2.849819	4.211391	-2.845027
26	6	0	2.354772	3.553703	-0.183343
27	6	0	0.916495	0.523302	4.345282
28	6	0	-4.160115	-0.928622	-2.234650
29	8	0	-4.783611	-0.426764	-3.133508
30	6	0	3.833540	-2.850271	1.133732
31	6	0	3.567948	-4.381565	-1.175584
32	6	0	2.206176	5.121867	-2.011932
33	6	0	3.801654	-4.238085	1.215548
34	6	0	3.666925	-5.006816	0.063416
35	6	0	-6.184498	-1.347873	-1.070548
36	6	0	-6.645494	-1.968035	0.230279
37	6	0	-1.437615	-2.848592	2.362098
38	1	0	-1.343379	-3.913550	2.136707
39	1	0	-0.762412	-2.623230	3.187887
40	1	0	-2.463281	-2.670698	2.694745
41	6	0	-2.402818	0.043402	1.660816
42	6	0	-2.444521	1.550197	1.511550
43	6	0	-2.634515	4.330127	1.206555
44	6	0	-2.923434	2.350010	2.547870
45	6	0	-2.060823	2.163059	0.317059
46	6	0	-2.153094	3.540887	0.165132
47	6	0	-3.020634	3.730892	2.399471
48	1	0	-2.758019	-0.223171	2.665308
49	1	0	-3.121222	-0.388402	0.962279
50	1	0	-3.223260	1.889885	3.483551
51	1	0	-1.691349	1.557001	-0.500971
52	1	0	-1.853724	3.998060	-0.770405
53	1	0	-2.708985	5.404541	1.086667
54	1	0	-3.394302	4.336030	3.217224
55	1	0	2.171414	3.279172	0.847273
56	1	0	1.457975	5.493372	-0.029885
57	1	0	1.897852	6.085976	-2.397557
58	1	0	3.041805	4.463511	-3.880947
59	1	0	3.747156	2.249943	-2.990886

60	1	0	0.499604	-0.225757	-0.263947
61	1	0	-1.110156	-0.067064	4.017708
62	1	0	0.774750	0.678352	5.407673
63	1	0	2.997812	1.062729	4.357223
64	1	0	3.288669	0.739823	1.941671
65	1	0	-0.068019	-2.258749	0.830215
66	1	0	-3.064086	-2.399514	0.246819
67	1	0	-1.795147	-3.490850	-0.249892
68	1	0	-6.470705	-0.298038	-1.148369
69	1	0	-6.590464	-1.868694	-1.939002
70	1	0	-6.349675	-3.017003	0.294290
71	1	0	-6.232028	-1.436141	1.089358
72	1	0	-7.734741	-1.917788	0.292908
73	1	0	3.938486	-2.235147	2.017881
74	1	0	3.883989	-4.717295	2.183740
75	1	0	3.643966	-6.087652	0.130517
76	1	0	3.466710	-4.974172	-2.076879
77	1	0	3.528404	-2.493010	-2.228922
78	1	0	0.206431	-0.565657	-3.445956

Calculated GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 P Isotropic = 304.3888 Anisotropy = 216.3719
XX= 220.7215 YX= 3.8770 ZX= 56.5217
XY= -0.4045 YY= 258.6372 ZY= 42.0294
XZ= 23.4905 YZ= 34.3847 ZZ= 433.8078
Eigenvalues: 212.7960 251.7337 448.6367
2 O Isotropic = 163.0857 Anisotropy = 94.4264
XX= 183.2433 YX= 46.7364 ZX= 9.6077
XY= 27.6026 YY= 186.8218 ZY= 6.3866
XZ= 19.9481 YZ= 21.0484 ZZ= 119.1921
Eigenvalues: 115.3559 147.8646 226.0367
3 O Isotropic = 177.9816 Anisotropy = 54.3792
XX= 178.9889 YX= -1.4166 ZX= -0.9327
XY= -0.1614 YY= 143.7483 ZY= 12.5054
XZ= -11.7096 YZ= 10.3124 ZZ= 211.2075
Eigenvalues: 141.8694 177.8410 214.2344
4 O Isotropic = 166.1808 Anisotropy = 89.2499
XX= 213.8614 YX= -40.2744 ZX= -1.2064
XY= -13.9895 YY= 160.9341 ZY= -18.0101
XZ= -1.7411 YZ= -20.4206 ZZ= 123.7469
Eigenvalues: 113.9994 158.8622 225.6807
5 N Isotropic = 163.3090 Anisotropy = 56.0480
XX= 141.5450 YX= -12.0349 ZX= -21.5870
XY= -3.6865 YY= 158.5323 ZY= -18.5367
XZ= -25.7059 YZ= -2.7471 ZZ= 189.8498
Eigenvalues: 127.6699 161.5828 200.6743

```
  6  C    Isotropic =    39.2578   Anisotropy =   152.2700
XX=    32.2398   YX=   -29.7123   ZX=     2.8199
XY=   -23.9224   YY=   130.7347   ZY=   -21.5969
XZ=    20.5353   YZ=   -22.8272   ZZ=   -45.2011
Eigenvalues:   -48.8551    25.8574   140.7711
  7  C    Isotropic =    25.6960   Anisotropy =    89.3306
XX=    31.7136   YX=   -16.3686   ZX=    37.2864
XY=   -10.7932   YY=    52.1772   ZY=    54.6805
XZ=    30.3736   YZ=    54.0020   ZZ=    -6.8027
Eigenvalues:   -54.2676    46.1060    85.2497
  8  O    Isotropic =   -12.4767   Anisotropy =   260.4488
XX=  -131.6323   YX=    -5.6584   ZX=    44.8863
XY=    23.4758   YY=   103.9513   ZY=    93.4566
XZ=     0.4544   YZ=   101.4316   ZZ=    -9.7492
Eigenvalues:  -136.1436   -62.4423   161.1558
  9  C    Isotropic =    41.4010   Anisotropy =   137.4014
XX=    -8.1161   YX=   -44.0652   ZX=   -10.6416
XY=   -40.0814   YY=   115.3732   ZY=   -31.2550
XZ=   -24.1169   YZ=   -27.2431   ZZ=    16.9458
Eigenvalues:   -34.3261    25.5271   133.0019
 10  C    Isotropic =    19.7376   Anisotropy =   125.6553
XX=   -31.0180   YX=   -14.7024   ZX=    48.8785
XY=     2.4605   YY=    75.0077   ZY=    45.7148
XZ=    22.8881   YZ=    51.8142   ZZ=    15.2231
Eigenvalues:   -57.7231    13.4281   103.5078
 11  C    Isotropic =    25.3993   Anisotropy =   113.9553
XX=    79.1215   YX=    50.3743   ZX=    -3.2113
XY=    51.6934   YY=   -37.5522   ZY=    41.7010
XZ=    -1.0465   YZ=    44.3370   ZZ=    34.6287
Eigenvalues:   -72.5698    47.3983   101.3696
 12  N    Isotropic =   179.3293   Anisotropy =    71.4717
XX=   178.7164   YX=   -12.7751   ZX=     7.5053
XY=    -8.5013   YY=   224.4536   ZY=    19.3140
XZ=    24.1269   YZ=   -20.2208   ZZ=   134.8178
Eigenvalues:   129.6265   181.3843   226.9770
 13  C    Isotropic =    53.5653   Anisotropy =   162.6971
XX=   116.2464   YX=    66.6272   ZX=    54.1938
XY=    69.7803   YY=    23.8178   ZY=   -19.7960
XZ=    45.5122   YZ=   -15.7894   ZZ=    20.6319
Eigenvalues:   -40.4090    39.0750   162.0301
 14  C    Isotropic =    55.3757   Anisotropy =   167.1585
XX=   165.6564   YX=    -1.7392   ZX=    -9.0487
XY=    -5.6602   YY=    21.9919   ZY=    36.0737
XZ=   -17.1112   YZ=    27.4305   ZZ=   -21.5210
Eigenvalues:   -38.7323    38.0448   166.8148
 15  C    Isotropic =    61.9110   Anisotropy =   162.9363
```

