Supporting Information

Electrophilic Iodination: A Gateway to High Iodine Compounds and Energetic Materials

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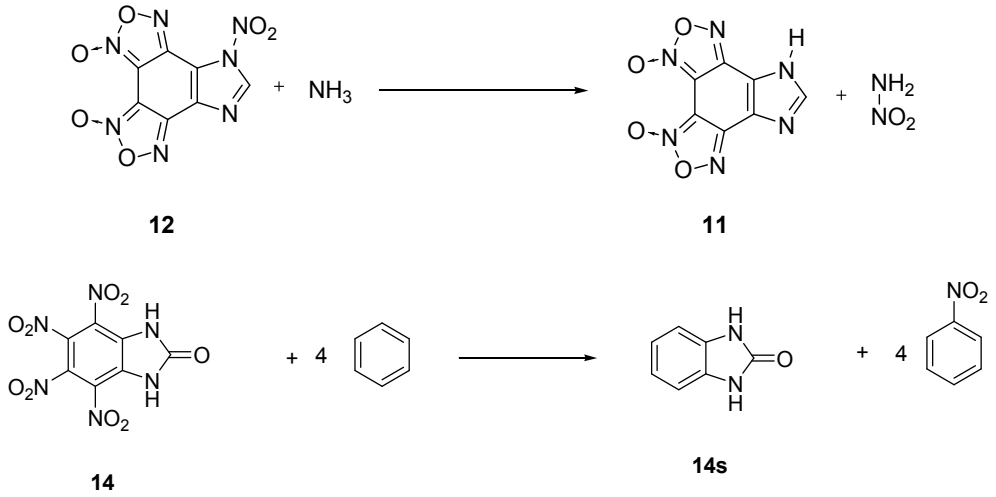
Calculations – University of Idaho

Gaussian Calculations

Geometric optimization and frequency analyses of the compounds in the isodesmic reactions were accomplished by using the B3LYP functional with the 6-31+G** basis set from Gaussian 03.[1] All of the optimized structures were characterized to be true local energy minima on the potential energy surface without imaginary frequencies. The enthalpy of reaction is obtained by combining the MP2/6– 311++G** energy difference for the reactions, the scaled zero point energies (ZPE), values of thermal correction (H_T), and other thermal factors. The gas phase heat of formation at 298.15K for compound **11** was calculated from the atomization energy at the G2 level, gas phase enthalpies of **12** and **14** were calculated based on isodesmic reactions in Scheme S1 at MP2/6-311++G(d,p)//B3LYP(6-31+G(d,p)) level. The gas phase enthalpies of formation of **11**, **12** and **14** were converted to the solid state enthalpies of formation by subtraction of sublimation enthalpy calculated according to Trouton's rule ($\Delta H_{sub} = 188T_m$) (Table S1).[2]



Scheme S1: Isodesmic reactions for compounds **12** and **14**.

Table S1. Calculated (MP2/6-311++G**//B3LYP/6-31+G**) total energy (E_0), corrected MP2 total energy (E_{corr}), zero-point energy (*ZPE*), thermal correction to enthalpy (H_T), heat of reaction for the isodesmic reaction (ΔH_R) and gas phase heats of formation ($\Delta_f H_m^\circ$) from Gaussian 03.[1]

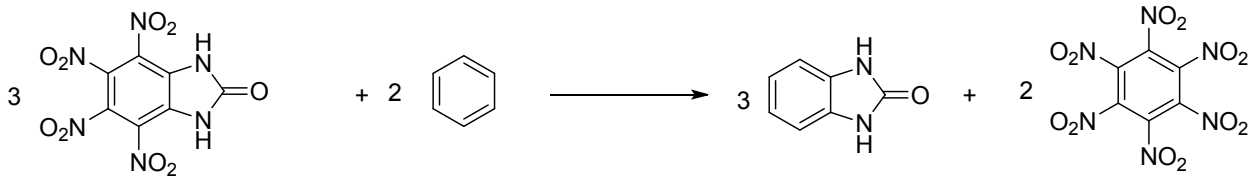
	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	E_0 [Hartree/Particle]	ΔH_R (Hartree/Particle)	ΔH_{Sub}[a] (kJ mol^{-1})	$\Delta_f H_m^\circ$(g) [kJ mol^{-1}]	$\Delta_f H_m^\circ$(s) [kJ mol^{-1}]
Benzene	0.100441	0.105785	-231.5842377	-	-	+82.9[b]	-
Nitrobenzene	0.103043	0.110809	-435.6906555	-	-	+68.5[b]	-
11	0.109795	0.1223	-895.031117	-	88.7	+604.2[c]	+515.5
12	0.110929	0.126049	-1099.084817	0.05495	79.1	+604.3	+525.2
14s	0.122904	0.131114	-453.9743248	-	-	-63.9[d]	-
14	0.131244	0.149867	-1270.361893	-0.03684	107.5	-24.8	-132.3

