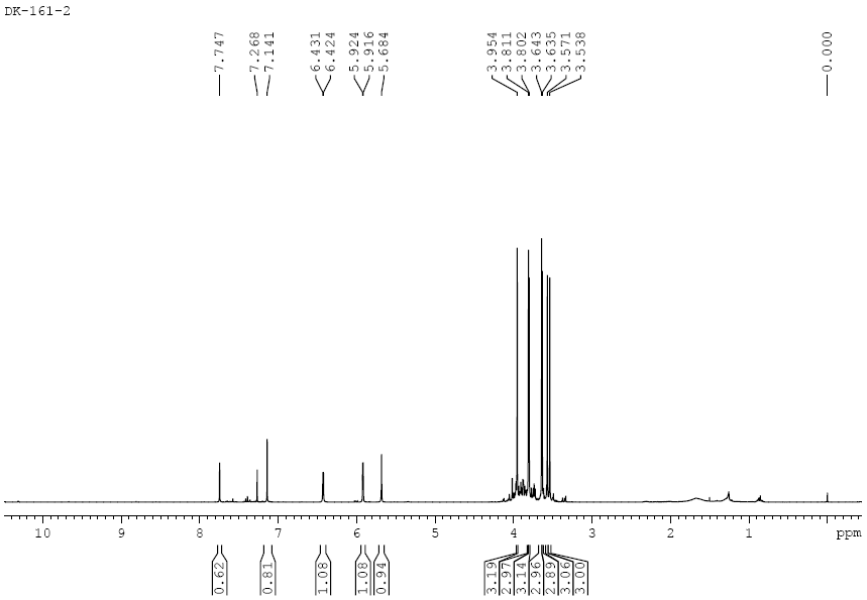
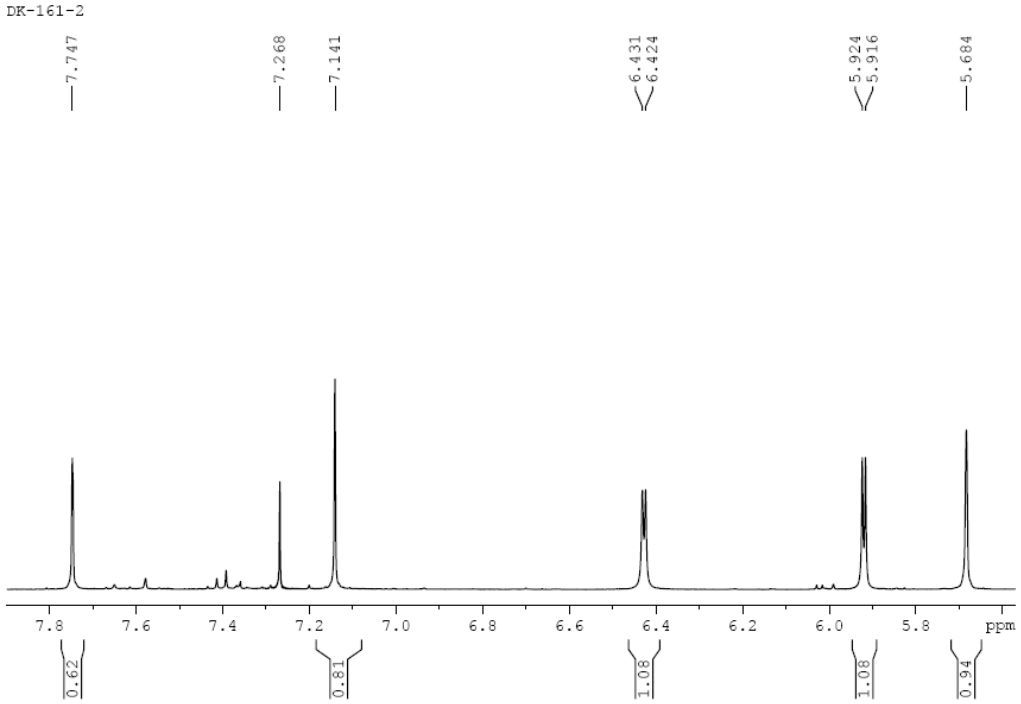
# Supplementary Material

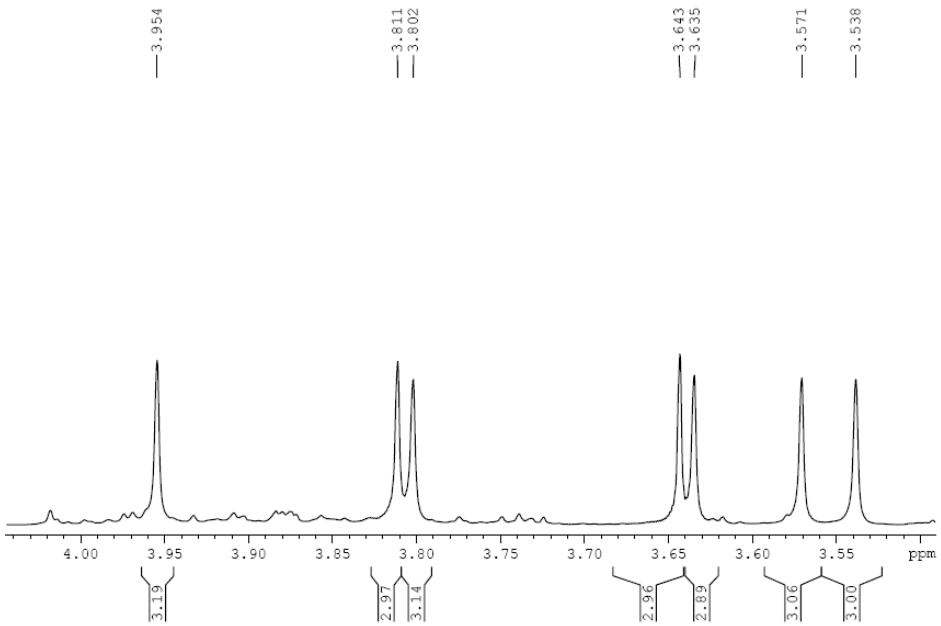
**Contents:** **Page No.**

## $^{1}$H-NMR spectrum for compound III

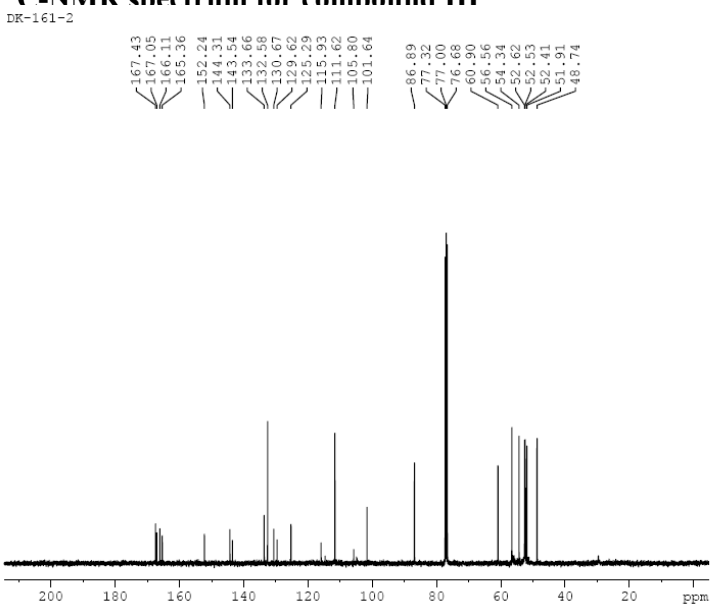


DK-161-2


3.954
3.811
3.802
3.643
3.635
3.571
3.538
4.00
3.95
3.90
3.85
3.80
3.75
3.70
3.65
3.60
3.55
ppm
3.19
2.97
3.14
2.96
2.89
3.06
3.00