XX= -8.2935 YX= -44.4422 ZX= 27.2884
XY= -46.3558 YY= 155.8182 ZY= -12.0247
XZ= 32.7988 YZ= -13.0314 ZZ= 38.2083
Eigenvalues: -30.1602 45.3580 170.5352
16 O Isotropic = 113.1391 Anisotropy = 173.1703
XX= 10.3273 YX= 37.2896 ZX= -44.5481
XY= 89.9295 YY= 156.8197 ZY= 2.6824
XZ= -157.4240 YZ= 10.9931 ZZ= 172.2703
Eigenvalues: -55.4108 166.2422 228.5859
17 N Isotropic = -36.2497 Anisotropy = 371.7783
XX= -171.1634 YX= -10.7923 ZX= 77.3174
XY= -9.7031 YY= 120.7586 ZY= 153.8790
XZ= 79.9296 YZ= 153.5553 ZZ= -58.3442
Eigenvalues: -234.4277 -85.9239 211.6025
18 C Isotropic = 24.9245 Anisotropy = 117.5529
XX= 101.7216 YX= -7.5865 ZX= -10.3748
XY= -7.0889 YY= -70.8942 ZY= 9.2435
XZ= -6.1145 YZ= 8.6576 ZZ= 43.9460
Eigenvalues: -71.8456 43.3260 103.2930
19 C Isotropic = 53.2211 Anisotropy = 179.1139
XX= -6.2091 YX= -54.5046 ZX= -35.9190
XY= -56.3078 YY= 151.7343 ZY= -32.8180
XZ= -38.8608 YZ= -37.7679 ZZ= 14.1382
Eigenvalues: -55.4902 42.5232 172.6304
20 C Isotropic = 122.4989 Anisotropy = 38.3487
XX= 101.5261 YX= 0.3817 ZX= 6.0339
XY= -1.4558 YY= 145.6316 ZY= 13.6583
XZ= 4.7634 YZ= 2.6858 ZZ= 120.3390
Eigenvalues: 99.9267 119.5053 148.0647
21 C Isotropic = 149.5342 Anisotropy = 35.9945
XX= 130.6604 YX= 8.0529 ZX= 13.6286
XY= 12.2068 YY= 143.1173 ZY= -1.0850
XZ= 7.0520 YZ= -7.0862 ZZ= 168.8249
Eigenvalues: 122.3784 148.6937 171.5305
22 C Isotropic = 48.7245 Anisotropy = 186.6124
XX= 120.8486 YX= 79.1614 ZX= 57.8799
XY= 76.8349 YY= 16.6091 ZY= -23.6524
XZ= 59.5895 YZ= -25.8324 ZZ= 8.7160
Eigenvalues: -63.0233 36.0641 173.1328
23 C Isotropic = 52.1021 Anisotropy = 188.4101
XX= -25.4721 YX= -43.5297 ZX= 39.2583
XY= -68.2484 YY= 153.0589 ZY= -32.5403
XZ= 39.4469 YZ= -18.2366 ZZ= 28.7195
Eigenvalues: -53.8567 32.4542 177.7088
24 C Isotropic = 46.4181 Anisotropy = 86.9503
XX= -2.4043 YX= -0.0629 ZX= 19.9899

XY= -7.8031 YY= 86.5251 ZY= 29.5758
XZ= 32.3244 YZ= 27.4505 ZZ= 55.1335
Eigenvalues: -14.6063 49.4757 104.3850
25 C Isotropic = 49.1156 Anisotropy = 184.2301
XX= 138.8909 YX= 42.9572 ZX= 47.1671
XY= 43.7537 YY= 52.5631 ZY= 33.4849
XZ= 46.9427 YZ= 36.0515 ZZ= -44.1072
Eigenvalues: -60.9781 36.3892 171.9357
26 C Isotropic = 56.4514 Anisotropy = 161.6919
XX= 135.7654 YX= 36.1770 ZX= 39.7864
XY= 39.7747 YY= 57.0957 ZY= 34.7695
XZ= 41.6641 YZ= 27.7336 ZZ= -23.5068
Eigenvalues: -38.7356 43.8438 164.2460
27 C Isotropic = 59.5944 Anisotropy = 168.3297
XX= 60.7739 YX= -27.2549 ZX= 13.2399
XY= -28.7942 YY= 158.1809 ZY= -33.0066
XZ= 17.8803 YZ= -33.3392 ZZ= -40.1717
Eigenvalues: -46.7146 53.6836 171.8142
28 C Isotropic = 16.5524 Anisotropy = 74.9199
XX= -38.5928 YX= -13.4979 ZX= 48.7269
XY= -28.9766 YY= 59.4495 ZY= 14.1778
XZ= 77.1075 YZ= 11.8326 ZZ= 28.8006
Eigenvalues: -80.6934 63.8517 66.4990
29 O Isotropic = -95.7758 Anisotropy = 598.7983
XX= -241.3659 YX= 64.0017 ZX= -32.2653
XY= 50.0523 YY= 171.0116 ZY= 256.9957
XZ= -18.1280 YZ= 260.7346 ZZ= -216.9733
Eigenvalues: -365.4375 -225.3131 303.4230
30 C Isotropic = 56.6955 Anisotropy = 159.7597
XX= 161.2789 YX= -6.6590 ZX= -16.1412
XY= -11.2472 YY= 19.0223 ZY= -37.9279
XZ= -18.3667 YZ= -35.3650 ZZ= -10.2146
Eigenvalues: -36.9317 43.8163 163.2020
31 C Isotropic = 49.1481 Anisotropy = 185.1157
XX= 170.3308 YX= -10.7990 ZX= -19.5832
XY= -10.4118 YY= 7.1366 ZY= -42.4845
XZ= -20.4368 YZ= -45.5324 ZZ= -30.0230
Eigenvalues: -61.4054 36.2911 172.5586
32 C Isotropic = 52.8729 Anisotropy = 183.4673
XX= 136.9645 YX= 74.2031 ZX= 18.2099
XY= 72.1260 YY= -16.1654 ZY= 43.9878
XZ= 19.7959 YZ= 45.2558 ZZ= 37.8194
Eigenvalues: -58.4559 41.8901 175.1844
33 C Isotropic = 49.6502 Anisotropy = 183.4192
XX= 170.0276 YX= -0.3181 ZX= -19.3390
XY= -2.5785 YY= 19.2933 ZY= 38.2735

XZ= -18.9941 YZ= 40.3295 ZZ= -40.3702
Eigenvalues: -61.0659 38.0869 171.9297
34 C Isotropic = 53.7815 Anisotropy = 182.4171
XX= 173.8444 YX= -7.7395 ZX= -13.3506
XY= -7.3187 YY= -56.0180 ZY= 6.4604
XZ= -12.4202 YZ= 6.8413 ZZ= 43.5180
Eigenvalues: -56.6542 42.6057 175.3929
35 C Isotropic = 120.3679 Anisotropy = 60.9566
XX= 158.8543 YX= -4.6296 ZX= 3.1438
XY= 0.1312 YY= 96.5742 ZY= -2.2934
XZ= -7.3538 YZ= -1.2254 ZZ= 99.6752
Eigenvalues: 95.6446 100.4535 159.0056
36 C Isotropic = 168.0811 Anisotropy = 21.8566
XX= 170.7120 YX= 1.6158 ZX= -2.5289
XY= 4.1016 YY= 158.9563 ZY= -10.1752
XZ= -8.8852 YZ= -9.2816 ZZ= 174.5751
Eigenvalues: 154.2897 167.3015 182.6522
37 C Isotropic = 168.8944 Anisotropy = 26.0133
XX= 160.4729 YX= 5.8777 ZX= -2.9811
XY= 0.6015 YY= 164.7542 ZY= -12.9914
XZ= 0.5611 YZ= -6.6593 ZZ= 181.4562
Eigenvalues: 157.8019 162.6448 186.2366
38 H Isotropic = 31.3990 Anisotropy = 9.8758
XX= 27.6614 YX= -0.4923 ZX= -0.6501
XY= 0.4969 YY= 37.6260 ZY= -1.4745
XZ= -0.1940 YZ= -2.1209 ZZ= 28.9096
Eigenvalues: 27.4986 28.7155 37.9829
39 H Isotropic = 30.7996 Anisotropy = 6.1885
XX= 28.2933 YX= 0.2513 ZX= 2.4585
XY= 3.5267 YY= 30.6388 ZY= -2.2102
XZ= 3.3763 YZ= -1.0730 ZZ= 33.4665
Eigenvalues: 25.7840 31.6895 34.9252
40 H Isotropic = 30.7481 Anisotropy = 8.0985
XX= 32.7739 YX= -0.1759 ZX= -3.4709
XY= 1.9144 YY= 29.1089 ZY= -1.9889
XZ= -4.3178 YZ= -1.9327 ZZ= 30.3615
Eigenvalues: 26.8761 29.2210 36.1471
41 C Isotropic = 128.0132 Anisotropy = 27.1518
XX= 133.4519 YX= -10.1896 ZX= -9.2462
XY= -13.3537 YY= 141.3229 ZY= -2.3220
XZ= -8.4995 YZ= -3.4433 ZZ= 121.2648
Eigenvalues: 113.9071 132.0181 150.1144
42 C Isotropic = 38.2982 Anisotropy = 195.2316
XX= 153.6781 YX= 16.3944 ZX= 37.9934
XY= 15.5718 YY= -62.4600 ZY= 6.8587
XZ= 49.4174 YZ= 13.6212 ZZ= 23.6764