[a] Heat of sublimation calculated according to Trouton's rule ($\Delta H_{Sub} = 0.188T_d$) ref: [2]. [b] Gas phase heat of formation NIST ref [3]; [c] Calculated from G2. [d] Experimental gas phase heat of formation ref [4]

Calculations – Dr. Jerry Boatz, Air Force Research Laboratory, Edwards Air Force Base, CA

GAMESS Calculations

The calculations for compound **14** were also performed by using GAMESS quantum chemistry program[5,6] with a different isodesmic reaction shown in Scheme S2. The heat of reaction is obtained by combining corrected



14 **14s**

Scheme S2: Isodesmic reaction for **14**

B3LYP/6-311++(d,p) energy difference of the products and reactants calculated at B3LYP /6-311++g(d,p)//B3LYP6-311++g(d,p)) level. The gas phase heats of fomation for the related species were calculated from the atomization energy at the G3(MP2) level. The heat of sublimation was obtained using an approach developed by Rice and Byrd (Table S2).[7,8]

Table S2: Calculation of heat of formation of **14**

	B3LYP/6-311++(d,p)	B3LYP ZPE	B3LYP scaled ZPE	b3lyp elect+scaled ZPE	b3lyp thermal correction	ΔH_R (Hartree/ Particle)	ΔH_f kcal /mol	ΔH_f kJ /mol	ΔH_{Sub} (kJ mol^{-1})	$\Delta_f H_m^\circ(s)$ [kJ mol^{-1}]
14	-1272.842640	0.130986	0.128759	-1272.713881	0.018791	0.07378	1.5	6.3	120.9	-114.6
14s	-454.987584	0.122195	0.120118	-454.867467	0.008385			-62.9[a]		
Hexanitro benzene	-1458.901699	0.111421	0.109527	-1458.792172	0.021663			279.1[a]		
Benzene	-232.157071	0.099939	0.098240	-232.058831	0.005412			78.2[a]		

[a] Calculated based on G3(MP2) using GAMESS.

[1] Gaussian03, RevisionD.01, M. J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery,Jr., T. Vreven, K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian, Inc., Wallingford CT, 2004.

[2] M. S. Westwell, M. S. Searle, D. J. Wales and D. H. Williams, *J. Am. Chem. Soc.,* 1995, **117**, 5013–5015.

[3] http://webbook.nist.gov/chemistry/

[4] V. M. F. Morais, M. S. Miranda, M. A. R. Matos, J. F Liebman, *Mol. Phys.* 2006, **104**, 325–334.

[5] M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, S. Koseki, N. Matsunaga, K. A. Nguyen, S. Su, T. L. Windus, M. Dupuis, J.A Montgomery. *J. Comput. Chem.* 1993, **14**, 1347– 1363

[6]. M. S. Gordon, M. W. Schmidt. Advances in Electronic Structure Theory, in Theory and Applications of Computational Chemistry: The First Forty Years; Dykstra, C.; Frenking, G.; Kim, K.; Scuseria, G., Eds.; Elsevier: Amsterdam, 2005; pp 1167– 1190.

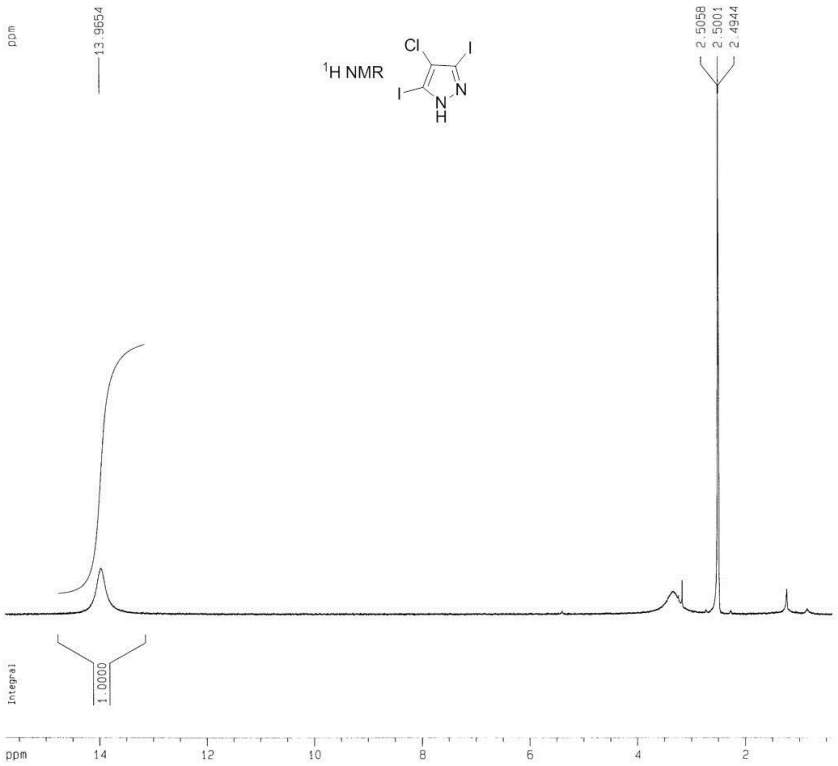
[7] E.F.C. Byrd, B. M. Rice. *J. Phys. Chem. A* 2006, **110** (3), 1005–1013; ibid 2009, ***113***, 5813.