## $^{13}$C-NMR spectrum for compound III

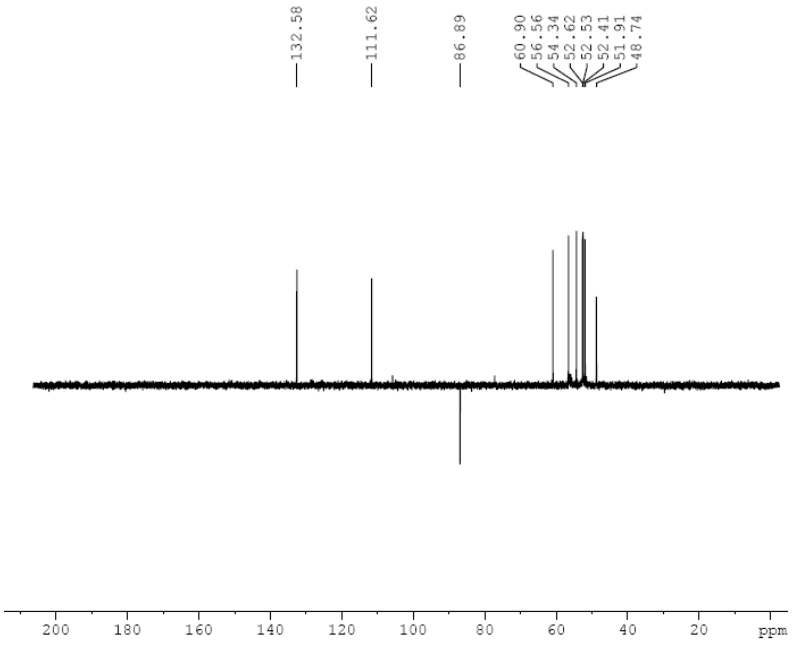



BRUKER

```
NAME          17_eswaran_delhi
EXPNO                       10
PROCNO                       1
Date_              20111018
Time                    8.06
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zgpg
TD                      22056
SOLVENT                 CDCl3
NS                       3072
DS                          4
SWH               22058.824 Hz
FIDRES             1.000128 Hz
AQ                 0.49998860 sec
RG                         203
DW                    22.667 usec
DE                     6.50 usec
TE                    298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.62 usec
PL1                     -2.00 dB
PL1W               58.25422241 W
SFO1              100.6494810 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                 100.00 usec
PL2                     -3.00 dB
PL12                    14.00 dB
PL13                    16.00 dB
PL2W              19.42244520 W
PL12W              0.26658249 W
PL13W              0.16897857 W
SFO2              400.2316009 MHz
SI                       32768
SF                100.6279183 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

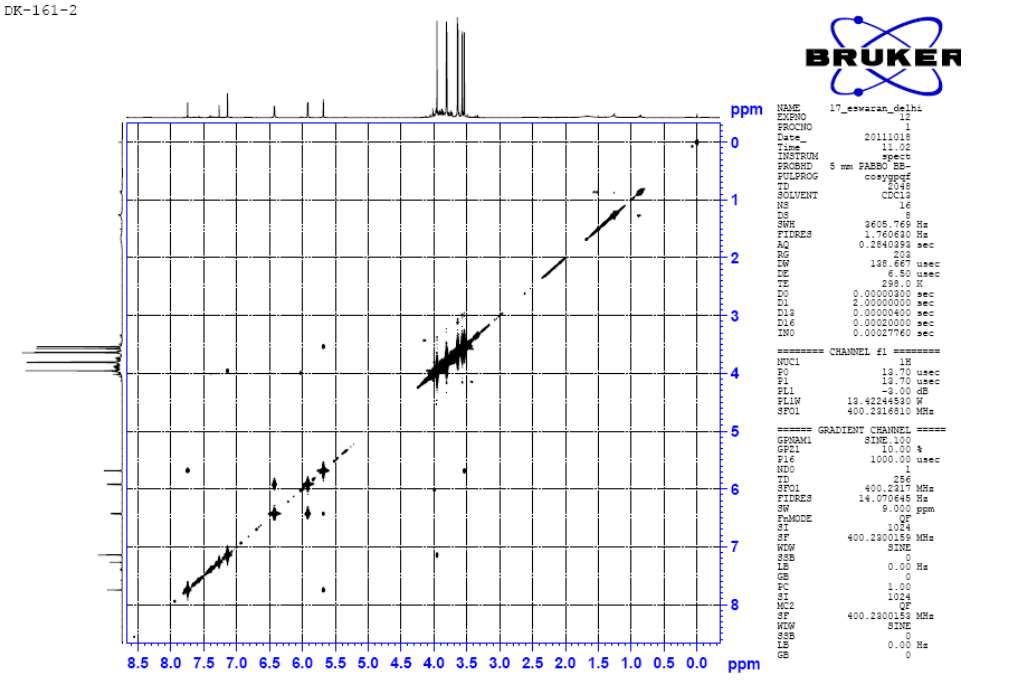
## DEPT Spectrum for compound III

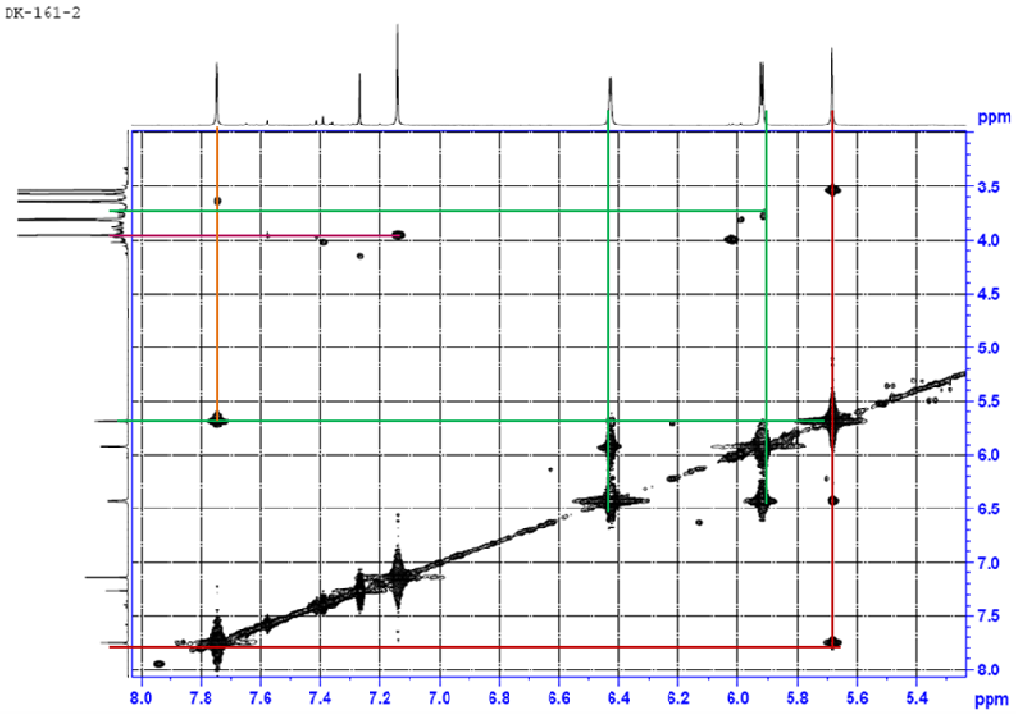
DK-161-2



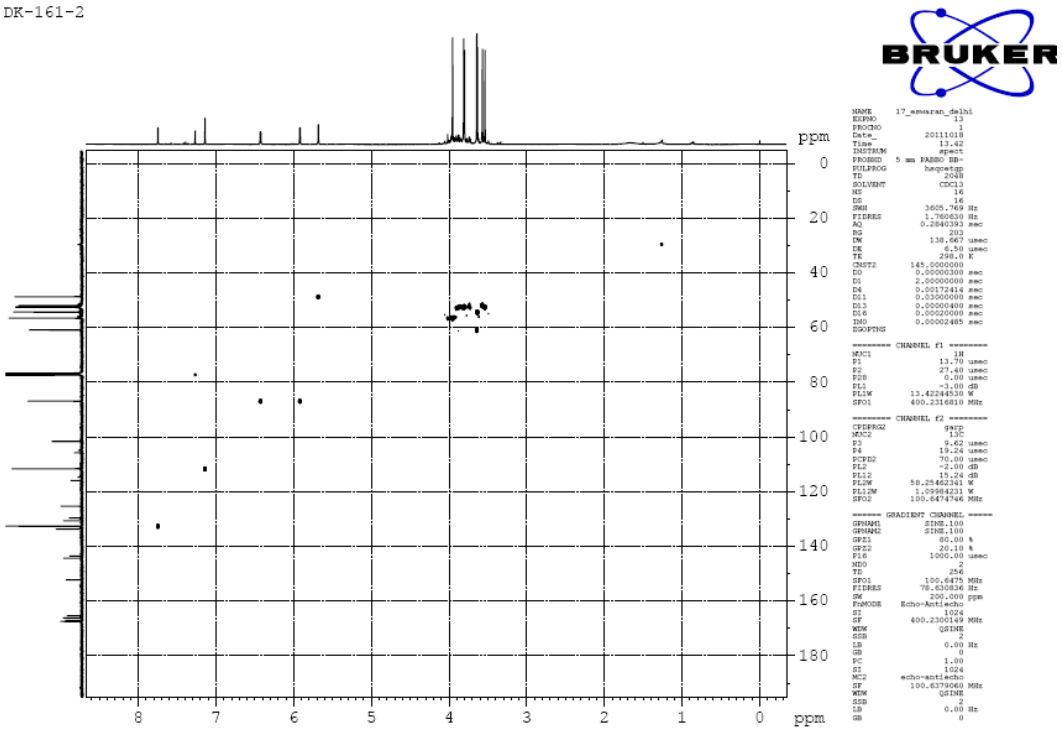

```
NAME          17_eswaran_delhi
EXPNO                       11
PROCNO                       1
Date_              20111018
Time                    11.01
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG              dept135
TD                      21006
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                21008.404 Hz
FIDRES             1.000114 Hz
AQ                 0.4999928 sec
RG                        202
DW                    23.800 usec
DE                     6.50 usec
TE                    298.0 K
CNST2              145.0000000
D1                  2.00000000 sec
D2                  0.00344828 sec
D12                 0.00002000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.62 usec
P2                       19.24 usec
PL1                     -2.00 dB
PL1W               58.25462241 W
SFO1              100.6481791 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
P3                       13.70 usec
P4                       27.40 usec
PCPD2                   100.00 usec
PL2                     -3.00 dB
PL12                    14.02 dB
PL2W               13.42244830 W
PL12W               0.26658249 W
SFO2              400.2316009 MHz
SI                       32768
SF                100.6379182 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