Eigenvalues: -64.2572 10.6992 168.4526
43 C Isotropic = 52.0299 Anisotropy = 183.1120
XX= 155.5749 YX= 21.1625 ZX= 43.2736
XY= 18.8187 YY= -55.1259 ZY= 14.3209
XZ= 42.8882 YZ= 16.0239 ZZ= 55.6407
Eigenvalues: -58.1765 40.1617 174.1046
44 C Isotropic = 49.7247 Anisotropy = 163.1837
XX= 138.6198 YX= -11.7150 ZX= 55.5607
XY= -4.1395 YY= 29.2467 ZY= 40.7389
XZ= 62.3666 YZ= 41.3636 ZZ= -18.6925
Eigenvalues: -58.0530 48.7132 158.5138
45 C Isotropic = 49.7268 Anisotropy = 186.5011
XX= 145.8096 YX= 29.9861 ZX= 64.7992
XY= 30.0828 YY= 6.4466 ZY= -32.9955
XZ= 72.5371 YZ= -38.4934 ZZ= -3.0758
Eigenvalues: -59.8471 34.9667 174.0609
46 C Isotropic = 49.6300 Anisotropy = 188.3723
XX= 150.6088 YX= 0.6568 ZX= 66.0215
XY= 0.9389 YY= 21.8043 ZY= 40.7627
XZ= 69.4994 YZ= 41.0384 ZZ= -23.5230
Eigenvalues: -64.1324 37.8109 175.2116
47 C Isotropic = 51.3209 Anisotropy = 180.8915
XX= 143.4606 YX= 30.8559 ZX= 67.1441
XY= 30.7441 YY= 10.4516 ZY= -38.6822
XZ= 68.8222 YZ= -38.9312 ZZ= 0.0504
Eigenvalues: -59.6063 41.6537 171.9152
48 H Isotropic = 27.7956 Anisotropy = 8.6351
XX= 28.2743 YX= -1.2272 ZX= -5.0287
XY= -2.3736 YY= 25.8324 ZY= 0.9545
XZ= -3.5814 YZ= 0.7586 ZZ= 29.2802
Eigenvalues: 24.0244 25.8102 33.5524
49 H Isotropic = 27.6486 Anisotropy = 6.4792
XX= 30.1842 YX= 2.6369 ZX= 2.6502
XY= -1.3203 YY= 26.7755 ZY= 3.9623
XZ= 1.3102 YZ= 3.2315 ZZ= 25.9861
Eigenvalues: 22.6120 28.3658 31.9681
50 H Isotropic = 24.6620 Anisotropy = 8.9408
XX= 22.9494 YX= -2.1581 ZX= -1.6299
XY= -3.8631 YY= 27.4495 ZY= 3.4672
XZ= -1.5439 YZ= 2.5977 ZZ= 23.5871
Eigenvalues: 21.4348 21.9286 30.6226
51 H Isotropic = 25.3726 Anisotropy = 7.9214
XX= 22.8758 YX= 0.1939 ZX= -0.0326
XY= -0.1845 YY= 29.7741 ZY= -3.5979
XZ= 0.1943 YZ= -1.4295 ZZ= 23.4679
Eigenvalues: 22.5687 22.8955 30.6535

52 H Isotropic = 24.9979 Anisotropy = 6.0727
XX= 24.0184 YX= -1.8586 ZX= -1.4697
XY= -1.1144 YY= 28.4217 ZY= 0.2595
XZ= -0.6268 YZ= 1.2765 ZZ= 22.5537
Eigenvalues: 22.0073 23.9401 29.0464
53 H Isotropic = 24.7482 Anisotropy = 4.4296
XX= 22.7966 YX= -1.2745 ZX= -2.4991
XY= -1.1695 YY= 25.0803 ZY= 0.0608
XZ= -2.1580 YZ= 0.2325 ZZ= 26.3678
Eigenvalues: 21.3566 25.1867 27.7013
54 H Isotropic = 24.6763 Anisotropy = 4.9683
XX= 22.1366 YX= -0.9232 ZX= -1.6854
XY= -1.0223 YY= 27.4972 ZY= -1.2148
XZ= -1.1281 YZ= -1.3245 ZZ= 24.3952
Eigenvalues: 21.1354 24.9051 27.9885
55 H Isotropic = 25.2568 Anisotropy = 7.9545
XX= 23.0685 YX= -2.2791 ZX= -1.2630
XY= -0.0924 YY= 30.3628 ZY= -0.7823
XZ= -0.6035 YZ= -0.0643 ZZ= 22.3392
Eigenvalues: 21.5803 23.6304 30.5598
56 H Isotropic = 24.8434 Anisotropy = 5.9147
XX= 22.5887 YX= 0.1709 ZX= -0.9674
XY= -0.0894 YY= 27.0965 ZY= -2.8269
XZ= -0.2300 YZ= -2.2887 ZZ= 24.8450
Eigenvalues: 22.3049 23.4386 28.7865
57 H Isotropic = 24.5369 Anisotropy = 4.3996
XX= 22.2752 YX= -0.4035 ZX= -2.4556
XY= -0.5697 YY= 24.8688 ZY= -0.2635
XZ= -2.0455 YZ= 0.3780 ZZ= 26.4668
Eigenvalues: 21.2461 24.8947 27.4700
58 H Isotropic = 24.2990 Anisotropy = 5.1311
XX= 22.2467 YX= -1.9051 ZX= -1.1987
XY= -1.6647 YY= 27.0979 ZY= -1.0116
XZ= -0.9975 YZ= -0.4971 ZZ= 23.5525
Eigenvalues: 21.0119 24.1654 27.7198
59 H Isotropic = 24.1916 Anisotropy = 9.2950
XX= 21.0636 YX= 0.7568 ZX= -2.1334
XY= 1.1783 YY= 25.7294 ZY= -4.5851
XZ= -1.6305 YZ= -3.8032 ZZ= 25.7817
Eigenvalues: 20.3130 21.8734 30.3882
60 H Isotropic = 25.6400 Anisotropy = 14.4183
XX= 33.9005 YX= 3.0295 ZX= -3.0121
XY= 6.6971 YY= 17.3968 ZY= 3.6329
XZ= 2.6869 YZ= 1.2464 ZZ= 25.6228
Eigenvalues: 15.5022 26.1657 35.2522
61 H Isotropic = 24.4796 Anisotropy = 9.9569