[8] E.F.C. Byrd, B. M Rice. *J. Phys. Chem. A* 2009, **113** (1), 345–352.

Table S3. Crystallographic data for **5**, **10** and **14**

Compound	**5**	**10•C_2H_6OS**	**14•$C_4H_8O_2$**
Formula	$C_8H_5I_2N_7O_4$	$C_9H_8I_2N_4O_5S$	$C_{11}H_{10}N_6O_{11}$
CCDC number	1424001	1424002	1424003
M_w	516.99	538.05	402.25
Crystal size [mm^3]	0.209 x 0.034 x 0.005	0.123 x 0.057 x 0.032	0.310 x 0.175 x 0.058
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$P2_1/c$	P-1
a [Å]	16.6797(6)	5.34160(10)	7.8304(7)
b [Å]	98.956(2)	25.7684(6)	9.3182(8)
c [Å]	9.1213(3)	11.3694(3)	12.2176(11)
α[°]	90	90	102.459(3)
β [°]	107.606(19)	97.2720(10)	104.030(3)
γ [°]	90	90	100.776(3)
V [Å^3]	1339.59(8)	1552.35(6)	817.12(13)
Z	4	4	2
T [K]	150(2)	273(2)	296(2)
ρ_{calcd} [Mg m^{-3}]	2.498	2.302	1.635
μ [mm^{-1}]	37.190	4.211	0.149
F(000)	960	1008	412
θ[°]	2.682 to 68.705	3.613 to 26.381	2.506 to 26.422
Index ranges	-17<=h<=20 -10<=k<=10 -10<=l<=10	-6<=h<=6 -32<=k<=32 -14<=l<=14	-8<=h<=9 -11<=k<=11 -15<=l<=15
Reflections collected	7543	14724	7885
Independent reflections (R_{int})	2389 [$R_{(int)}$ = 0.0453]	3168 [$R_{(int)}$ = 0.0346]	3321 [$R_{(int)}$ = 0.0157]
Data/restraints/parameters	2389 / 1 / 193	3168 / 0 / 196	3321 / 0 / 275
GOF on F^2	1.024	0.827	1.069
R_1 ($I > 2\delta(I)$)[a]	0.0322	0.0275	0.0381
wR_2 ($I > 2\delta$ (I))[b]	0.0718	0.0758	0.1067
R_1 (all data)	R_1 = 0.0536	0.0410	0.0536
wR_2 (all data)	0.0797	0.0853	0.1197
Largest diff. peak and hole [e. Å-3]	0.830 and -0.874	0.855 and -0.449	0.257 and -0.203

[a] $R_1 = \Sigma||F_0| - |F_c|| / \Sigma|F_0|$ [b] $R_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum w(F_0^2)^2]^{1/2}$