**COSY Spectrum of compound III**

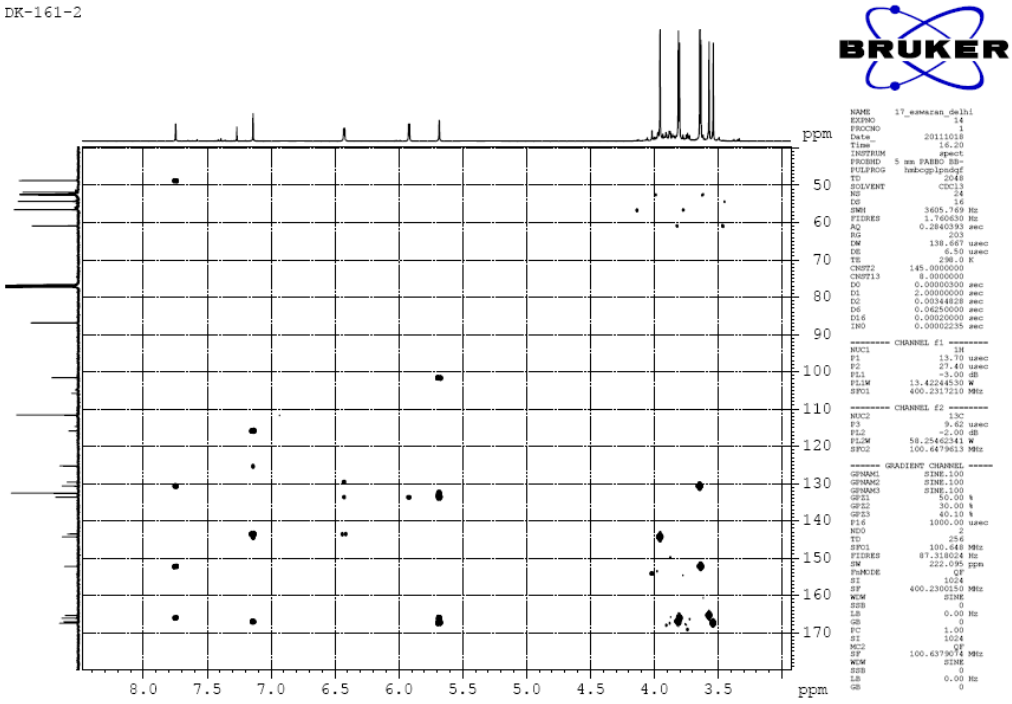


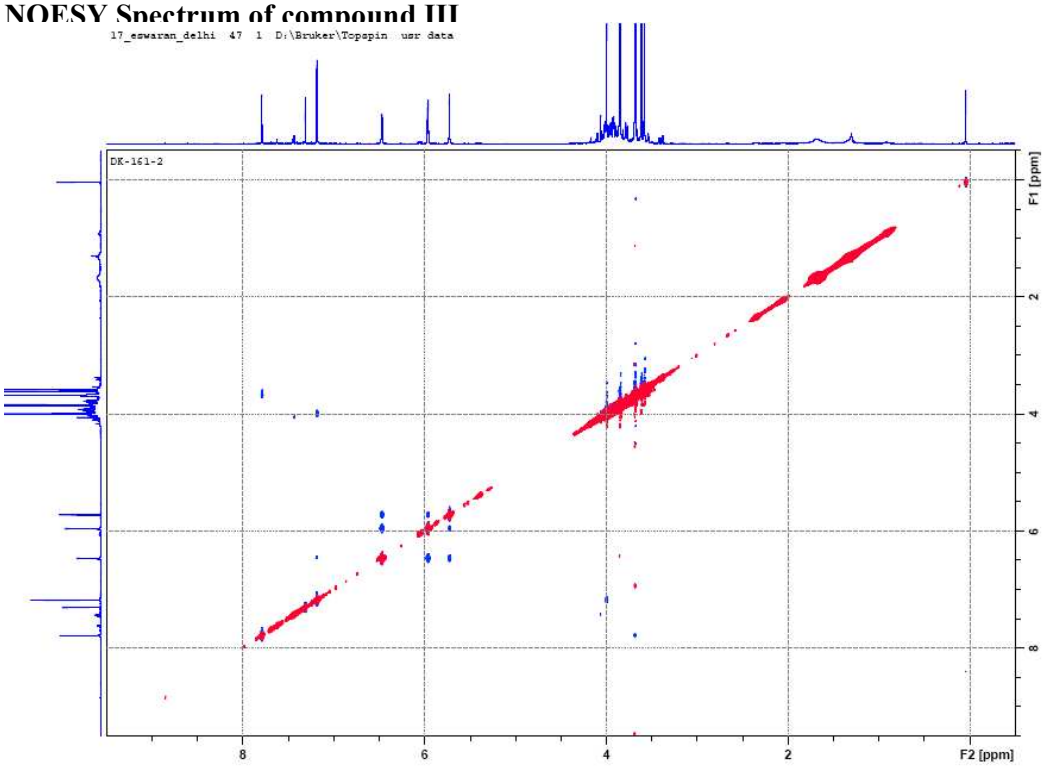
## HSQC Spectrum of compound III



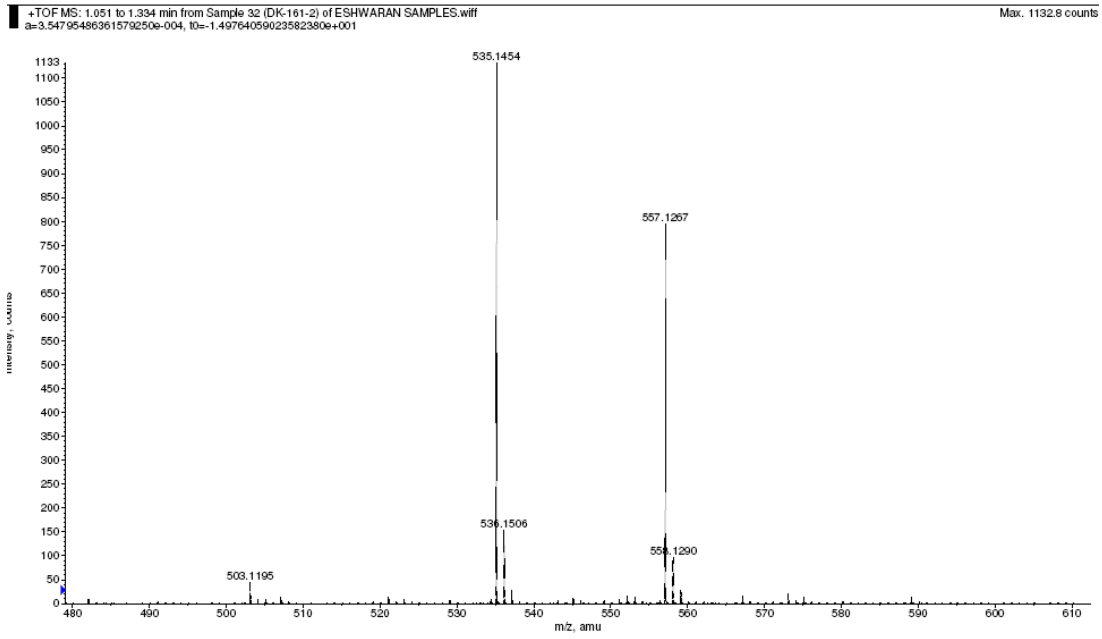
**HMBC Spectrum of compound III**



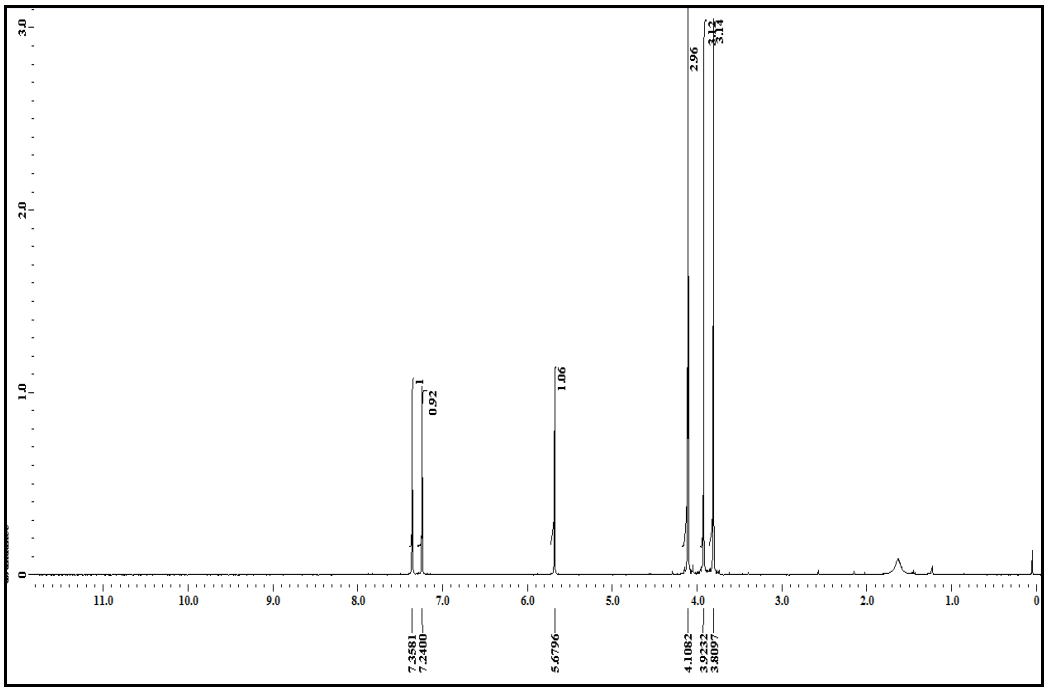
**NOESY Spectrum of compound III**



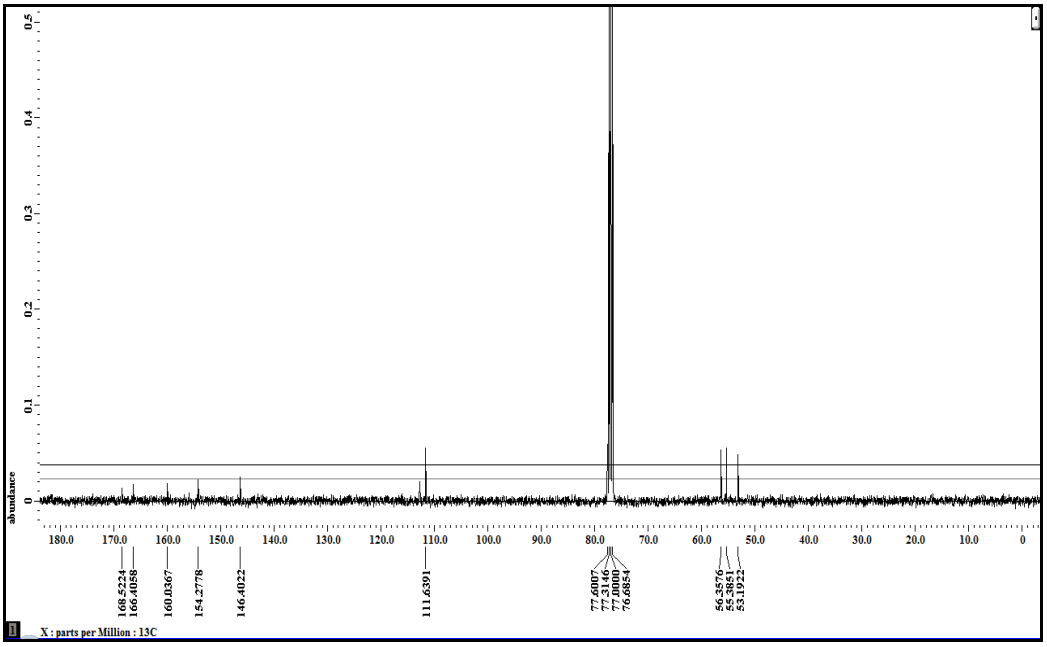
## HRMS Spectrum of compound III



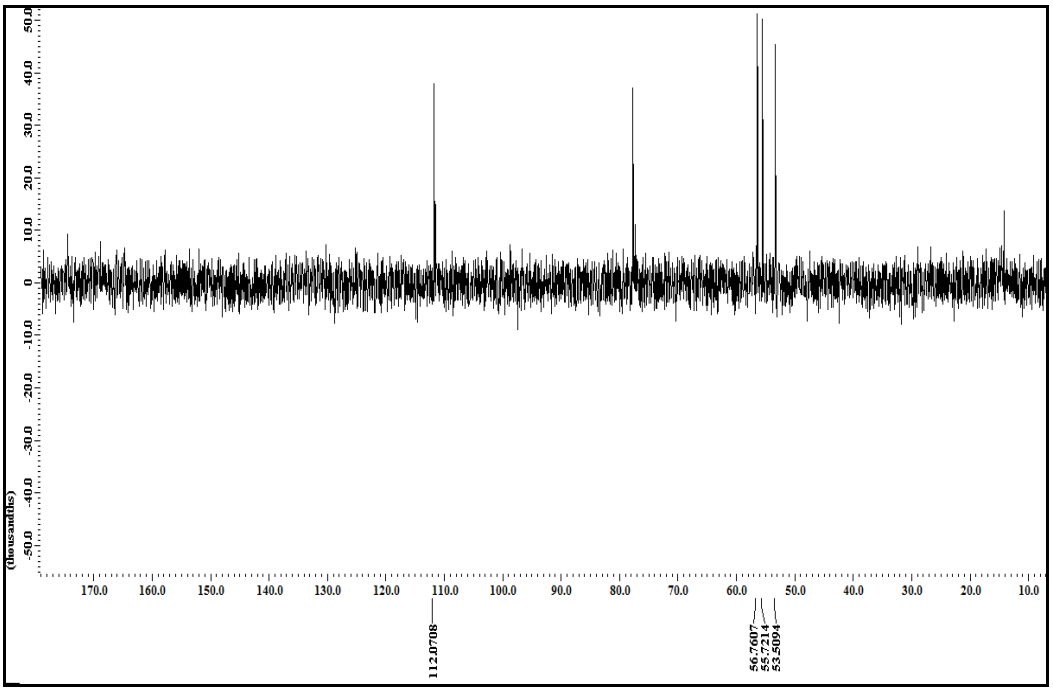
**$^{1}$H- NMR spectrum of compound IV**



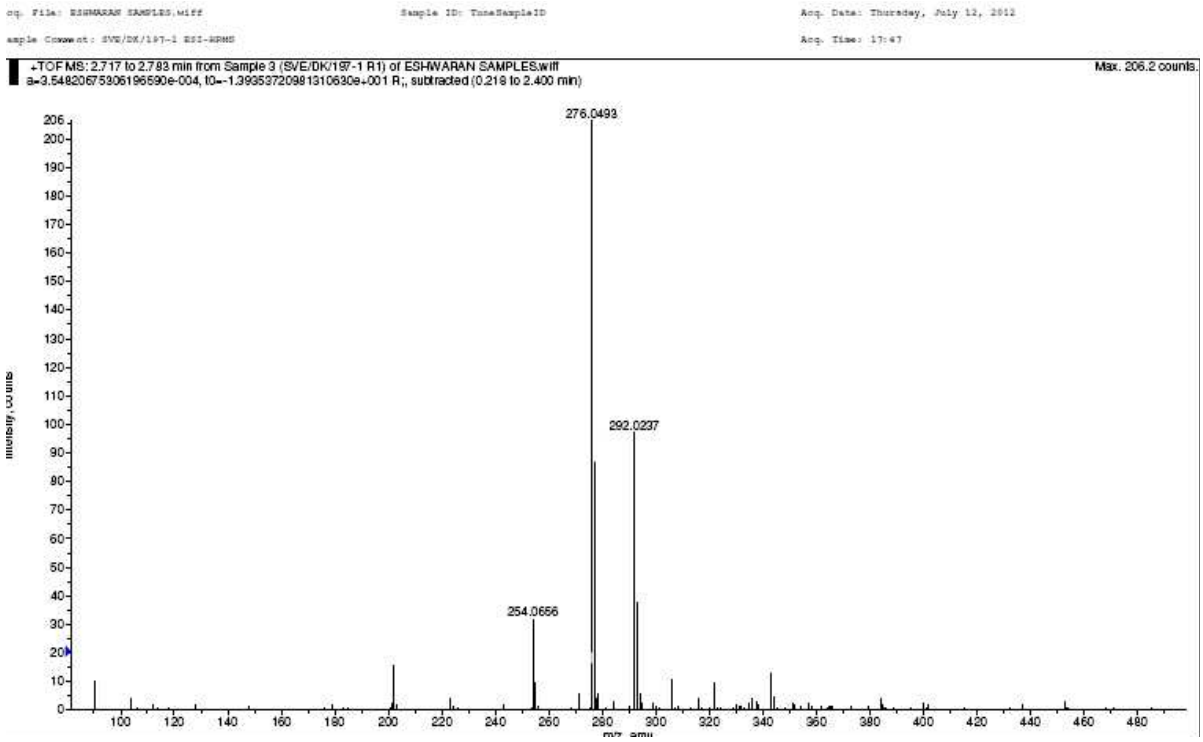
## $^{13}$C- NMR spectrum of compound IV