XX= 22.8436 YX= -1.0978 ZX= 3.8145
XY= -0.3968 YY= 21.1326 ZY= 3.8460
XZ= 2.2045 YZ= 1.4120 ZZ= 29.4627
Eigenvalues: 19.4768 22.8445 31.1176
62 H Isotropic = 24.8673 Anisotropy = 4.5585
XX= 27.2476 YX= 0.8766 ZX= 0.7420
XY= 1.4022 YY= 21.4724 ZY= 1.0827
XZ= 0.8147 YZ= 0.6651 ZZ= 25.8820
Eigenvalues: 21.1452 25.5505 27.9063
63 H Isotropic = 24.4842 Anisotropy = 5.0998
XX= 24.7646 YX= 0.0844 ZX= -0.8653
XY= 0.5421 YY= 21.1692 ZY= 1.1691
XZ= -1.0275 YZ= 0.4658 ZZ= 27.5190
Eigenvalues: 21.0148 24.5539 27.8841
64 H Isotropic = 23.9478 Anisotropy = 9.6927
XX= 21.6813 YX= -0.2738 ZX= 1.4742
XY= 1.3215 YY= 20.4469 ZY= 1.9362
XZ= 1.9733 YZ= 1.6062 ZZ= 29.7153
Eigenvalues: 20.0878 21.3461 30.4096
65 H Isotropic = 28.6845 Anisotropy = 7.8849
XX= 32.2764 YX= -1.8393 ZX= -4.2596
XY= 0.0314 YY= 28.5945 ZY= 2.3052
XZ= -2.8334 YZ= -1.3219 ZZ= 25.1827
Eigenvalues: 23.7114 28.4011 33.9412
66 H Isotropic = 27.8710 Anisotropy = 9.4308
XX= 33.6778 YX= 0.3299 ZX= 2.0379
XY= 1.0963 YY= 23.7000 ZY= -1.3722
XZ= 1.7935 YZ= -1.0398 ZZ= 26.2354
Eigenvalues: 23.0299 26.4250 34.1583
67 H Isotropic = 29.3742 Anisotropy = 6.9833
XX= 26.7904 YX= 0.8254 ZX= 0.2603
XY= 0.4287 YY= 33.8292 ZY= 0.3944
XZ= 0.6824 YZ= 1.4734 ZZ= 27.5031
Eigenvalues: 26.5525 27.5405 34.0298
68 H Isotropic = 27.8895 Anisotropy = 5.8439
XX= 30.5156 YX= -2.3333 ZX= 0.0261
XY= -2.1305 YY= 27.7630 ZY= -2.0433
XZ= -1.1715 YZ= -1.5350 ZZ= 25.3901
Eigenvalues: 24.0163 27.8668 31.7855
69 H Isotropic = 27.7684 Anisotropy = 7.7715
XX= 30.6804 YX= 3.0247 ZX= 2.8251
XY= 2.9592 YY= 23.6143 ZY= 0.4467
XZ= 1.3154 YZ= 0.7418 ZZ= 29.0106
Eigenvalues: 22.5136 27.8422 32.9495
70 H Isotropic = 30.5672 Anisotropy = 6.6224
XX= 29.6079 YX= 0.6250 ZX= -0.6861

XY= 0.1343 YY= 34.2655 ZY= -2.0502
XZ= 0.0616 YZ= -2.3432 ZZ= 27.8283
Eigenvalues: 27.1359 29.5836 34.9822
71 H Isotropic = 30.6109 Anisotropy = 6.5867
XX= 30.6572 YX= 2.6503 ZX= 0.4741
XY= 1.3104 YY= 27.4614 ZY= 1.9539
XZ= 1.2595 YZ= 2.6970 ZZ= 33.7142
Eigenvalues: 26.0926 30.7381 35.0020
72 H Isotropic = 30.8085 Anisotropy = 10.9483
XX= 37.4910 YX= 1.1572 ZX= -2.0144
XY= 1.0074 YY= 26.7409 ZY= -0.7495
XZ= -2.3675 YZ= -0.5290 ZZ= 28.1937
Eigenvalues: 26.4925 27.8257 38.1074
73 H Isotropic = 24.7805 Anisotropy = 8.0581
XX= 22.5945 YX= -2.2364 ZX= 0.5151
XY= -3.7987 YY= 27.6340 ZY= -2.1363
XZ= 1.1983 YZ= -2.7680 ZZ= 24.1130
Eigenvalues: 21.1504 23.0386 30.1526
74 H Isotropic = 24.5677 Anisotropy = 5.8123
XX= 21.8258 YX= -0.9456 ZX= 0.5474
XY= -1.2202 YY= 28.1187 ZY= 1.0351
XZ= 0.6122 YZ= 0.8032 ZZ= 23.7586
Eigenvalues: 21.4121 23.8483 28.4426
75 H Isotropic = 24.5758 Anisotropy = 3.7669
XX= 21.7240 YX= -0.8207 ZX= 0.3572
XY= -0.9543 YY= 24.9743 ZY= 0.3508
XZ= 0.4933 YZ= 0.2274 ZZ= 27.0290
Eigenvalues: 21.4554 25.1848 27.0870
76 H Isotropic = 24.2731 Anisotropy = 5.5483
XX= 21.1507 YX= -0.8021 ZX= -0.2797
XY= -1.2287 YY= 27.4631 ZY= -1.0773
XZ= -0.3444 YZ= -1.3324 ZZ= 24.2055
Eigenvalues: 20.9123 23.9351 27.9719
77 H Isotropic = 23.6691 Anisotropy = 9.5592
XX= 20.1372 YX= -2.5653 ZX= -1.4224
XY= -2.4595 YY= 27.9983 ZY= 3.1103
XZ= -0.8438 YZ= 2.6081 ZZ= 22.8717
Eigenvalues: 19.3703 21.5951 30.0419
78 H Isotropic = 23.4786 Anisotropy = 5.9523
XX= 25.8905 YX= 1.6624 ZX= 1.3686
XY= 0.3373 YY= 19.5074 ZY= -1.8682
XZ= 2.4830 YZ= -1.4753 ZZ= 25.0380
Eigenvalues: 18.7191 24.2699 27.4468

B3LYP /6-311+g(2d,p) calculated optimal geometry, energy (in a.u.), GIAO nuclear magnetic shielding tensors of **2b** compound R optical isomer

E = -2273.72652382

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.978853	1.388408	-0.321360
2	8	0	-4.010635	0.884846	0.799539
3	8	0	-3.452960	1.405533	-1.709993
4	8	0	-2.690946	2.793641	0.399538
5	7	0	-1.587349	0.497225	-0.201770
6	6	0	-0.750737	0.204398	0.885673
7	6	0	5.120489	-1.461246	-2.577820
8	8	0	4.017930	-0.660732	-2.635372
9	6	0	0.462718	-0.464391	0.606027
10	6	0	3.905632	-0.115875	-1.383444
11	6	0	-4.752778	-0.292251	0.629360
12	7	0	0.773098	-0.742775	-0.765799
13	6	0	-5.786192	-0.340376	-0.296297
14	6	0	-1.992966	4.247949	-1.417087
15	6	0	-1.077711	0.525286	2.203906
16	8	0	4.711915	0.702313	1.287053
17	7	0	5.703544	-1.474006	-1.437904
18	6	0	-1.808797	3.734974	-0.138887
19	6	0	-0.233043	0.158556	3.245215
20	6	0	1.333448	0.413963	-1.506158
21	6	0	2.788238	0.830860	-1.125692
22	6	0	-5.238949	-2.521752	1.353742
23	6	0	1.280600	-0.836686	1.669505
24	6	0	4.950058	-0.608024	-0.648147
25	6	0	-6.547773	-1.500210	-0.390016
26	6	0	-4.466663	-1.369295	1.455252
27	6	0	0.940231	-0.536589	2.984667
28	6	0	5.348733	-0.366081	0.754838
29	8	0	6.150896	-1.034489	1.355812
30	6	0	-0.783430	4.185970	0.681181
31	6	0	-1.118470	5.227434	-1.877859
32	6	0	-6.279266	-2.590181	0.432779
33	6	0	0.078179	5.170248	0.209380
34	6	0	-0.084646	5.691458	-1.070638
35	6	0	5.046146	1.011610	2.663049
36	6	0	4.281678	2.256926	3.054727
37	6	0	1.101511	0.295875	-3.015432
38	1	0	1.667134	-0.510958	-3.478098

39	1	0	0.041330	0.136922	-3.221099
40	1	0	1.402356	1.224081	-3.505886
41	6	0	1.351817	-2.064422	-1.044185
42	6	0	0.410385	-3.207481	-0.722170
43	6	0	-1.292430	-5.368262	-0.186250
44	6	0	0.816676	-4.243145	0.117237
45	6	0	-0.862414	-3.270122	-1.293184
46	6	0	-1.708737	-4.339083	-1.027214
47	6	0	-0.026329	-5.318773	0.384090
48	1	0	2.302285	-2.232776	-0.523660
49	1	0	1.582858	-2.092336	-2.109489
50	1	0	1.802553	-4.210076	0.568460
51	1	0	-1.192791	-2.474763	-1.951439
52	1	0	-2.694136	-4.369942	-1.476739
53	1	0	-1.952198	-6.202364	0.021520
54	1	0	0.306405	-6.113519	1.041418
55	1	0	-3.650943	-1.299011	2.162899
56	1	0	-5.021829	-3.366964	1.995498
57	1	0	-6.879398	-3.488739	0.356736
58	1	0	-7.355978	-1.548430	-1.109854
59	1	0	-5.974268	0.512339	-0.934067
60	1	0	-1.304529	0.026683	-1.053855
61	1	0	2.202110	-1.367680	1.469403
62	1	0	1.590084	-0.842817	3.795148
63	1	0	-0.507967	0.405425	4.263748
64	1	0	-2.004471	1.039974	2.417337
65	1	0	0.737374	1.267233	-1.174077
66	1	0	2.818972	1.079512	-0.067209
67	1	0	2.996138	1.762881	-1.665399
68	1	0	4.781618	0.155168	3.285456
69	1	0	6.125626	1.152277	2.731968
70	1	0	4.552466	3.099899	2.416203
71	1	0	3.204616	2.096189	2.984145
72	1	0	4.520765	2.521225	4.087307
73	1	0	-0.674037	3.767069	1.673016
74	1	0	0.877356	5.529965	0.846352
75	1	0	0.587182	6.459081	-1.434810
76	1	0	-1.254014	5.632315	-2.873611
77	1	0	-2.800586	3.876317	-2.032957
78	1	0	5.384831	-1.989865	-3.479162