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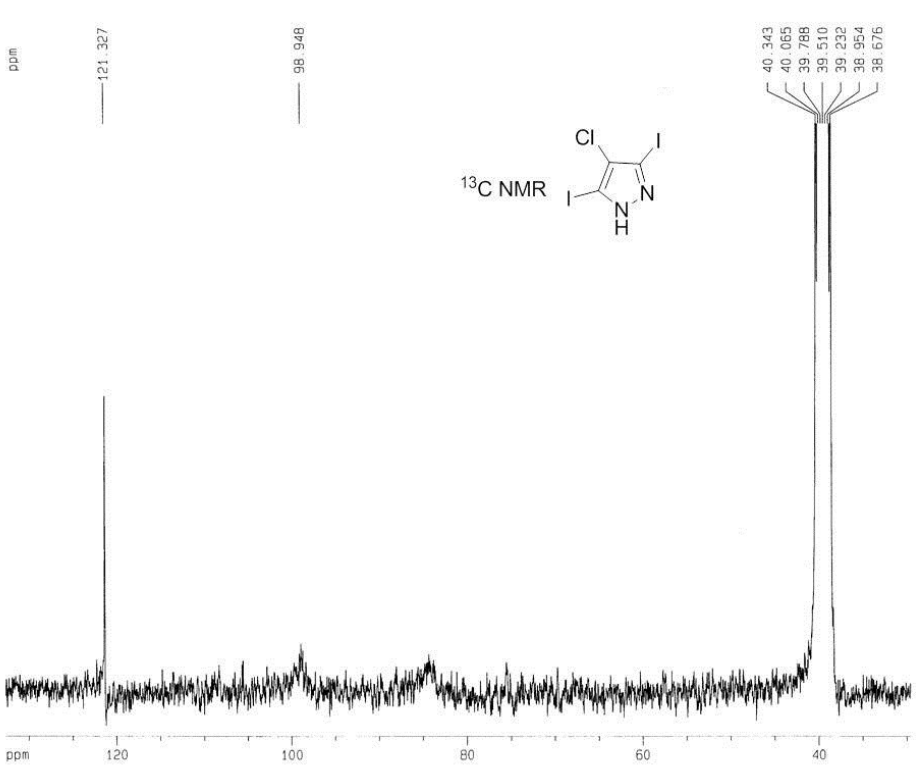