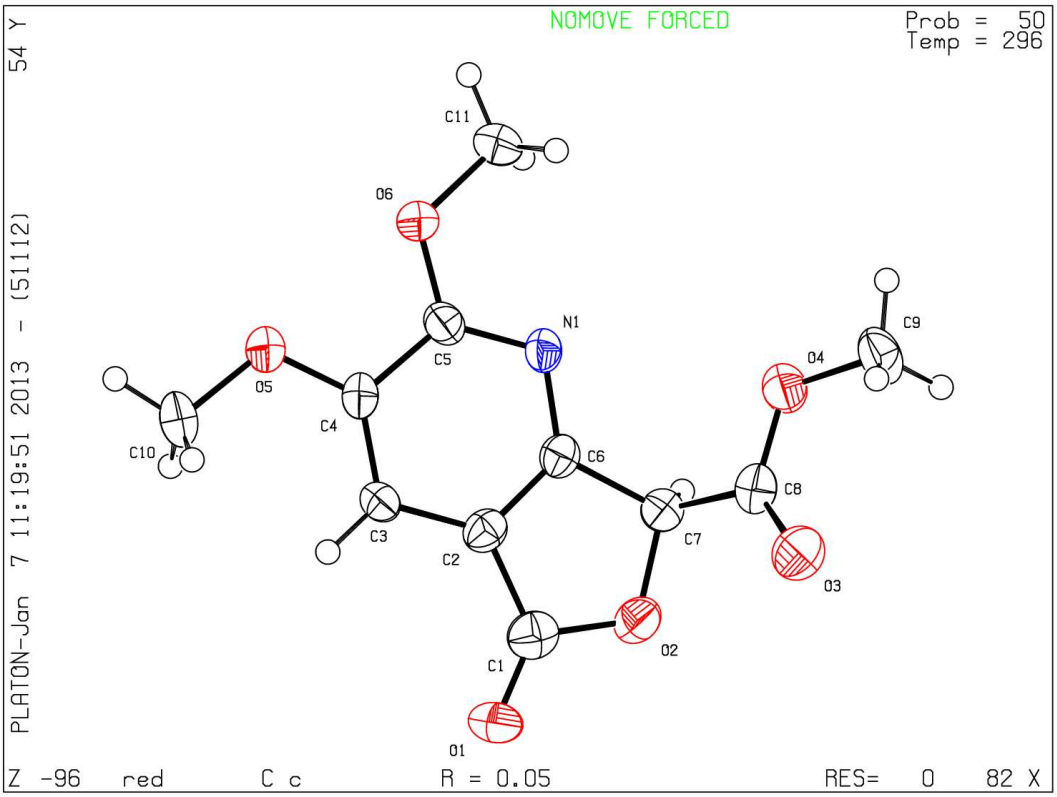
**DEPT- 135 spectrum of compound IV**



**HRMS spectrum of compound IV**



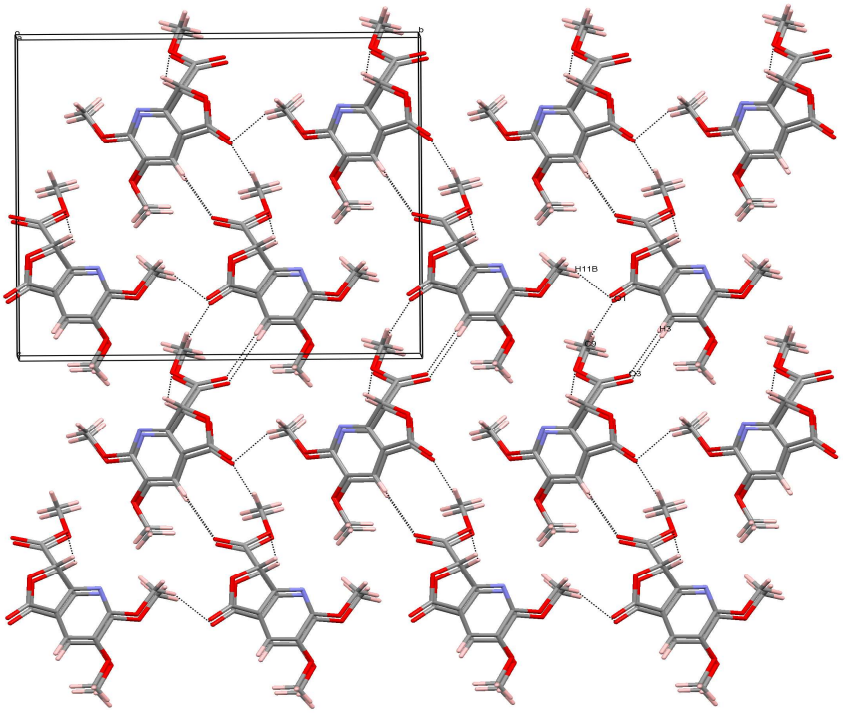
**Molecular diagram of Compound IV along with the atomic numbering scheme**



**Crystallographic table**

| Compound | IV |
|---|---|
| ***CCDC No.*** | **918314** |
| ***Molecular formula*** | $C_{11}H_{11}N_1O_6$ |
| ***Formula weight*** | 253.21 |
| ***Crystal system*** | Monoclinic |
| ***Space group*** | *C*c |
| ***a (Å)*** | 4.3177(2) |
| ***b (Å)*** | 16.1033(9) |
| ***c (Å)*** | 15.989(1) |
| ***α (°)*** | 90 |
| ***β (°)*** | 94.126(5) |
| ***γ (°)*** | 90 |
| ***V (Å$^3$)*** | 1108.8(1) |
| ***Z*** | 4 |
| ***$\rho_{calc}$ (g/cm$^3$)*** | 1.517 |
| ***F(000)*** | 528 |
| ***μ (mm$^{-1}$)*** | 0.13 |
| ***T (K)*** | 298(2) |
| ***λ (Å)*** | 0.71073 |
| ***$\theta_{min}$, $\theta_{max}$ (°)*** | 2.5, 26.0 |
| ***Reflns. collected*** | 2365 |
| ***Unique reflns.*** | 1637 |
| ***Completeness (%)*** | 99.9 |
| ***$R_{int}$*** | 0.024 |
| ***$R_{obs}$, $R_{all}$*** | 0.050, 0.065 |
| ***$wR_2$ ($F^2$)*** | 0.123 |
| ***Goodness-of-fit*** | 1.07 |

**Packing diagram of IV depicting the C-HPPPO and CPPPO contacts**



**Tables of (a) Bond Distances (b) Bond Angles and(c) Torsion angles**

**(a)**

| | Bond distances(♦) | | Bond distances(♦) |
|---|---|---|---|
| O1—C1 | 1.209 (6) | C3—C4 | 1.369 (5) |
| O2—C1 | 1.380 (6) | C4—C5 | 1.430 (6) |
| O2—C7 | 1.429 (4) | C6—C7 | 1.504 (5) |
| O3—C8 | 1.192 (4) | C7—C8 | 1.525 (6) |
| O4—C8 | 1.329 (5) | C3—H3 | 0.9300 |
| O4—C9 | 1.464 (6) | C7—H7 | 0.9800 |
| O5—C4 | 1.358 (5) | C9—H9A | 0.9600 |
| O5—C10 | 1.432 (6) | C9—H9B | 0.9600 |
| O6—C5 | 1.341 (4) | C9—H9C | 0.9600 |
| O6—C11 | 1.447 (6) | C10—H10A | 0.9600 |
| N1—C5 | 1.328 (6) | C10—H10B | 0.9600 |
| N1—C6 | 1.353 (4) | C10—H10C | 0.9600 |
| C1—C2 | 1.466 (6) | C11—H11A | 0.9600 |
| C2—C3 | 1.408 (6) | C11—H11B | 0.9600 |
| C2—C6 | 1.353 (5) | C11—H11C | 0.9600 |

**(b)**

| | Bond Angles (°) | | Bond Angles (°) |
|---|---|---|---|
| C1—O2—C7 | 110.6 (3) | O3—C8—C7 | 125.0 (4) |
| C8—O4—C9 | 116.8 (3) | O4—C8—C7 | 109.1 (3) |
| C4—O5—C10 | 116.2 (3) | C2—C3—H3 | 122.00 |
| C5—O6—C11 | 117.5 (3) | C4—C3—H3 | 122.00 |
| C5—N1—C6 | 113.8 (3) | O2—C7—H7 | 109.00 |
| O1—C1—O2 | 121.6 (4) | C6—C7—H7 | 109.00 |
| O1—C1—C2 | 131.0 (4) | C8—C7—H7 | 109.00 |
| O2—C1—C2 | 107.4 (4) | O4—C9—H9A | 110.00 |
| C1—C2—C3 | 130.3 (4) | O4—C9—H9B | 109.00 |
| C1—C2—C6 | 108.9 (4) | O4—C9—H9C | 109.00 |
| C3—C2—C6 | 120.8 (3) | H9A—C9—H9B | 109.00 |
| C2—C3—C4 | 115.8 (4) | H9A—C9—H9C | 109.00 |
| O5—C4—C3 | 126.5 (4) | H9B—C9—H9C | 109.00 |
| O5—C4—C5 | 114.5 (3) | O5—C10—H10A | 110.00 |
| C3—C4—C5 | 119.0 (4) | O5—C10—H10B | 110.00 |
| O6—C5—N1 | 119.7 (4) | O5—C10—H10C | 109.00 |
| O6—C5—C4 | 115.2 (4) | H10A—C10—H10B | 109.00 |
| N1—C5—C4 | 125.1 (3) | H10A—C10—H10C | 109.00 |
| N1—C6—C2 | 125.4 (3) | H10B—C10—H10C | 109.00 |
| N1—C6—C7 | 125.9 (3) | O6—C11—H11A | 109.00 |

| | | | |
|---|---|---|---|
| C2—C6—C7 | 108.7 (3) | O6—C11—H11B | 109.00 |
| O2—C7—C6 | 104.4 (3) | O6—C11—H11C | 109.00 |
| O2—C7—C8 | 109.2 (3) | H11A—C11—H11B | 109.00 |
| C6—C7—C8 | 117.1 (3) | H11A—C11—H11C | 109.00 |
| O3—C8—O4 | 125.8 (4) | H11B—C11—H11C | 110.00 |

**(c)**

| | Torsion Angles (°) | | Torsion Angles (°) |
|---|---|---|---|
| C7—O2—C1—O1 | −179.2 (4) | C3—C2—C6—N1 | −1.0 (6) |
| C7—O2—C1—C2 | 1.9 (4) | C1—C2—C6—C7 | 1.0 (4) |
| C1—O2—C7—C8 | 124.6 (3) | C1—C2—C6—N1 | 178.1 (3) |
| C1—O2—C7—C6 | −1.3 (4) | C1—C2—C3—C4 | −178.4 (4) |
| C9—O4—C8—C7 | −174.0 (3) | C6—C2—C3—C4 | 0.4 (5) |
| C9—O4—C8—O3 | 3.6 (6) | C2—C3—C4—O5 | 179.4 (4) |
| C10—O5—C4—C3 | 0.2 (6) | C2—C3—C4—C5 | 0.8 (5) |
| C10—O5—C4—C5 | 178.9 (3) | C3—C4—C5—N1 | −1.7 (6) |
| C11—O6—C5—N1 | 5.2 (5) | O5—C4—C5—N1 | 179.5 (3) |
| C11—O6—C5—C4 | −175.9 (3) | C3—C4—C5—O6 | 179.5 (3) |
| C5—N1—C6—C7 | 176.8 (3) | O5—C4—C5—O6 | 0.7 (5) |
| C5—N1—C6—C2 | 0.2 (5) | N1—C6—C7—O2 | −176.9 (3) |
| C6—N1—C5—C4 | 1.2 (5) | N1—C6—C7—C8 | 62.3 (5) |
| C6—N1—C5—O6 | 179.9 (3) | C2—C6—C7—C8 | −120.7 (3) |

| | | | |
|---|---|---|---|
| O2—C1—C2—C3 | 177.1 (4) | C2—C6—C7—O2 | 0.2 (4) |
| O1—C1—C2—C3 | −1.7 (7) | O2—C7—C8—O3 | −3.0 (6) |
| O1—C1—C2—C6 | 179.4 (4) | C6—C7—C8—O4 | −67.1 (4) |
| O2—C1—C2—C6 | −1.8 (4) | O2—C7—C8—O4 | 174.6 (3) |
| C3—C2—C6—C7 | −178.1 (3) | C6—C7—C8—O3 | 115.3 (4) |

**Intermolecular contacts in compound IV**

| Interaction | H···A (Å) | X···A (Å) | Symmetry Operator |
|---|---|---|---|
| C7-H7PPPO4 | 2.661 | 3.389(5) | 1+x,y,z |
| C3-H3PPPO3 | 2.584 | 3.385(5) | x,-1-y,1/2+z |
| C11-H11BPPPO3 | 2.687 | 3.413(7) | -1.5+x,-1/2+y,z |
| O1PPP C9 | - | 3.069(6) | -1+x,-1-y,1/2+z |