Calculated GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 P Isotropic = 304.3888 Anisotropy = 216.3719
XX= 220.7215 YX= 3.8770 ZX= 56.5217
XY= -0.4045 YY= 258.6372 ZY= 42.0294
XZ= 23.4905 YZ= 34.3847 ZZ= 433.8078

Eigenvalues: 212.7960 251.7337 448.6367
2 O Isotropic = 163.0857 Anisotropy = 94.4264
XX= 183.2433 YX= 46.7364 ZX= 9.6077
XY= 27.6026 YY= 186.8218 ZY= 6.3866
XZ= 19.9481 YZ= 21.0484 ZZ= 119.1921
Eigenvalues: 115.3559 147.8646 226.0367
3 O Isotropic = 177.9816 Anisotropy = 54.3792
XX= 178.9889 YX= -1.4166 ZX= -0.9327
XY= -0.1614 YY= 143.7483 ZY= 12.5054
XZ= -11.7096 YZ= 10.3124 ZZ= 211.2075
Eigenvalues: 141.8694 177.8410 214.2344
4 O Isotropic = 166.1808 Anisotropy = 89.2499
XX= 213.8614 YX= -40.2744 ZX= -1.2064
XY= -13.9895 YY= 160.9341 ZY= -18.0101
XZ= -1.7411 YZ= -20.4206 ZZ= 123.7469
Eigenvalues: 113.9994 158.8622 225.6807
5 N Isotropic = 163.3090 Anisotropy = 56.0480
XX= 141.5450 YX= -12.0349 ZX= -21.5870
XY= -3.6865 YY= 158.5323 ZY= -18.5367
XZ= -25.7059 YZ= -2.7471 ZZ= 189.8498
Eigenvalues: 127.6699 161.5828 200.6743
6 C Isotropic = 39.2578 Anisotropy = 152.2700
XX= 32.2398 YX= -29.7123 ZX= 2.8199
XY= -23.9224 YY= 130.7347 ZY= -21.5969
XZ= 20.5353 YZ= -22.8272 ZZ= -45.2011
Eigenvalues: -48.8551 25.8574 140.7711
7 C Isotropic = 25.6960 Anisotropy = 89.3306
XX= 31.7136 YX= -16.3686 ZX= 37.2864
XY= -10.7932 YY= 52.1772 ZY= 54.6805
XZ= 30.3736 YZ= 54.0020 ZZ= -6.8027
Eigenvalues: -54.2676 46.1060 85.2497
8 O Isotropic = -12.4767 Anisotropy = 260.4488
XX= -131.6323 YX= -5.6584 ZX= 44.8863
XY= 23.4758 YY= 103.9513 ZY= 93.4566
XZ= 0.4544 YZ= 101.4316 ZZ= -9.7492
Eigenvalues: -136.1436 -62.4423 161.1558
9 C Isotropic = 41.4010 Anisotropy = 137.4014
XX= -8.1161 YX= -44.0652 ZX= -10.6416
XY= -40.0814 YY= 115.3732 ZY= -31.2550
XZ= -24.1169 YZ= -27.2431 ZZ= 16.9458
Eigenvalues: -34.3261 25.5271 133.0019
10 C Isotropic = 19.7376 Anisotropy = 125.6553
XX= -31.0180 YX= -14.7024 ZX= 48.8785
XY= 2.4605 YY= 75.0077 ZY= 45.7148
XZ= 22.8881 YZ= 51.8142 ZZ= 15.2231
Eigenvalues: -57.7231 13.4281 103.5078

```
 11  C    Isotropic =    25.3993   Anisotropy =   113.9553
XX=    79.1215   YX=    50.3743   ZX=    -3.2113
XY=    51.6934   YY=   -37.5522   ZY=    41.7010
XZ=    -1.0465   YZ=    44.3370   ZZ=    34.6287
Eigenvalues:   -72.5698    47.3983   101.3696
 12  N    Isotropic =   179.3293   Anisotropy =    71.4717
XX=   178.7164   YX=   -12.7751   ZX=     7.5053
XY=    -8.5013   YY=   224.4536   ZY=    19.3140
XZ=    24.1269   YZ=   -20.2208   ZZ=   134.8178
Eigenvalues:   129.6265   181.3843   226.9770
 13  C    Isotropic =    53.5653   Anisotropy =   162.6971
XX=   116.2464   YX=    66.6272   ZX=    54.1938
XY=    69.7803   YY=    23.8178   ZY=   -19.7960
XZ=    45.5122   YZ=   -15.7894   ZZ=    20.6319
Eigenvalues:   -40.4090    39.0750   162.0301
 14  C    Isotropic =    55.3757   Anisotropy =   167.1585
XX=   165.6564   YX=    -1.7392   ZX=    -9.0487
XY=    -5.6602   YY=    21.9919   ZY=    36.0737
XZ=   -17.1112   YZ=    27.4305   ZZ=   -21.5210
Eigenvalues:   -38.7323    38.0448   166.8148
 15  C    Isotropic =    61.9110   Anisotropy =   162.9363
XX=    -8.2935   YX=   -44.4422   ZX=    27.2884
XY=   -46.3558   YY=   155.8182   ZY=   -12.0247
XZ=    32.7988   YZ=   -13.0314   ZZ=    38.2083
Eigenvalues:   -30.1602    45.3580   170.5352
 16  O    Isotropic =   113.1391   Anisotropy =   173.1703
XX=    10.3273   YX=    37.2896   ZX=   -44.5481
XY=    89.9295   YY=   156.8197   ZY=     2.6824
XZ=  -157.4240   YZ=    10.9931   ZZ=   172.2703
Eigenvalues:   -55.4108   166.2422   228.5859
 17  N    Isotropic =   -36.2497   Anisotropy =   371.7783
XX=  -171.1634   YX=   -10.7923   ZX=    77.3174
XY=    -9.7031   YY=   120.7586   ZY=   153.8790
XZ=    79.9296   YZ=   153.5553   ZZ=   -58.3442
Eigenvalues:  -234.4277   -85.9239   211.6025
 18  C    Isotropic =    24.9245   Anisotropy =   117.5529
XX=   101.7216   YX=    -7.5865   ZX=   -10.3748
XY=    -7.0889   YY=   -70.8942   ZY=     9.2435
XZ=    -6.1145   YZ=     8.6576   ZZ=    43.9460
Eigenvalues:   -71.8456    43.3260   103.2930
 19  C    Isotropic =    53.2211   Anisotropy =   179.1139
XX=    -6.2091   YX=   -54.5046   ZX=   -35.9190
XY=   -56.3078   YY=   151.7343   ZY=   -32.8180
XZ=   -38.8608   YZ=   -37.7679   ZZ=    14.1382
Eigenvalues:   -55.4902    42.5232   172.6304
 20  C    Isotropic =   122.4989   Anisotropy =    38.3487
```