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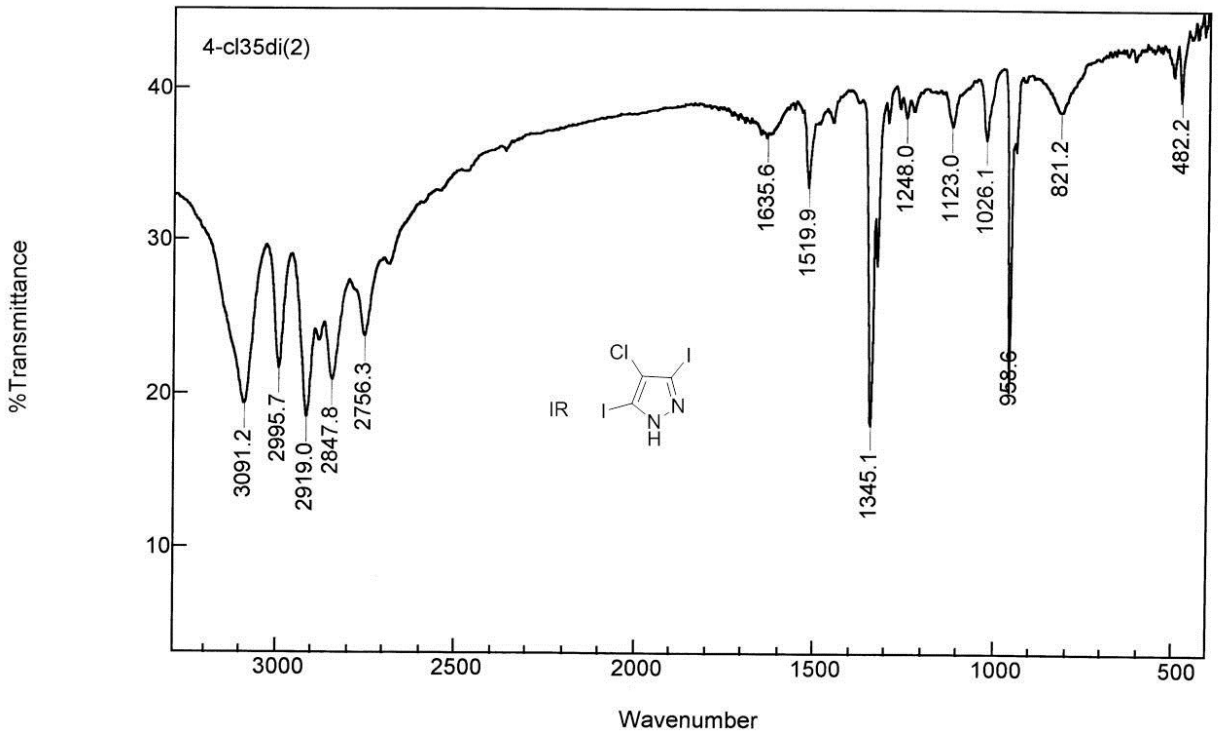
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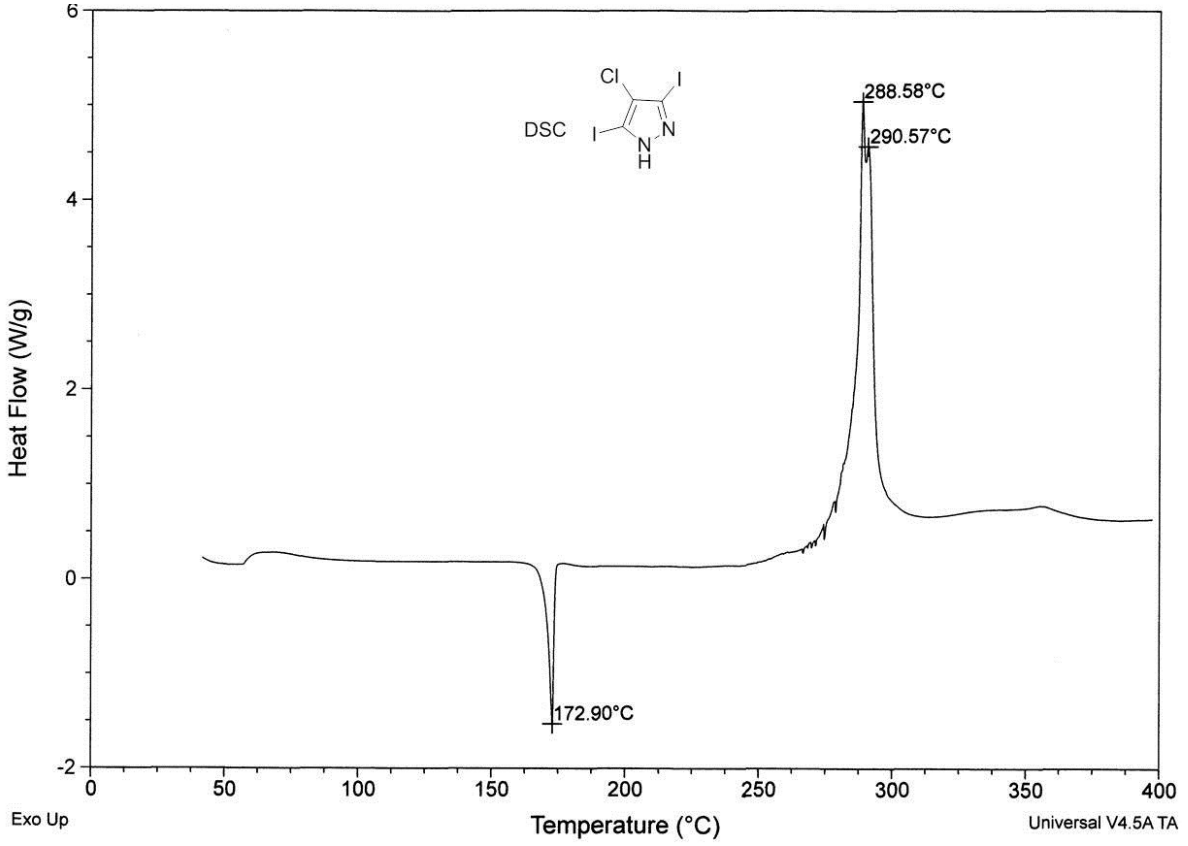
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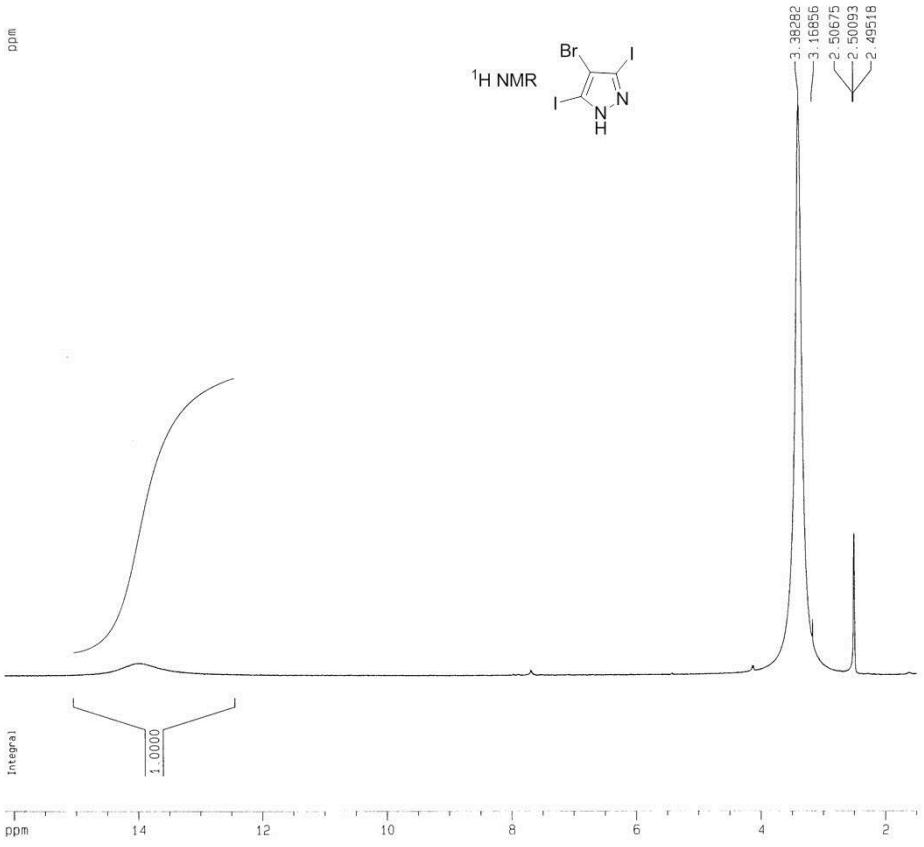