**Coorindates for Open-shell singlet nitrene (1n)**

Energy = -971.1213463 Hartrees ($S^2$ = 0.94665)

| | | | |
|---|---|---|---|
| C | 2.11910600 | 0.54224000 | -0.01783300 |
| C | 1.95306700 | -0.86115700 | -0.10377900 |
| C | 0.62079800 | -1.40983500 | -0.19333200 |
| C | -0.51661900 | -0.52629000 | -0.16605400 |
| C | -0.31881500 | 0.84323300 | -0.04025700 |
| C | 0.99529500 | 1.35698400 | 0.02704700 |
| H | 1.09153300 | 2.43306800 | 0.09327300 |
| N | 0.44164100 | -2.72679300 | -0.28906400 |
| C | -1.86010800 | -1.18446900 | -0.36041200 |
| O | -2.33040400 | -1.69321800 | 0.78866400 |
| O | -2.41117700 | -1.27551300 | -1.43572500 |
| C | -3.56879700 | -2.42492200 | 0.68736800 |
| H | -3.44762100 | -3.27544100 | 0.01280900 |
| H | -3.78730200 | -2.76238400 | 1.69982900 |
| H | -4.36377900 | -1.77501900 | 0.31396700 |
| C | -1.40603000 | 1.86673500 | 0.02276700 |
| O | -1.20217900 | 3.06810000 | -0.01692200 |
| O | -2.63154800 | 1.33021000 | 0.14338400 |
| C | -3.73326400 | 2.25887100 | 0.15970900 |
| H | -3.65129900 | 2.92756900 | 1.01958100 |
| H | -3.74331400 | 2.84824500 | -0.75969500 |
| H | -4.62785800 | 1.64179800 | 0.23209100 |
| O | 2.94236400 | -1.76064700 | -0.17248900 |
| O | 3.40128700 | 1.01482200 | -0.01568800 |
| C | 3.60652100 | 2.42636100 | 0.02945700 |
| H | 4.68768200 | 2.56488200 | 0.00683400 |
| H | 3.15491100 | 2.91978700 | -0.83883800 |
| H | 3.20066900 | 2.85790000 | 0.95195100 |
| C | 4.21798500 | -1.57237500 | 0.46859100 |
| H | 4.86503400 | -0.92580200 | -0.12463800 |
| H | 4.08895700 | -1.15336900 | 1.46986800 |
| H | 4.63932600 | -2.57596800 | 0.53699800 |

**Coordinates for transition state for conversion of nitrene to azirine (TS 1n-1a)**

Energy = -971.0986586 Hartrees

| | | | |
|---|---|---|---|
| C | -1.942895 | -0.796986 | -0.226832 |
| C | -0.617943 | -1.409173 | 0.046119 |
| C | 0.544674 | -0.503058 | 0.103118 |
| C | 0.347493 | 0.854618 | 0.046004 |
| C | -0.977052 | 1.394570 | 0.043123 |
| C | -2.109913 | 0.605604 | -0.041719 |
| H | -1.052722 | 2.474171 | 0.088067 |
| N | -0.610258 | -2.647141 | 0.384691 |
| O | -2.941723 | -1.585025 | -0.591998 |
| C | -4.091568 | -1.787294 | 0.256215 |

| | | | |
|---|---|---|---|
| H | -4.819226 | -2.314617 | -0.360161 |
| H | -3.782170 | -2.421811 | 1.093513 |
| H | -4.501443 | -0.839182 | 0.606901 |
| C | 1.871550 | -1.157276 | 0.347307 |
| O | 2.203320 | -1.993202 | -0.646302 |
| C | 3.402909 | -2.767798 | -0.441665 |
| H | 3.289695 | -3.401934 | 0.440229 |
| H | 3.511296 | -3.372119 | -1.341278 |
| H | 4.263445 | -2.107736 | -0.309672 |
| O | 2.523998 | -0.982092 | 1.355322 |
| C | 1.442806 | 1.877212 | 0.063735 |
| O | 2.596779 | 1.413246 | -0.436938 |
| C | 3.721675 | 2.313763 | -0.375860 |
| H | 4.550080 | 1.768715 | -0.826148 |
| H | 3.506219 | 3.226634 | -0.935415 |
| H | 3.943098 | 2.564974 | 0.663729 |
| O | 1.282089 | 3.018372 | 0.457868 |
| O | -3.383051 | 1.084683 | -0.109654 |
| C | -3.580415 | 2.499811 | -0.105777 |
| H | -3.083929 | 2.968459 | -0.963423 |
| H | -4.657800 | 2.645186 | -0.183299 |
| H | -3.213938 | 2.947446 | 0.825126 |

**Coordinates for azirine (1a)**

Energy = -971.1308768 Hartrees

| | | | |
|---|---|---|---|
| C | -1.733870 | -0.344506 | 0.008584 |
| C | -0.359986 | -0.658829 | 0.401886 |
| C | 0.789763 | 0.195484 | 0.452268 |
| C | 0.372263 | 1.497291 | 0.665457 |
| C | -1.014972 | 1.876867 | 0.754276 |
| C | -2.059051 | 1.032597 | 0.419011 |
| H | -1.212302 | 2.904346 | 1.033521 |
| N | -1.215577 | -1.332933 | 1.056726 |
| O | -2.289863 | -0.830926 | -1.157552 |
| C | -3.472123 | -1.624389 | -0.972249 |
| H | -3.756363 | -1.976950 | -1.964988 |
| H | -3.263393 | -2.479770 | -0.320811 |
| H | -4.282547 | -1.022449 | -0.546804 |
| C | 2.187945 | -0.266580 | 0.441875 |
| O | 2.260861 | -1.565008 | 0.071324 |
| C | 3.579640 | -2.143452 | 0.068923 |
| H | 4.019089 | -2.091174 | 1.067847 |
| H | 3.438193 | -3.179201 | -0.237580 |
| H | 4.224703 | -1.615337 | -0.637403 |
| O | 3.156752 | 0.405778 | 0.746409 |

| | | | |
|---|---|---|---|
| C | 1.357735 | 2.618897 | 0.892558 |
| O | 2.033052 | 2.915200 | -0.224586 |
| C | 3.067294 | 3.912680 | -0.088012 |
| H | 3.473472 | 4.043536 | -1.090089 |
| H | 2.648609 | 4.848550 | 0.288709 |
| H | 3.836009 | 3.548675 | 0.597159 |
| O | 1.450834 | 3.214835 | 1.944960 |
| O | -3.344774 | 1.400275 | 0.293426 |
| C | -3.701304 | 2.775402 | 0.474912 |
| H | -3.154509 | 3.411756 | -0.229278 |
| H | -4.770678 | 2.830332 | 0.273306 |
| H | -3.501794 | 3.095919 | 1.502919 |

**Coordinates for transition state for conversion of azirine to ketenimine (TS 1a-1k)**

Energy = -971.1216764 Hartrees

| | | | |
|---|---|---|---|
| C | 2.170910 | 0.341695 | 0.270808 |
| C | 0.719553 | 1.158169 | 0.674493 |
| C | -0.533785 | 0.791878 | 0.239063 |
| C | -0.658695 | -0.622952 | 0.307226 |
| C | 0.463036 | -1.462772 | 0.352746 |
| C | 1.791697 | -1.022851 | 0.165990 |
| H | 0.276330 | -2.527832 | 0.403668 |
| N | 1.732270 | 1.182911 | 1.409885 |
| O | 3.111981 | 0.842207 | -0.564678 |
| C | 4.203009 | 1.552195 | 0.052029 |
| H | 4.821141 | 1.908340 | -0.772072 |
| H | 3.838281 | 2.397705 | 0.641640 |
| H | 4.783258 | 0.877563 | 0.690247 |
| C | -1.546484 | 1.707179 | -0.316573 |
| O | -1.210329 | 3.000512 | -0.096090 |
| C | -2.118276 | 3.980307 | -0.633658 |
| H | -3.103861 | 3.875594 | -0.174051 |
| H | -1.678692 | 4.946151 | -0.386480 |
| H | -2.210709 | 3.861947 | -1.716068 |
| O | -2.543521 | 1.358599 | -0.918289 |
| C | -2.025088 | -1.233391 | 0.458500 |
| O | -2.161246 | -2.345771 | -0.295921 |
| C | -3.438525 | -3.008217 | -0.193010 |
| H | -3.377275 | -3.859182 | -0.870701 |
| H | -3.613971 | -3.340027 | 0.833200 |
| H | -4.238308 | -2.328391 | -0.494609 |
| O | -2.882752 | -0.811361 | 1.203486 |
| O | 2.770078 | -1.843416 | -0.297219 |
| C | 2.415888 | -3.092401 | -0.896545 |
| H | 1.617721 | -2.960728 | -1.634772 |
| H | 3.322545 | -3.449535 | -1.386246 |

| | | | |
|---|---|---|---|
| H | 2.104526 | -3.821173 | -0.139674 |

**Coordinates for ketenimine (1k)**

Energy = -971.1379435 Hartrees

| | | | |
|---|---|---|---|
| C | -0.418022 | 0.888895 | -0.034224 |
| C | -0.062844 | -0.764128 | -1.553012 |
| C | 2.080501 | -0.752549 | -1.189783 |
| C | 2.023614 | 0.152395 | -0.138468 |
| C | 0.925837 | 1.043545 | 0.181168 |
| H | 1.245578 | 1.972897 | 0.645704 |
| N | 1.032835 | -0.784666 | -2.141332 |
| C | -0.918619 | -0.371568 | -0.615538 |
| C | -2.039506 | -1.147497 | -0.059615 |
| O | -2.581555 | -0.898626 | 1.000017 |
| O | -2.374714 | -2.186991 | -0.858112 |
| C | -3.441543 | -3.024442 | -0.374677 |
| H | -4.356430 | -2.439875 | -0.253344 |
| H | -3.572852 | -3.791417 | -1.137407 |
| H | -3.171629 | -3.474382 | 0.584066 |
| C | -1.388147 | 1.996878 | 0.196514 |
| O | -0.925047 | 2.926914 | 1.065102 |
| O | -2.476346 | 2.061976 | -0.339994 |
| C | -1.817804 | 4.027053 | 1.326901 |
| H | -2.756581 | 3.660143 | 1.748035 |
| H | -1.294104 | 4.659678 | 2.043152 |
| H | -2.026585 | 4.576092 | 0.405524 |
| O | 3.103332 | -1.529645 | -1.549808 |
| O | 3.225018 | 0.436099 | 0.494600 |
| C | 3.224395 | 0.295317 | 1.920110 |
| H | 4.211323 | 0.615979 | 2.257975 |
| H | 2.457778 | 0.923633 | 2.386664 |
| H | 3.053933 | -0.749934 | 2.209612 |
| C | 4.063068 | -2.011342 | -0.592957 |
| H | 3.557586 | -2.350093 | 0.316797 |
| H | 4.545906 | -2.856642 | -1.084342 |
| H | 4.792376 | -1.238669 | -0.351366 |