XX= 101.5261 YX= 0.3817 ZX= 6.0339
XY= -1.4558 YY= 145.6316 ZY= 13.6583
XZ= 4.7634 YZ= 2.6858 ZZ= 120.3390
Eigenvalues: 99.9267 119.5053 148.0647
21 C Isotropic = 149.5342 Anisotropy = 35.9945
XX= 130.6604 YX= 8.0529 ZX= 13.6286
XY= 12.2068 YY= 143.1173 ZY= -1.0850
XZ= 7.0520 YZ= -7.0862 ZZ= 168.8249
Eigenvalues: 122.3784 148.6937 171.5305
22 C Isotropic = 48.7245 Anisotropy = 186.6124
XX= 120.8486 YX= 79.1614 ZX= 57.8799
XY= 76.8349 YY= 16.6091 ZY= -23.6524
XZ= 59.5895 YZ= -25.8324 ZZ= 8.7160
Eigenvalues: -63.0233 36.0641 173.1328
23 C Isotropic = 52.1021 Anisotropy = 188.4101
XX= -25.4721 YX= -43.5297 ZX= 39.2583
XY= -68.2484 YY= 153.0589 ZY= -32.5403
XZ= 39.4469 YZ= -18.2366 ZZ= 28.7195
Eigenvalues: -53.8567 32.4542 177.7088
24 C Isotropic = 46.4181 Anisotropy = 86.9503
XX= -2.4043 YX= -0.0629 ZX= 19.9899
XY= -7.8031 YY= 86.5251 ZY= 29.5758
XZ= 32.3244 YZ= 27.4505 ZZ= 55.1335
Eigenvalues: -14.6063 49.4757 104.3850
25 C Isotropic = 49.1156 Anisotropy = 184.2301
XX= 138.8909 YX= 42.9572 ZX= 47.1671
XY= 43.7537 YY= 52.5631 ZY= 33.4849
XZ= 46.9427 YZ= 36.0515 ZZ= -44.1072
Eigenvalues: -60.9781 36.3892 171.9357
26 C Isotropic = 56.4514 Anisotropy = 161.6919
XX= 135.7654 YX= 36.1770 ZX= 39.7864
XY= 39.7747 YY= 57.0957 ZY= 34.7695
XZ= 41.6641 YZ= 27.7336 ZZ= -23.5068
Eigenvalues: -38.7356 43.8438 164.2460
27 C Isotropic = 59.5944 Anisotropy = 168.3297
XX= 60.7739 YX= -27.2549 ZX= 13.2399
XY= -28.7942 YY= 158.1809 ZY= -33.0066
XZ= 17.8803 YZ= -33.3392 ZZ= -40.1717
Eigenvalues: -46.7146 53.6836 171.8142
28 C Isotropic = 16.5524 Anisotropy = 74.9199
XX= -38.5928 YX= -13.4979 ZX= 48.7269
XY= -28.9766 YY= 59.4495 ZY= 14.1778
XZ= 77.1075 YZ= 11.8326 ZZ= 28.8006
Eigenvalues: -80.6934 63.8517 66.4990
29 O Isotropic = -95.7758 Anisotropy = 598.7983
XX= -241.3659 YX= 64.0017 ZX= -32.2653

XY= 50.0523 YY= 171.0116 ZY= 256.9957
XZ= -18.1280 YZ= 260.7346 ZZ= -216.9733
Eigenvalues: -365.4375 -225.3131 303.4230
30 C Isotropic = 56.6955 Anisotropy = 159.7597
XX= 161.2789 YX= -6.6590 ZX= -16.1412
XY= -11.2472 YY= 19.0223 ZY= -37.9279
XZ= -18.3667 YZ= -35.3650 ZZ= -10.2146
Eigenvalues: -36.9317 43.8163 163.2020
31 C Isotropic = 49.1481 Anisotropy = 185.1157
XX= 170.3308 YX= -10.7990 ZX= -19.5832
XY= -10.4118 YY= 7.1366 ZY= -42.4845
XZ= -20.4368 YZ= -45.5324 ZZ= -30.0230
Eigenvalues: -61.4054 36.2911 172.5586
32 C Isotropic = 52.8729 Anisotropy = 183.4673
XX= 136.9645 YX= 74.2031 ZX= 18.2099
XY= 72.1260 YY= -16.1654 ZY= 43.9878
XZ= 19.7959 YZ= 45.2558 ZZ= 37.8194
Eigenvalues: -58.4559 41.8901 175.1844
33 C Isotropic = 49.6502 Anisotropy = 183.4192
XX= 170.0276 YX= -0.3181 ZX= -19.3390
XY= -2.5785 YY= 19.2933 ZY= 38.2735
XZ= -18.9941 YZ= 40.3295 ZZ= -40.3702
Eigenvalues: -61.0659 38.0869 171.9297
34 C Isotropic = 53.7815 Anisotropy = 182.4171
XX= 173.8444 YX= -7.7395 ZX= -13.3506
XY= -7.3187 YY= -56.0180 ZY= 6.4604
XZ= -12.4202 YZ= 6.8413 ZZ= 43.5180
Eigenvalues: -56.6542 42.6057 175.3929
35 C Isotropic = 120.3679 Anisotropy = 60.9566
XX= 158.8543 YX= -4.6296 ZX= 3.1438
XY= 0.1312 YY= 96.5742 ZY= -2.2934
XZ= -7.3538 YZ= -1.2254 ZZ= 99.6752
Eigenvalues: 95.6446 100.4535 159.0056
36 C Isotropic = 168.0811 Anisotropy = 21.8566
XX= 170.7120 YX= 1.6158 ZX= -2.5289
XY= 4.1016 YY= 158.9563 ZY= -10.1752
XZ= -8.8852 YZ= -9.2816 ZZ= 174.5751
Eigenvalues: 154.2897 167.3015 182.6522
37 C Isotropic = 168.8944 Anisotropy = 26.0133
XX= 160.4729 YX= 5.8777 ZX= -2.9811
XY= 0.6015 YY= 164.7542 ZY= -12.9914
XZ= 0.5611 YZ= -6.6593 ZZ= 181.4562
Eigenvalues: 157.8019 162.6448 186.2366
38 H Isotropic = 31.3990 Anisotropy = 9.8758
XX= 27.6614 YX= -0.4923 ZX= -0.6501
XY= 0.4969 YY= 37.6260 ZY= -1.4745

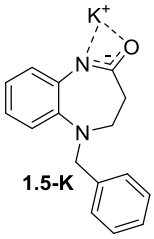
XZ= -0.1940 YZ= -2.1209 ZZ= 28.9096
Eigenvalues: 27.4986 28.7155 37.9829
39 H Isotropic = 30.7996 Anisotropy = 6.1885
XX= 28.2933 YX= 0.2513 ZX= 2.4585
XY= 3.5267 YY= 30.6388 ZY= -2.2102
XZ= 3.3763 YZ= -1.0730 ZZ= 33.4665
Eigenvalues: 25.7840 31.6895 34.9252
40 H Isotropic = 30.7481 Anisotropy = 8.0985
XX= 32.7739 YX= -0.1759 ZX= -3.4709
XY= 1.9144 YY= 29.1089 ZY= -1.9889
XZ= -4.3178 YZ= -1.9327 ZZ= 30.3615
Eigenvalues: 26.8761 29.2210 36.1471
41 C Isotropic = 128.0132 Anisotropy = 27.1518
XX= 133.4519 YX= -10.1896 ZX= -9.2462
XY= -13.3537 YY= 141.3229 ZY= -2.3220
XZ= -8.4995 YZ= -3.4433 ZZ= 121.2648
Eigenvalues: 113.9071 132.0181 150.1144
42 C Isotropic = 38.2982 Anisotropy = 195.2316
XX= 153.6781 YX= 16.3944 ZX= 37.9934
XY= 15.5718 YY= -62.4600 ZY= 6.8587
XZ= 49.4174 YZ= 13.6212 ZZ= 23.6764
Eigenvalues: -64.2572 10.6992 168.4526
43 C Isotropic = 52.0299 Anisotropy = 183.1120
XX= 155.5749 YX= 21.1625 ZX= 43.2736
XY= 18.8187 YY= -55.1259 ZY= 14.3209
XZ= 42.8882 YZ= 16.0239 ZZ= 55.6407
Eigenvalues: -58.1765 40.1617 174.1046
44 C Isotropic = 49.7247 Anisotropy = 163.1837
XX= 138.6198 YX= -11.7150 ZX= 55.5607
XY= -4.1395 YY= 29.2467 ZY= 40.7389
XZ= 62.3666 YZ= 41.3636 ZZ= -18.6925
Eigenvalues: -58.0530 48.7132 158.5138
45 C Isotropic = 49.7268 Anisotropy = 186.5011
XX= 145.8096 YX= 29.9861 ZX= 64.7992
XY= 30.0828 YY= 6.4466 ZY= -32.9955
XZ= 72.5371 YZ= -38.4934 ZZ= -3.0758
Eigenvalues: -59.8471 34.9667 174.0609
46 C Isotropic = 49.6300 Anisotropy = 188.3723
XX= 150.6088 YX= 0.6568 ZX= 66.0215
XY= 0.9389 YY= 21.8043 ZY= 40.7627
XZ= 69.4994 YZ= 41.0384 ZZ= -23.5230
Eigenvalues: -64.1324 37.8109 175.2116
47 C Isotropic = 51.3209 Anisotropy = 180.8915
XX= 143.4606 YX= 30.8559 ZX= 67.1441
XY= 30.7441 YY= 10.4516 ZY= -38.6822
XZ= 68.8222 YZ= -38.9312 ZZ= 0.0504