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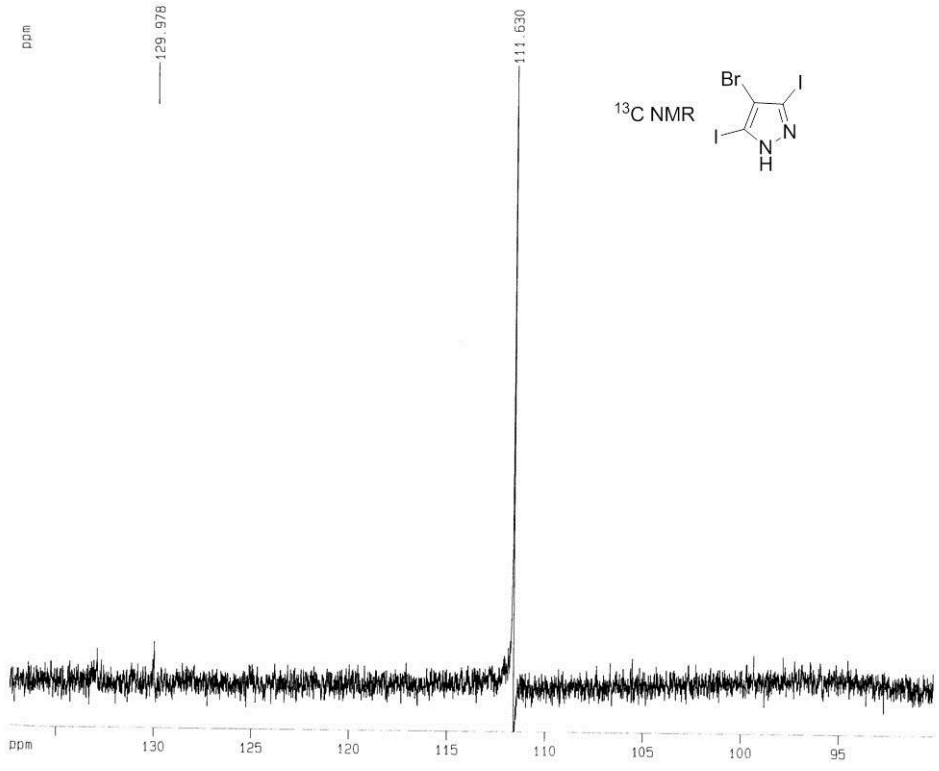