**Coordinates for transition state for the ring-closing of ketenimine (TS 1k-1a')**

Energy = -971.1100851 Hartrees

| | | | |
|---|---|---|---|
| C | -0.552957 | 0.776123 | 0.070077 |
| C | -0.294320 | -0.427288 | -1.174730 |
| C | 1.863283 | -0.649831 | -0.867496 |
| C | 1.720509 | -0.127509 | 0.476285 |
| C | 0.655525 | 0.679611 | 0.841809 |
| H | 0.830982 | 1.358433 | 1.674180 |
| N | 0.852665 | -0.687991 | -1.732006 |

| | | | |
|---|---|---|---|
| C | -1.299745 | -0.452225 | -0.360940 |
| C | -2.308296 | -1.306417 | 0.265759 |
| O | -2.742907 | -1.131775 | 1.388153 |
| O | -2.690259 | -2.301557 | -0.560806 |
| C | -3.703064 | -3.186791 | -0.043167 |
| H | -4.609288 | -2.626146 | 0.197856 |
| H | -3.893062 | -3.902725 | -0.841951 |
| H | -3.342984 | -3.694801 | 0.854739 |
| C | -1.196009 | 2.094673 | -0.198161 |
| O | -0.531690 | 3.110506 | 0.407049 |
| O | -2.194756 | 2.252620 | -0.871889 |
| C | -1.113424 | 4.418757 | 0.245981 |
| H | -2.130203 | 4.435132 | 0.645508 |
| H | -0.467210 | 5.093738 | 0.806586 |
| H | -1.137915 | 4.695192 | -0.810671 |
| O | 3.029574 | -1.095464 | -1.359656 |
| O | 2.812738 | -0.192725 | 1.319806 |
| C | 2.818053 | -1.347414 | 2.172414 |
| H | 3.714111 | -1.266507 | 2.790329 |
| H | 1.927954 | -1.360279 | 2.812152 |
| H | 2.856789 | -2.272353 | 1.583189 |
| C | 4.286202 | -0.466525 | -1.031823 |
| H | 4.720952 | -0.903288 | -0.132157 |
| H | 4.926049 | -0.658710 | -1.894266 |
| H | 4.159654 | 0.609463 | -0.892772 |

**Coordinates for ring-closing product from ketenimine (1a')**

Energy = -971.1137475 Hartrees

| | | | |
|---|---|---|---|
| C | -1.657205 | -0.352743 | 0.145233 |
| C | -0.176391 | -0.278322 | 0.543785 |
| C | 0.245981 | 1.741136 | -0.202415 |
| C | -1.199581 | 2.040322 | -0.078126 |
| C | -2.124934 | 1.043952 | 0.020404 |
| H | -3.176469 | 1.301694 | -0.071978 |
| N | 0.762282 | 0.587812 | 0.132916 |
| C | -0.961678 | -0.840558 | 1.418758 |
| C | -1.309466 | -1.084217 | 2.812328 |
| O | -2.424418 | -0.925195 | 3.275279 |
| O | -0.241930 | -1.514994 | 3.516395 |
| C | -0.490360 | -1.817127 | 4.903534 |
| H | -1.256533 | -2.590959 | 4.992595 |
| H | 0.462974 | -2.170910 | 5.294370 |
| H | -0.818438 | -0.921319 | 5.436449 |
| C | -2.174226 | -1.404445 | -0.796125 |
| O | -3.040853 | -0.873073 | -1.691255 |
| O | -1.868664 | -2.577559 | -0.770006 |
| C | -3.623868 | -1.802706 | -2.626140 |
| H | -4.171825 | -2.583126 | -2.093080 |

| | | | |
|---|---|---|---|
| H | -4.298067 | -1.208849 | -3.242668 |
| H | -2.844921 | -2.263802 | -3.237780 |
| O | 1.118696 | 2.677343 | -0.612129 |
| O | -1.607599 | 3.348436 | -0.202623 |
| C | -1.408113 | 4.144713 | 0.977280 |
| H | -1.772824 | 5.143861 | 0.734063 |
| H | -1.982472 | 3.735571 | 1.816165 |
| H | -0.346372 | 4.193605 | 1.248584 |
| C | 0.786760 | 3.581126 | -1.687859 |
| H | 0.355611 | 4.505658 | -1.301650 |
| H | 1.735067 | 3.786867 | -2.186431 |
| H | 0.091152 | 3.117156 | -2.390772 |

**Coordinates for ring-opening from 1a' to pyridylcarbene (TS-1a'-1c)**

Energy = -971.0935363 Hartrees

| | | | |
|---|---|---|---|
| C | -0.390223 | 0.980203 | -0.222506 |
| C | -0.339055 | -0.281611 | -0.897376 |
| C | 1.884719 | -0.549015 | -0.591778 |
| C | 1.868254 | 0.477566 | 0.448723 |
| C | 0.740917 | 1.242134 | 0.615988 |
| H | 0.748402 | 2.074697 | 1.310847 |
| N | 0.801053 | -0.970005 | -1.177524 |
| C | -1.603808 | -0.603343 | -0.521591 |
| C | -2.008968 | -1.722059 | 0.309111 |
| O | -1.929552 | -1.730779 | 1.528006 |
| O | -2.549390 | -2.711533 | -0.435946 |
| C | -3.029792 | -3.857650 | 0.296889 |
| H | -3.810941 | -3.559018 | 0.999793 |
| H | -3.429002 | -4.531625 | -0.460301 |
| H | -2.211957 | -4.333323 | 0.843376 |
| C | -1.403849 | 2.042697 | -0.513847 |
| O | -1.676012 | 2.757604 | 0.600447 |
| O | -1.859707 | 2.289991 | -1.609244 |
| C | -2.610223 | 3.842829 | 0.431652 |
| H | -3.573137 | 3.459574 | 0.086635 |
| H | -2.706193 | 4.295963 | 1.417714 |
| H | -2.228100 | 4.565379 | -0.293356 |
| O | 3.048706 | -1.176967 | -0.890332 |
| O | 2.995858 | 0.753136 | 1.164815 |
| C | 3.430598 | -0.278841 | 2.076959 |
| H | 4.345643 | 0.098862 | 2.533931 |
| H | 2.669614 | -0.439836 | 2.847979 |
| H | 3.633150 | -1.212720 | 1.545153 |
| C | 4.077443 | -0.374111 | -1.507891 |
| H | 4.340528 | 0.483728 | -0.883172 |
| H | 4.937206 | -1.034983 | -1.618355 |

| | | | |
|---|---|---|---|
| H | 3.742112 | -0.041078 | -2.495528 |

**Coordinates for pyridylcarbene (1c)**

Energy = -971.1310958 Hartrees

| | | | |
|---|---|---|---|
| C | -0.386293 | 0.121486 | 0.114103 |
| C | 0.650811 | 1.083198 | 0.109633 |
| C | 1.987679 | 0.674212 | 0.047831 |
| C | 2.271327 | -0.683021 | -0.049439 |
| C | 1.160185 | -1.606564 | -0.078283 |
| N | -0.080418 | -1.220047 | 0.005439 |
| H | 2.779207 | 1.412114 | 0.086412 |
| O | 1.489104 | -2.903903 | -0.188138 |
| O | 3.490928 | -1.223928 | -0.116207 |
| C | 4.636943 | -0.363799 | -0.062297 |
| H | 4.660480 | 0.192245 | 0.880644 |
| H | 5.498337 | -1.027488 | -0.123036 |
| H | 4.641349 | 0.329575 | -0.910009 |
| C | 0.402515 | -3.847970 | -0.195024 |
| H | -0.258048 | -3.665088 | -1.046485 |
| H | 0.879822 | -4.824002 | -0.277684 |
| H | -0.176060 | -3.772825 | 0.728954 |
| C | -1.720867 | 0.566292 | 0.282649 |
| C | -2.769388 | -0.407037 | 0.423033 |
| O | -3.068696 | -0.831363 | 1.536379 |
| O | -3.447658 | -0.695684 | -0.710502 |
| C | -4.612531 | -1.528041 | -0.548151 |
| H | -5.331722 | -1.054033 | 0.124558 |
| H | -5.033662 | -1.630174 | -1.548237 |
| H | -4.335710 | -2.506118 | -0.146924 |
| C | 0.364014 | 2.552434 | 0.244296 |
| O | -0.269773 | 3.046726 | -0.825113 |
| O | 0.740663 | 3.207265 | 1.195927 |
| C | -0.649638 | 4.437016 | -0.744432 |
| H | 0.230945 | 5.065739 | -0.593823 |
| H | -1.128455 | 4.658210 | -1.697180 |
| H | -1.348653 | 4.580022 | 0.082449 |

**Coordinates for transition state of formation of ylide (TS 1c-1y)**

Energy = -971.1246238 Hartrees

| | | | |
|---|---|---|---|
| C | -0.410336 | 0.168779 | -0.170665 |
| C | 0.823977 | 0.847018 | -0.044915 |
| C | 2.005295 | 0.101876 | 0.087901 |
| C | 1.943524 | -1.283650 | 0.058716 |
| C | 0.647671 | -1.887744 | -0.066894 |
| N | -0.468085 | -1.196823 | -0.123182 |

| | | | |
|---|---|---|---|
| H | 2.945321 | 0.623531 | 0.212332 |
| O | 0.621840 | -3.229169 | -0.081381 |
| O | 2.990625 | -2.128372 | 0.169795 |
| C | 4.298804 | -1.570170 | 0.292973 |
| H | 4.386378 | -0.968806 | 1.205662 |
| H | 4.975898 | -2.422131 | 0.350164 |
| H | 4.549363 | -0.957323 | -0.580837 |
| C | -0.666824 | -3.861332 | -0.171300 |
| H | -1.184430 | -3.553210 | -1.083037 |
| H | -0.453598 | -4.929909 | -0.187990 |
| H | -1.282943 | -3.602621 | 0.693632 |
| C | -1.615051 | 0.849865 | -0.496860 |
| C | -2.874026 | 0.560791 | 0.126725 |
| O | -3.191846 | 1.156169 | 1.152252 |
| O | -3.679044 | -0.274068 | -0.562200 |
| C | -4.998854 | -0.461309 | -0.010922 |
| H | -5.539089 | 0.488022 | 0.015083 |
| H | -5.490612 | -1.164297 | -0.682784 |
| H | -4.940549 | -0.871836 | 1.000091 |
| C | 0.779109 | 2.317441 | -0.033261 |
| O | 1.984115 | 2.897853 | -0.238966 |
| O | -0.255554 | 2.945484 | 0.126760 |
| C | 1.989842 | 4.339734 | -0.226722 |
| H | 1.591648 | 4.713250 | 0.719698 |
| H | 3.034332 | 4.624998 | -0.348844 |
| H | 1.385004 | 4.727135 | -1.049629 |

**Coordinates for ylide (1y)**

Energy = -971.2030265 Hartrees

| | | | |
|---|---|---|---|
| C | -0.232528 | 0.056424 | 0.014948 |
| C | 1.054245 | 0.699736 | 0.037771 |
| C | 2.242832 | -0.086144 | 0.040753 |
| C | 2.088953 | -1.446594 | 0.021189 |
| C | 0.734408 | -2.001821 | -0.001249 |
| N | -0.367132 | -1.302881 | -0.004398 |
| H | 3.217217 | 0.385690 | 0.057838 |
| O | 0.685873 | -3.342255 | -0.019385 |
| O | 3.085179 | -2.369988 | 0.020221 |
| C | 4.424245 | -1.890086 | 0.041512 |
| H | 4.620145 | -1.302676 | 0.947749 |
| H | 5.057877 | -2.777242 | 0.036968 |
| H | 4.640215 | -1.279164 | -0.844392 |
| C | -0.617547 | -3.947434 | -0.041916 |
| H | -1.169172 | -3.637980 | -0.933229 |
| H | -0.428620 | -5.020837 | -0.053899 |
| H | -1.189064 | -3.661328 | 0.844651 |
| C | -1.201554 | 1.056040 | 0.017237 |
| C | -2.645310 | 1.143366 | 0.002439 |

| | | | |
|---|---|---|---|
| O | -3.284650 | 2.186230 | 0.009118 |
| O | -3.219803 | -0.087279 | -0.020122 |
| C | -4.655635 | -0.092188 | -0.036020 |
| H | -5.034656 | 0.421772 | -0.923386 |
| H | -4.939172 | -1.144735 | -0.052981 |
| H | -5.054276 | 0.398384 | 0.855974 |
| C | 0.780768 | 2.055217 | 0.052521 |
| O | 1.623757 | 3.085696 | 0.075446 |
| O | -0.534439 | 2.283493 | 0.040829 |
| C | 1.054280 | 4.411283 | 0.086585 |
| H | 0.433354 | 4.553498 | 0.974868 |
| H | 1.908944 | 5.085957 | 0.104954 |
| H | 0.453170 | 4.577023 | -0.811199 |