Eigenvalues: -59.6063 41.6537 171.9152
48 H Isotropic = 27.7956 Anisotropy = 8.6351
XX= 28.2743 YX= -1.2272 ZX= -5.0287
XY= -2.3736 YY= 25.8324 ZY= 0.9545
XZ= -3.5814 YZ= 0.7586 ZZ= 29.2802
Eigenvalues: 24.0244 25.8102 33.5524
49 H Isotropic = 27.6486 Anisotropy = 6.4792
XX= 30.1842 YX= 2.6369 ZX= 2.6502
XY= -1.3203 YY= 26.7755 ZY= 3.9623
XZ= 1.3102 YZ= 3.2315 ZZ= 25.9861
Eigenvalues: 22.6120 28.3658 31.9681
50 H Isotropic = 24.6620 Anisotropy = 8.9408
XX= 22.9494 YX= -2.1581 ZX= -1.6299
XY= -3.8631 YY= 27.4495 ZY= 3.4672
XZ= -1.5439 YZ= 2.5977 ZZ= 23.5871
Eigenvalues: 21.4348 21.9286 30.6226
51 H Isotropic = 25.3726 Anisotropy = 7.9214
XX= 22.8758 YX= 0.1939 ZX= -0.0326
XY= -0.1845 YY= 29.7741 ZY= -3.5979
XZ= 0.1943 YZ= -1.4295 ZZ= 23.4679
Eigenvalues: 22.5687 22.8955 30.6535
52 H Isotropic = 24.9979 Anisotropy = 6.0727
XX= 24.0184 YX= -1.8586 ZX= -1.4697
XY= -1.1144 YY= 28.4217 ZY= 0.2595
XZ= -0.6268 YZ= 1.2765 ZZ= 22.5537
Eigenvalues: 22.0073 23.9401 29.0464
53 H Isotropic = 24.7482 Anisotropy = 4.4296
XX= 22.7966 YX= -1.2745 ZX= -2.4991
XY= -1.1695 YY= 25.0803 ZY= 0.0608
XZ= -2.1580 YZ= 0.2325 ZZ= 26.3678
Eigenvalues: 21.3566 25.1867 27.7013
54 H Isotropic = 24.6763 Anisotropy = 4.9683
XX= 22.1366 YX= -0.9232 ZX= -1.6854
XY= -1.0223 YY= 27.4972 ZY= -1.2148
XZ= -1.1281 YZ= -1.3245 ZZ= 24.3952
Eigenvalues: 21.1354 24.9051 27.9885
55 H Isotropic = 25.2568 Anisotropy = 7.9545
XX= 23.0685 YX= -2.2791 ZX= -1.2630
XY= -0.0924 YY= 30.3628 ZY= -0.7823
XZ= -0.6035 YZ= -0.0643 ZZ= 22.3392
Eigenvalues: 21.5803 23.6304 30.5598
56 H Isotropic = 24.8434 Anisotropy = 5.9147
XX= 22.5887 YX= 0.1709 ZX= -0.9674
XY= -0.0894 YY= 27.0965 ZY= -2.8269
XZ= -0.2300 YZ= -2.2887 ZZ= 24.8450
Eigenvalues: 22.3049 23.4386 28.7865

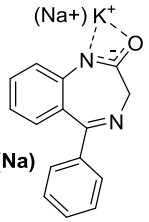
57 H Isotropic = 24.5369 Anisotropy = 4.3996
XX= 22.2752 YX= -0.4035 ZX= -2.4556
XY= -0.5697 YY= 24.8688 ZY= -0.2635
XZ= -2.0455 YZ= 0.3780 ZZ= 26.4668
Eigenvalues: 21.2461 24.8947 27.4700
58 H Isotropic = 24.2990 Anisotropy = 5.1311
XX= 22.2467 YX= -1.9051 ZX= -1.1987
XY= -1.6647 YY= 27.0979 ZY= -1.0116
XZ= -0.9975 YZ= -0.4971 ZZ= 23.5525
Eigenvalues: 21.0119 24.1654 27.7198
59 H Isotropic = 24.1916 Anisotropy = 9.2950
XX= 21.0636 YX= 0.7568 ZX= -2.1334
XY= 1.1783 YY= 25.7294 ZY= -4.5851
XZ= -1.6305 YZ= -3.8032 ZZ= 25.7817
Eigenvalues: 20.3130 21.8734 30.3882
60 H Isotropic = 25.6400 Anisotropy = 14.4183
XX= 33.9005 YX= 3.0295 ZX= -3.0121
XY= 6.6971 YY= 17.3968 ZY= 3.6329
XZ= 2.6869 YZ= 1.2464 ZZ= 25.6228
Eigenvalues: 15.5022 26.1657 35.2522
61 H Isotropic = 24.4796 Anisotropy = 9.9569
XX= 22.8436 YX= -1.0978 ZX= 3.8145
XY= -0.3968 YY= 21.1326 ZY= 3.8460
XZ= 2.2045 YZ= 1.4120 ZZ= 29.4627
Eigenvalues: 19.4768 22.8445 31.1176
62 H Isotropic = 24.8673 Anisotropy = 4.5585
XX= 27.2476 YX= 0.8766 ZX= 0.7420
XY= 1.4022 YY= 21.4724 ZY= 1.0827
XZ= 0.8147 YZ= 0.6651 ZZ= 25.8820
Eigenvalues: 21.1452 25.5505 27.9063
63 H Isotropic = 24.4842 Anisotropy = 5.0998
XX= 24.7646 YX= 0.0844 ZX= -0.8653
XY= 0.5421 YY= 21.1692 ZY= 1.1691
XZ= -1.0275 YZ= 0.4658 ZZ= 27.5190
Eigenvalues: 21.0148 24.5539 27.8841
64 H Isotropic = 23.9478 Anisotropy = 9.6927
XX= 21.6813 YX= -0.2738 ZX= 1.4742
XY= 1.3215 YY= 20.4469 ZY= 1.9362
XZ= 1.9733 YZ= 1.6062 ZZ= 29.7153
Eigenvalues: 20.0878 21.3461 30.4096
65 H Isotropic = 28.6845 Anisotropy = 7.8849
XX= 32.2764 YX= -1.8393 ZX= -4.2596
XY= 0.0314 YY= 28.5945 ZY= 2.3052
XZ= -2.8334 YZ= -1.3219 ZZ= 25.1827
Eigenvalues: 23.7114 28.4011 33.9412
66 H Isotropic = 27.8710 Anisotropy = 9.4308

XX= 33.6778 YX= 0.3299 ZX= 2.0379
XY= 1.0963 YY= 23.7000 ZY= -1.3722
XZ= 1.7935 YZ= -1.0398 ZZ= 26.2354
Eigenvalues: 23.0299 26.4250 34.1583
67 H Isotropic = 29.3742 Anisotropy = 6.9833
XX= 26.7904 YX= 0.8254 ZX= 0.2603
XY= 0.4287 YY= 33.8292 ZY= 0.3944
XZ= 0.6824 YZ= 1.4734 ZZ= 27.5031
Eigenvalues: 26.5525 27.5405 34.0298
68 H Isotropic = 27.8895 Anisotropy = 5.8439
XX= 30.5156 YX= -2.3333 ZX= 0.0261
XY= -2.1305 YY= 27.7630 ZY= -2.0433
XZ= -1.1715 YZ= -1.5350 ZZ= 25.3901
Eigenvalues: 24.0163 27.8668 31.7855
69 H Isotropic = 27.7684 Anisotropy = 7.7715
XX= 30.6804 YX= 3.0247 ZX= 2.8251
XY= 2.9592 YY= 23.6143 ZY= 0.4467
XZ= 1.3154 YZ= 0.7418 ZZ= 29.0106
Eigenvalues: 22.5136 27.8422 32.9495
70 H Isotropic = 30.5672 Anisotropy = 6.6224
XX= 29.6079 YX= 0.6250 ZX= -0.6861
XY= 0.1343 YY= 34.2655 ZY= -2.0502
XZ= 0.0616 YZ= -2.3432 ZZ= 27.8283
Eigenvalues: 27.1359 29.5836 34.9822
71 H Isotropic = 30.6109 Anisotropy = 6.5867
XX= 30.6572 YX= 2.6503 ZX= 0.4741
XY= 1.3104 YY= 27.4614 ZY= 1.9539
XZ= 1.2595 YZ= 2.6970 ZZ= 33.7142
Eigenvalues: 26.0926 30.7381 35.0020
72 H Isotropic = 30.8085 Anisotropy = 10.9483
XX= 37.4910 YX= 1.1572 ZX= -2.0144
XY= 1.0074 YY= 26.7409 ZY= -0.7495
XZ= -2.3675 YZ= -0.5290 ZZ= 28.1937
Eigenvalues: 26.4925 27.8257 38.1074
73 H Isotropic = 24.7805 Anisotropy = 8.0581
XX= 22.5945 YX= -2.2364 ZX= 0.5151
XY= -3.7987 YY= 27.6340 ZY= -2.1363
XZ= 1.1983 YZ= -2.7680 ZZ= 24.1130
Eigenvalues: 21.1504 23.0386 30.1526
74 H Isotropic = 24.5677 Anisotropy = 5.8123
XX= 21.8258 YX= -0.9456 ZX= 0.5474
XY= -1.2202 YY= 28.1187 ZY= 1.0351
XZ= 0.6122 YZ= 0.8032 ZZ= 23.7586
Eigenvalues: 21.4121 23.8483 28.4426
75 H Isotropic = 24.5758 Anisotropy = 3.7669
XX= 21.7240 YX= -0.8207 ZX= 0.3572