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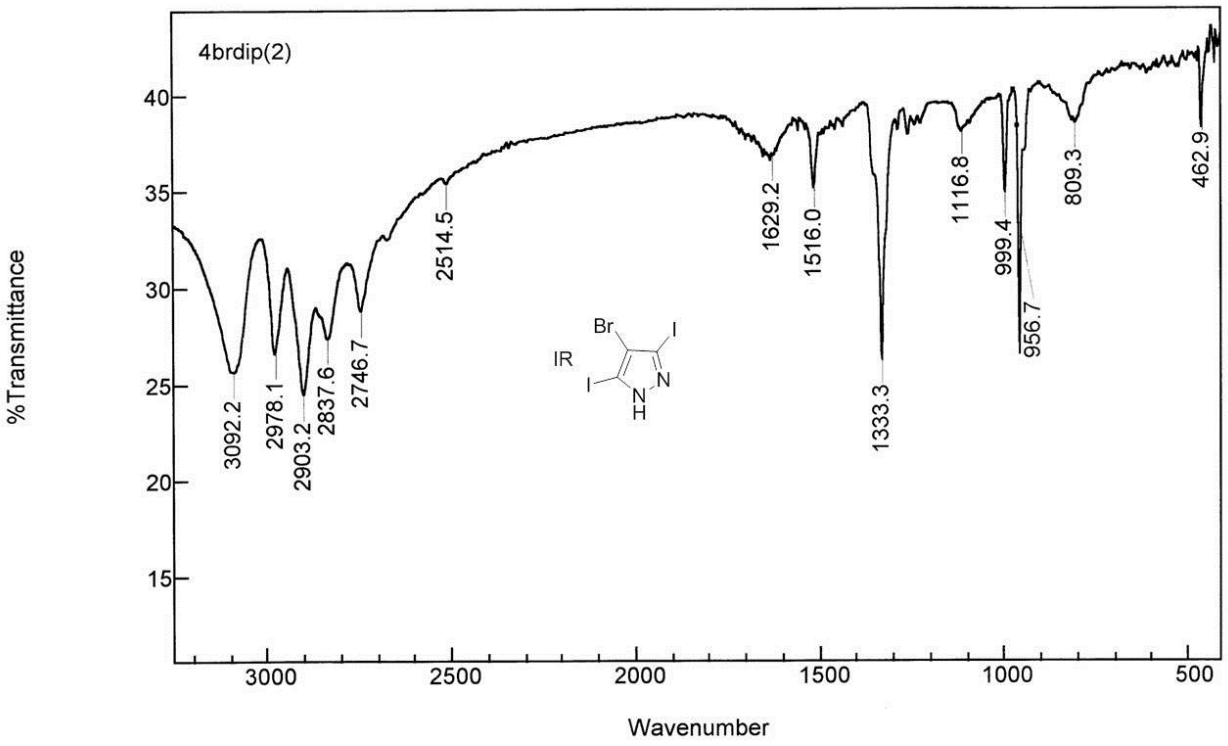
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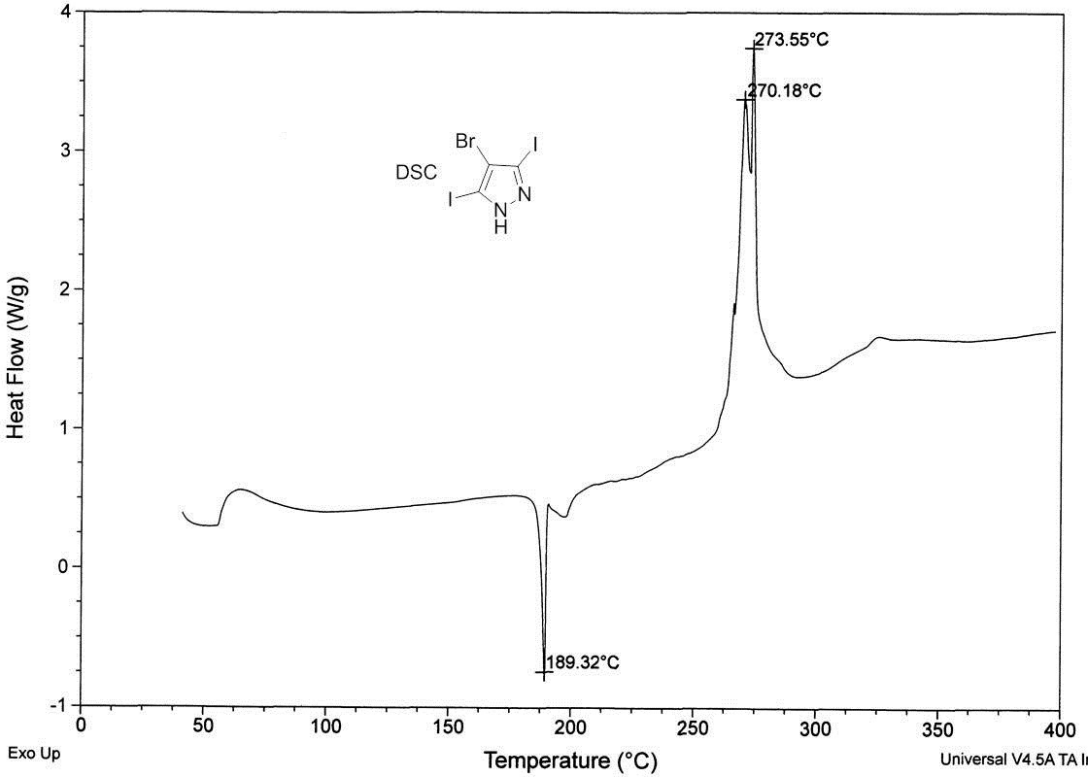
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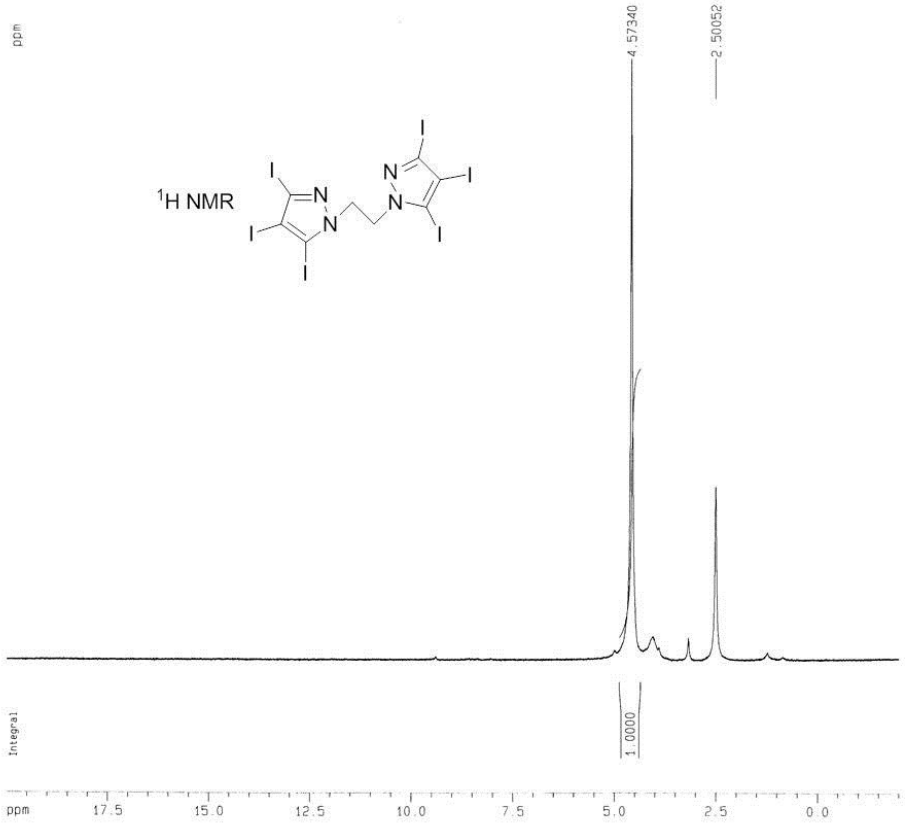