**Coordinates for transition state of formation of oxazolidine from nitrene (TS 1n-1o)**

Energy = -971.10524615 Hartrees

| | | | |
|---|---|---|---|
| C | 2.066913 | 0.903521 | 0.092497 |
| C | 2.117773 | -0.475826 | -0.074457 |
| C | 0.928106 | -1.292993 | -0.094718 |
| C | -0.323013 | -0.596820 | 0.066645 |
| C | -0.354029 | 0.809125 | 0.138086 |
| C | 0.818655 | 1.554678 | 0.176616 |
| H | 0.756204 | 2.631918 | 0.243274 |
| N | 0.962191 | -2.617031 | -0.194300 |
| C | -1.433961 | -1.525870 | 0.170961 |
| O | -2.614573 | -1.015895 | 0.566142 |
| O | -1.266872 | -2.731562 | -0.036026 |
| C | -3.698531 | -1.956551 | 0.691388 |
| H | -3.913649 | -2.420627 | -0.274278 |
| H | -3.446947 | -2.732382 | 1.418050 |
| H | -4.549062 | -1.368696 | 1.035399 |
| C | -1.623002 | 1.611244 | 0.087083 |
| O | -1.915034 | 2.475187 | 0.890090 |
| O | -2.352542 | 1.328679 | -1.009138 |
| C | -3.591506 | 2.050346 | -1.138563 |
| H | -4.244791 | 1.834301 | -0.289524 |
| H | -3.405327 | 3.126069 | -1.183958 |
| H | -4.036001 | 1.696496 | -2.068354 |
| O | 3.318184 | -1.133758 | 0.032616 |
| O | 3.266361 | 1.538307 | 0.142091 |
| C | 3.284976 | 2.954996 | 0.314524 |
| H | 4.339855 | 3.227627 | 0.352889 |
| H | 2.806756 | 3.464991 | -0.529793 |
| H | 2.795686 | 3.247696 | 1.250262 |
| C | 3.316085 | -2.350679 | -0.600916 |
| H | 2.244820 | -2.909793 | -0.347935 |
| H | 3.267013 | -2.294400 | -1.693786 |
| H | 4.115127 | -2.982668 | -0.213223 |

**Coordinates for oxazolidine (1o)**

Energy = -971.235838 Hartrees

| | | | |
|---|---|---|---|
| C | 0.838100 | -1.219518 | 0.050228 |
| C | 2.027132 | -0.484880 | 0.023131 |
| C | 2.041789 | 0.901859 | -0.002191 |
| C | 0.788918 | 1.552020 | -0.043803 |
| C | -0.403855 | 0.829086 | -0.048177 |
| C | -0.412280 | -0.588469 | 0.022689 |
| H | 0.739181 | 2.631084 | -0.102891 |
| H | 0.569240 | -3.242279 | -0.212453 |
| C | 2.624300 | -2.650517 | -0.095110 |
| H | 2.819007 | -2.959065 | -1.136418 |
| H | 3.151587 | -3.311299 | 0.597386 |
| N | 1.190587 | -2.560449 | 0.203114 |
| O | 3.119250 | -1.313917 | 0.097339 |
| O | 3.251916 | 1.518695 | 0.002241 |
| C | 3.287402 | 2.943585 | -0.024715 |
| H | 2.783165 | 3.371062 | 0.850037 |
| H | 4.344408 | 3.209827 | -0.001698 |
| H | 2.832084 | 3.335878 | -0.942009 |
| C | -1.675578 | -1.339119 | 0.202106 |
| C | -1.668813 | 1.588936 | -0.313683 |
| O | -2.457964 | 1.323533 | -1.196869 |
| O | -2.688417 | -0.903727 | 0.711103 |
| O | -1.575651 | -2.627219 | -0.239498 |
| O | -1.790285 | 2.663661 | 0.498197 |
| C | -2.757606 | -3.432807 | -0.059484 |
| H | -3.597010 | -2.998111 | -0.606373 |
| H | -2.504570 | -4.414496 | -0.460123 |
| H | -3.014408 | -3.501355 | 1.000171 |
| C | -2.958239 | 3.477752 | 0.275326 |
| H | -3.863536 | 2.881609 | 0.409967 |
| H | -2.903596 | 4.271332 | 1.020204 |
| H | -2.948074 | 3.893169 | -0.735606 |

**Unscaled vibrational frequencies in ($cm^{-1}$) for transition states and different possible species formed from singlet nitrene**

| 1n | TS 1n-1a | 1a | TS 1a-1k | 1k | TS 1k-1a' |
|---|---|---|---|---|---|
| 26.63 | 22.1884*i* | 30.37 | 342.9743*i* | 40.78 | 393.1187*i* |
| 42.31 | 41.88 | 39.05 | 28.52 | 44.95 | 35.82 |
| 50.03 | 47.69 | 61.82 | 45.53 | 48.19 | 40.13 |
| 61.86 | 52.33 | 73.49 | 55.37 | 65.13 | 46.27 |
| 83.61 | 64.65 | 80.71 | 69.54 | 84.54 | 57.66 |
| 88.50 | 79.04 | 90.91 | 71.05 | 96.17 | 63.75 |
| 101.07 | 99.34 | 108.19 | 95.42 | 106.89 | 71.92 |
| 114.39 | 103.85 | 116.30 | 107.65 | 120.84 | 85.44 |
| 116.32 | 111.62 | 127.98 | 110.43 | 127.88 | 96.90 |
| 129.50 | 121.69 | 133.89 | 126.19 | 136.25 | 127.26 |
| 139.44 | 126.69 | 137.16 | 135.96 | 143.80 | 129.32 |
| 172.88 | 137.03 | 152.07 | 139.35 | 154.11 | 149.08 |
| 181.28 | 171.78 | 175.38 | 146.87 | 159.20 | 153.93 |
| 198.47 | 185.57 | 196.41 | 171.07 | 173.00 | 163.77 |
| 202.99 | 207.31 | 216.72 | 192.89 | 194.80 | 172.84 |
| 215.81 | 219.97 | 234.78 | 211.64 | 215.67 | 192.22 |
| 248.26 | 233.72 | 263.07 | 229.24 | 248.59 | 217.88 |
| 256.95 | 247.89 | 269.80 | 251.25 | 252.64 | 247.60 |
| 275.40 | 275.54 | 286.27 | 259.88 | 302.45 | 264.39 |
| 305.35 | 296.09 | 291.53 | 292.94 | 316.35 | 285.44 |
| 307.82 | 309.82 | 295.05 | 308.42 | 332.45 | 312.49 |
| 337.32 | 330.92 | 328.18 | 312.91 | 364.63 | 334.66 |
| 339.78 | 355.63 | 342.45 | 355.57 | 373.62 | 357.51 |
| 371.45 | 378.88 | 372.52 | 382.28 | 406.56 | 389.58 |
| 403.53 | 401.89 | 392.27 | 389.23 | 425.40 | 426.56 |
| 452.13 | 412.95 | 506.26 | 430.53 | 480.97 | 443.48 |
| 468.02 | 477.73 | 524.15 | 490.98 | 496.25 | 477.37 |
| 524.35 | 511.44 | 566.82 | 531.15 | 504.21 | 520.11 |
| 538.92 | 531.31 | 621.34 | 564.10 | 532.66 | 568.45 |
| 611.84 | 608.39 | 641.49 | 587.94 | 611.90 | 604.81 |
| 631.83 | 630.87 | 657.25 | 620.13 | 650.07 | 625.64 |
| 669.97 | 664.56 | 692.61 | 665.51 | 658.74 | 666.13 |
| 741.26 | 719.05 | 720.56 | 703.45 | 710.36 | 721.05 |
| 756.00 | 761.11 | 777.35 | 727.47 | 745.39 | 752.06 |
| 779.57 | 785.99 | 784.07 | 768.29 | 764.41 | 760.45 |
| 790.49 | 793.51 | 792.39 | 783.25 | 779.97 | 773.29 |
| 806.07 | 807.83 | 822.86 | 784.63 | 793.77 | 795.98 |
| 853.49 | 855.84 | 851.75 | 825.15 | 836.05 | 836.39 |
| 907.23 | 907.37 | 884.00 | 872.21 | 908.82 | 872.61 |

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|---|---|---|---|---|---|
| 938.00 | 933.10 | 926.75 | 913.75 | 937.08 | 916.04 |
| 986.76 | 979.09 | 988.24 | 977.41 | 978.59 | 978.73 |
| 1006.77 | 993.54 | 1001.80 | 990.30 | 998.65 | 1014.67 |
| 1037.19 | 1019.34 | 1038.41 | 1007.04 | 1032.30 | 1025.73 |
| 1071.93 | 1049.88 | 1057.95 | 1064.71 | 1067.62 | 1051.32 |
| 1158.87 | 1138.51 | 1124.17 | 1095.41 | 1130.40 | 1102.89 |
| 1165.19 | 1155.25 | 1151.77 | 1167.36 | 1163.51 | 1162.95 |
| 1170.00 | 1166.94 | 1169.06 | 1168.06 | 1168.40 | 1167.69 |
| 1171.37 | 1170.27 | 1171.27 | 1170.62 | 1171.83 | 1173.09 |
| 1172.60 | 1171.13 | 1172.60 | 1173.40 | 1174.10 | 1173.36 |
| 1180.16 | 1172.77 | 1174.37 | 1174.45 | 1174.17 | 1173.78 |
| 1204.78 | 1202.07 | 1193.44 | 1179.40 | 1192.86 | 1180.19 |
| 1205.74 | 1206.10 | 1199.81 | 1203.58 | 1208.17 | 1202.13 |
| 1216.41 | 1216.20 | 1212.95 | 1209.78 | 1213.29 | 1209.46 |
| 1217.93 | 1216.90 | 1215.55 | 1216.66 | 1217.15 | 1213.45 |
| 1260.32 | 1248.82 | 1221.63 | 1219.94 | 1249.17 | 1224.29 |
| 1278.23 | 1269.29 | 1238.03 | 1249.27 | 1252.28 | 1249.61 |
| 1297.92 | 1296.76 | 1286.06 | 1282.92 | 1280.42 | 1267.14 |
| 1330.52 | 1323.15 | 1308.52 | 1318.45 | 1314.78 | 1309.29 |
| 1346.46 | 1366.76 | 1372.42 | 1342.59 | 1364.56 | 1369.18 |
| 1385.10 | 1418.64 | 1424.16 | 1431.84 | 1397.70 | 1415.84 |
| 1436.92 | 1468.55 | 1467.39 | 1471.77 | 1465.05 | 1425.82 |
| 1472.05 | 1475.33 | 1472.98 | 1472.87 | 1473.88 | 1472.42 |
| 1476.39 | 1478.47 | 1475.22 | 1477.55 | 1476.10 | 1474.70 |
| 1485.46 | 1481.41 | 1476.36 | 1481.28 | 1481.88 | 1478.65 |
| 1486.56 | 1487.47 | 1487.99 | 1486.53 | 1486.85 | 1487.08 |
| 1488.30 | 1488.54 | 1488.25 | 1487.29 | 1487.72 | 1488.52 |
| 1491.33 | 1493.43 | 1492.52 | 1493.17 | 1491.83 | 1490.41 |
| 1497.56 | 1496.83 | 1496.97 | 1494.02 | 1492.87 | 1492.25 |
| 1498.59 | 1497.73 | 1498.51 | 1500.27 | 1501.54 | 1499.89 |
| 1498.75 | 1498.73 | 1500.04 | 1501.48 | 1501.74 | 1500.23 |
| 1499.15 | 1500.03 | 1506.77 | 1505.26 | 1502.87 | 1501.01 |
| 1504.40 | 1507.20 | 1509.53 | 1511.25 | 1509.77 | 1507.72 |
| 1509.35 | 1528.79 | 1511.54 | 1524.56 | 1547.81 | 1508.44 |
| 1587.13 | 1574.18 | 1603.68 | 1545.50 | 1624.96 | 1590.84 |
| 1601.29 | 1620.90 | 1766.56 | 1770.52 | 1765.64 | 1766.31 |
| 1762.48 | 1769.30 | 1790.73 | 1795.34 | 1783.72 | 1781.82 |
| 1795.28 | 1784.96 | 1797.48 | 1910.29 | 1965.01 | 1973.23 |
| 3028.56 | 3029.66 | 3036.18 | 3032.88 | 3019.49 | 3021.30 |
| 3062.63 | 3051.70 | 3038.31 | 3046.42 | 3055.23 | 3064.81 |
| 3066.21 | 3067.58 | 3065.13 | 3064.13 | 3063.55 | 3065.04 |
| 3068.31 | 3069.15 | 3068.39 | 3066.08 | 3065.00 | 3066.46 |
| 3097.94 | 3099.84 | 3108.15 | 3105.17 | 3090.45 | 3090.38 |
| 3146.57 | 3144.77 | 3112.09 | 3123.94 | 3142.54 | 3144.01 |