XY= -0.9543 YY= 24.9743 ZY= 0.3508
XZ= 0.4933 YZ= 0.2274 ZZ= 27.0290
Eigenvalues: 21.4554 25.1848 27.0870
76 H Isotropic = 24.2731 Anisotropy = 5.5483
XX= 21.1507 YX= -0.8021 ZX= -0.2797
XY= -1.2287 YY= 27.4631 ZY= -1.0773
XZ= -0.3444 YZ= -1.3324 ZZ= 24.2055
Eigenvalues: 20.9123 23.9351 27.9719
77 H Isotropic = 23.6691 Anisotropy = 9.5592
XX= 20.1372 YX= -2.5653 ZX= -1.4224
XY= -2.4595 YY= 27.9983 ZY= 3.1103
XZ= -0.8438 YZ= 2.6081 ZZ= 22.8717
Eigenvalues: 19.3703 21.5951 30.0419
78 H Isotropic = 23.4786 Anisotropy = 5.9523
XX= 25.8905 YX= 1.6624 ZX= 1.3686
XY= 0.3373 YY= 19.5074 ZY= -1.8682
XZ= 2.4830 YZ= -1.4753 ZZ= 25.0380
Eigenvalues: 18.7191 24.2699 27.4468



1.5-K



1.4-K (Na)

Optimal geometry of Model complexes of 1,4-benzodiazepine coordinated with Na^+ or K^+ (**1.4-Na** or **1.4-K**) and 1,5- benzodiazepine coordinated to K+ (**1,5-K)** and Phosphorylated benzodiazepine intermediate

B3LYP/311G+(d,p) optimized geometry and energy (in a.u.) of the model **1.4-K** intermediate

E = -1363.14597014

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.862942	2.354751	0.088250
2	6	0	0.834858	2.239966	-0.504281
3	6	0	-1.290092	1.083777	-0.157229
4	6	0	-1.125661	3.522198	0.014164
5	6	0	0.238941	3.472650	-0.296323
6	6	0	0.104617	1.036445	-0.445932
7	7	0	-2.125061	-0.014098	-0.014657
8	6	0	-2.035959	-1.087379	-0.806111
9	6	0	0.807967	-0.252438	-0.667432
10	7	0	0.325413	-1.243786	-1.327703
11	6	0	-0.991486	-1.098242	-1.925583
12	1	0	-2.921827	2.386753	0.321600
13	1	0	-1.609681	4.477081	0.191276
14	1	0	0.822703	4.382768	-0.369743
15	1	0	1.893756	2.191518	-0.730614

16	1	0	-1.071997	-0.167175	-2.505510
17	1	0	-1.186030	-1.949600	-2.575301
18	19	0	-3.834150	-1.323031	1.482480
19	8	0	-2.780799	-2.092496	-0.648451
20	6	0	2.174927	-0.443546	-0.083950
21	6	0	4.717273	-0.910687	1.020558
22	6	0	2.548692	0.149054	1.129564
23	6	0	3.096005	-1.277910	-0.733140
24	6	0	4.355943	-1.504881	-0.189544
25	6	0	3.807386	-0.087158	1.680079
26	1	0	2.800839	-1.746225	-1.663619
27	1	0	5.059117	-2.145925	-0.710175
28	1	0	5.699454	-1.088745	1.444561
29	1	0	4.075710	0.372601	2.625083
30	1	0	1.847928	0.790088	1.650910

B3LYP/311G+(d,p) optimized geometry and energy (in a.u.) of the model **1.4-Na** intermediate

E = -925.501764478

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.273645	2.082106	0.170293
2	6	0	0.356304	2.124351	-0.680878
3	6	0	-1.608163	0.846289	0.001965
4	6	0	-1.659551	3.290746	-0.104374
5	6	0	-0.332633	3.318688	-0.548502
6	6	0	-0.248098	0.879926	-0.416556
7	7	0	-2.321141	-0.299304	0.332582
8	6	0	-2.196258	-1.445030	-0.345783
9	6	0	0.556597	-0.361643	-0.557012
10	7	0	0.121212	-1.463010	-1.054454
11	6	0	-1.248623	-1.505394	-1.541376
12	1	0	-3.303917	2.053845	0.508364
13	1	0	-2.212432	4.215976	0.019442
14	1	0	0.153123	4.259362	-0.779822
15	1	0	1.390352	2.137715	-1.005112
16	1	0	-1.464634	-0.663020	-2.214729
17	1	0	-1.412488	-2.443218	-2.068714
18	8	0	-2.845759	-2.475471	-0.012149
19	6	0	1.978500	-0.359335	-0.085713
20	6	0	4.634140	-0.467138	0.825301
21	6	0	2.385618	0.394124	1.023212
22	6	0	2.923437	-1.171080	-0.728852
23	6	0	4.239494	-1.219910	-0.281672

24	6	0	3.701631	0.335725	1.478719
25	1	0	2.603744	-1.763427	-1.576889
26	1	0	4.959960	-1.846088	-0.796568
27	1	0	5.659980	-0.506753	1.174791
28	1	0	3.996896	0.917474	2.345129
29	1	0	1.667565	1.019671	1.539828
30	11	0	-3.738642	-1.426920	1.704722

B3LYP/311G+(d,p) optimized geometry and energy (in a.u.) of the model **1.5-K** intermediate

E = -1403.66565860

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.536170	2.067026	0.079981
2	6	0	-0.168950	2.404905	-0.170959
3	6	0	1.737698	0.896585	0.098493
4	6	0	2.031011	3.345285	-0.093108
5	6	0	0.654684	3.518867	-0.243398
6	6	0	0.327136	1.101009	0.008400
7	7	0	2.475526	-0.288072	0.139685
8	19	0	4.978773	-1.021299	-0.166075
9	6	0	2.102369	-1.564929	0.171944
10	8	0	2.990581	-2.476148	0.082208
11	7	0	-0.611697	0.055817	0.120141
12	6	0	-0.294835	-1.084556	0.960978
13	6	0	0.680057	-2.074756	0.332214
14	1	0	3.608722	1.926346	0.175089
15	1	0	2.702883	4.196408	-0.116152
16	1	0	0.227220	4.505234	-0.382576
17	1	0	-1.244758	2.533891	-0.227822
18	1	0	-1.232868	-1.594402	1.201406
19	1	0	0.107753	-0.712432	1.908291
20	1	0	0.742518	-2.990946	0.927334
21	1	0	0.316715	-2.384339	-0.655472
22	6	0	-1.597403	-0.161233	-0.926225
23	6	0	-3.034985	-0.278003	-0.435632
24	6	0	-5.720103	-0.436456	0.378514
25	6	0	-3.474998	0.401982	0.703249
26	6	0	-3.956085	-1.047039	-1.153660
27	6	0	-5.289482	-1.124009	-0.755151
28	6	0	-4.806876	0.324221	1.107478
29	1	0	-1.358111	-1.065322	-1.510367
30	1	0	-1.528131	0.672037	-1.629798
31	1	0	-5.989007	-1.726699	-1.324257

32	1	0	-3.625640	-1.593572	-2.032238
33	1	0	-2.760952	0.982008	1.277117
34	1	0	-5.131551	0.856870	1.994920
35	1	0	-6.755388	-0.498827	0.694798