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|---|---|---|---|---|---|
| 3149.21 | 3148.96 | 3144.14 | 3143.34 | 3145.19 | 3144.83 |
| 3150.81 | 3151.01 | 3150.65 | 3147.42 | 3145.72 | 3148.33 |
| 3159.40 | 3163.87 | 3151.71 | 3157.07 | 3149.33 | 3155.40 |
| 3167.45 | 3179.64 | 3169.21 | 3166.79 | 3174.16 | 3162.76 |
| 3178.64 | 3181.42 | 3178.37 | 3175.60 | 3174.25 | 3174.33 |
| 3180.74 | 3182.45 | 3181.70 | 3176.68 | 3174.99 | 3177.88 |
| 3242.30 | 3235.23 | 3228.06 | 3232.98 | 3189.87 | 3178.33 |

| **1a'** | **TS 1a'-1c** | **1c** | **TS 1c-1y** | **1y** | **TS 1n-1o** | **1o** |
|---|---|---|---|---|---|---|
| 34.38 | 156.7377*i* | 40.78 | 58.193*i* | 41.28 | 392.9597*i* | 18.46 |
| 37.70 | 35.22 | 44.95 | 35.18 | 56.09 | 35.60 | 42.60 |
| 47.32 | 40.66 | 48.19 | 46.83 | 61.21 | 56.97 | 67.24 |
| 54.31 | 52.25 | 65.13 | 57.62 | 81.99 | 76.10 | 76.66 |
| 65.18 | 58.62 | 84.54 | 69.69 | 92.17 | 82.33 | 96.14 |
| 72.93 | 60.96 | 96.17 | 89.71 | 94.84 | 84.19 | 117.27 |
| 83.59 | 79.58 | 106.89 | 106.02 | 125.38 | 109.77 | 121.11 |
| 93.39 | 88.69 | 120.84 | 115.63 | 136.19 | 132.72 | 140.13 |
| 125.31 | 95.77 | 127.88 | 121.84 | 141.39 | 134.63 | 148.46 |
| 130.38 | 113.26 | 136.25 | 134.27 | 156.44 | 150.36 | 157.67 |
| 132.77 | 131.25 | 143.80 | 138.63 | 159.30 | 162.66 | 169.72 |
| 152.73 | 138.20 | 154.11 | 151.24 | 180.35 | 181.82 | 182.84 |
| 155.98 | 141.91 | 159.20 | 162.11 | 181.58 | 193.74 | 197.39 |
| 165.64 | 147.54 | 173.00 | 176.24 | 195.99 | 197.17 | 212.72 |
| 189.49 | 163.99 | 194.80 | 191.86 | 213.31 | 222.78 | 236.59 |
| 210.41 | 177.05 | 215.67 | 195.26 | 249.41 | 231.43 | 252.44 |
| 245.34 | 196.18 | 248.59 | 231.32 | 270.03 | 269.62 | 279.93 |
| 259.48 | 244.80 | 252.64 | 241.64 | 273.95 | 288.12 | 290.99 |
| 272.29 | 263.49 | 302.45 | 278.88 | 317.21 | 303.65 | 303.19 |
| 303.91 | 288.61 | 316.35 | 293.31 | 345.82 | 309.21 | 335.96 |
| 326.68 | 305.02 | 332.45 | 312.65 | 374.82 | 334.65 | 339.90 |
| 351.72 | 313.43 | 364.63 | 344.32 | 406.73 | 359.20 | 384.67 |
| 372.51 | 358.08 | 373.62 | 373.03 | 410.28 | 392.43 | 410.92 |
| 421.70 | 407.99 | 406.56 | 384.49 | 435.04 | 422.56 | 457.47 |
| 440.28 | 477.84 | 425.40 | 469.60 | 462.65 | 460.83 | 523.59 |
| 458.43 | 495.48 | 480.97 | 482.54 | 508.22 | 474.88 | 565.19 |
| 510.29 | 503.95 | 496.25 | 494.41 | 543.56 | 522.35 | 582.20 |
| 567.25 | 528.23 | 504.21 | 517.55 | 563.56 | 582.41 | 613.25 |
| 595.68 | 567.09 | 532.66 | 564.44 | 639.04 | 605.78 | 644.52 |
| 617.16 | 611.01 | 611.90 | 638.74 | 688.41 | 619.93 | 687.91 |
| 649.29 | 650.33 | 650.07 | 670.02 | 720.63 | 638.76 | 711.31 |
| 710.85 | 678.69 | 658.74 | 682.29 | 723.86 | 692.50 | 748.33 |
| 727.57 | 714.90 | 710.36 | 749.21 | 739.96 | 694.27 | 782.27 |

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|---|---|---|---|---|---|---|
| 763.10 | 746.20 | 745.39 | 762.73 | 759.47 | 755.50 | 788.78 |
| 777.77 | 777.55 | 764.41 | 770.11 | 765.87 | 777.75 | 803.85 |
| 786.76 | 783.68 | 779.97 | 776.95 | 782.61 | 782.41 | 814.99 |
| 816.54 | 803.68 | 793.77 | 796.49 | 863.13 | 804.02 | 847.31 |
| 847.29 | 855.54 | 836.05 | 860.34 | 884.30 | 819.86 | 891.40 |
| 874.89 | 899.31 | 908.82 | 899.21 | 921.70 | 859.38 | 952.71 |
| 913.92 | 921.33 | 937.08 | 908.28 | 1001.20 | 947.64 | 987.50 |
| 974.36 | 966.99 | 978.59 | 979.54 | 1019.41 | 964.89 | 1004.90 |
| 1001.73 | 1000.47 | 998.65 | 1017.31 | 1036.67 | 997.26 | 1033.25 |
| 1019.88 | 1032.27 | 1032.30 | 1041.86 | 1066.57 | 1036.94 | 1044.08 |
| 1051.52 | 1039.51 | 1067.62 | 1060.61 | 1144.46 | 1061.95 | 1062.52 |
| 1090.78 | 1116.08 | 1130.40 | 1120.21 | 1163.02 | 1086.34 | 1134.83 |
| 1147.72 | 1154.52 | 1163.51 | 1167.78 | 1170.37 | 1153.59 | 1152.59 |
| 1166.65 | 1167.22 | 1168.40 | 1170.38 | 1171.86 | 1170.98 | 1170.69 |
| 1170.68 | 1168.71 | 1171.83 | 1172.47 | 1172.94 | 1171.59 | 1173.82 |
| 1171.97 | 1170.13 | 1174.10 | 1174.13 | 1173.55 | 1172.24 | 1174.08 |
| 1173.67 | 1174.26 | 1174.17 | 1200.91 | 1202.58 | 1177.07 | 1181.31 |
| 1174.27 | 1183.05 | 1192.86 | 1204.57 | 1205.10 | 1200.70 | 1199.13 |
| 1196.82 | 1201.52 | 1208.17 | 1208.03 | 1209.15 | 1205.59 | 1202.68 |
| 1199.14 | 1206.28 | 1213.29 | 1214.98 | 1211.76 | 1214.47 | 1211.02 |
| 1211.73 | 1212.73 | 1217.15 | 1240.94 | 1241.98 | 1228.21 | 1212.61 |
| 1216.93 | 1230.14 | 1249.17 | 1252.02 | 1273.42 | 1236.65 | 1220.30 |
| 1236.76 | 1257.60 | 1252.28 | 1291.42 | 1312.99 | 1262.94 | 1274.71 |
| 1265.21 | 1288.11 | 1280.42 | 1306.67 | 1337.25 | 1293.25 | 1297.09 |
| 1295.90 | 1305.78 | 1314.78 | 1377.68 | 1388.29 | 1308.44 | 1344.37 |
| 1328.90 | 1362.73 | 1364.56 | 1409.94 | 1415.76 | 1363.81 | 1360.29 |
| 1379.28 | 1423.73 | 1397.70 | 1426.49 | 1454.48 | 1372.53 | 1400.14 |
| 1472.50 | 1470.05 | 1465.05 | 1454.80 | 1469.23 | 1395.32 | 1435.71 |
| 1472.67 | 1473.48 | 1473.88 | 1474.67 | 1478.49 | 1459.35 | 1471.11 |
| 1475.81 | 1476.18 | 1476.10 | 1477.95 | 1481.08 | 1472.38 | 1473.58 |
| 1484.80 | 1478.87 | 1481.88 | 1485.83 | 1484.02 | 1477.44 | 1480.91 |
| 1487.78 | 1487.54 | 1486.85 | 1486.31 | 1485.34 | 1486.32 | 1485.03 |
| 1487.89 | 1487.84 | 1487.72 | 1487.16 | 1490.74 | 1488.13 | 1485.76 |
| 1490.48 | 1494.37 | 1491.83 | 1489.10 | 1496.57 | 1488.46 | 1487.04 |
| 1493.78 | 1496.50 | 1492.87 | 1498.80 | 1498.20 | 1491.17 | 1498.38 |
| 1500.06 | 1500.81 | 1501.54 | 1499.74 | 1502.55 | 1499.37 | 1501.24 |
| 1501.11 | 1501.17 | 1501.74 | 1501.78 | 1502.98 | 1500.33 | 1502.61 |
| 1501.89 | 1507.67 | 1502.87 | 1502.92 | 1507.97 | 1501.68 | 1508.54 |
| 1508.78 | 1511.64 | 1509.77 | 1505.69 | 1522.11 | 1508.72 | 1538.05 |
| 1531.63 | 1513.37 | 1547.81 | 1526.99 | 1555.80 | 1541.71 | 1550.42 |
| 1632.43 | 1611.41 | 1624.96 | 1559.74 | 1590.90 | 1566.52 | 1627.65 |
| 1758.80 | 1634.38 | 1765.64 | 1612.63 | 1630.45 | 1631.16 | 1672.53 |
| 1795.62 | 1724.60 | 1783.72 | 1667.50 | 1689.12 | 1653.42 | 1773.75 |
| 1913.96 | 1791.31 | 1965.01 | 1728.00 | 1746.17 | 1680.16 | 1794.04 |

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|---|---|---|---|---|---|---|
| 3026.26 | 3044.50 | 3019.49 | 3026.85 | 3015.45 | 1779.36 | 2963.13 |
| 3064.13 | 3047.41 | 3055.23 | 3060.73 | 3057.15 | 3030.12 | 3024.64 |
| 3065.63 | 3064.78 | 3063.55 | 3063.14 | 3060.17 | 3058.77 | 3063.58 |
| 3066.07 | 3066.34 | 3065.00 | 3065.99 | 3060.37 | 3063.01 | 3066.24 |
| 3096.06 | 3124.37 | 3090.45 | 3095.55 | 3078.55 | 3064.43 | 3091.74 |
| 3143.00 | 3126.74 | 3142.54 | 3139.04 | 3132.05 | 3099.94 | 3101.76 |
| 3146.11 | 3144.31 | 3145.19 | 3141.78 | 3137.91 | 3141.21 | 3143.51 |
| 3152.84 | 3146.74 | 3145.72 | 3146.90 | 3139.12 | 3144.10 | 3148.37 |
| 3154.33 | 3165.26 | 3149.33 | 3165.92 | 3158.05 | 3159.45 | 3158.16 |
| 3160.64 | 3167.84 | 3174.16 | 3172.14 | 3165.37 | 3174.51 | 3170.79 |
| 3175.58 | 3176.66 | 3174.25 | 3173.06 | 3169.82 | 3174.59 | 3173.56 |
| 3177.90 | 3178.09 | 3174.99 | 3176.03 | 3180.07 | 3178.93 | 3242.36 |
| 3198.07 | 3226.96 | 3189.87 | 3244.58 | 3234.32 | 3249.71 | 3622.50 |