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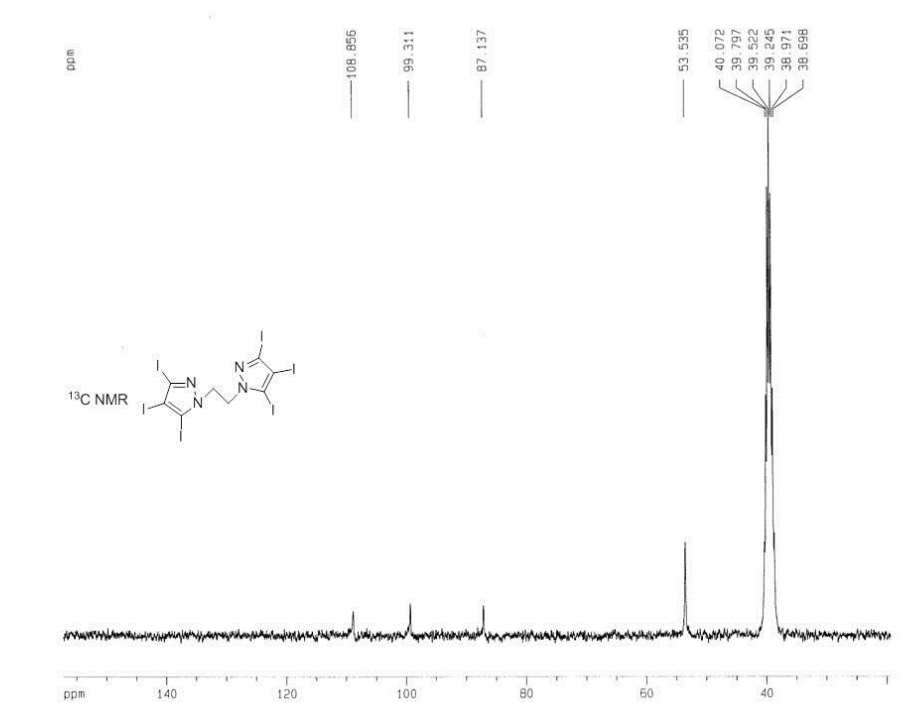


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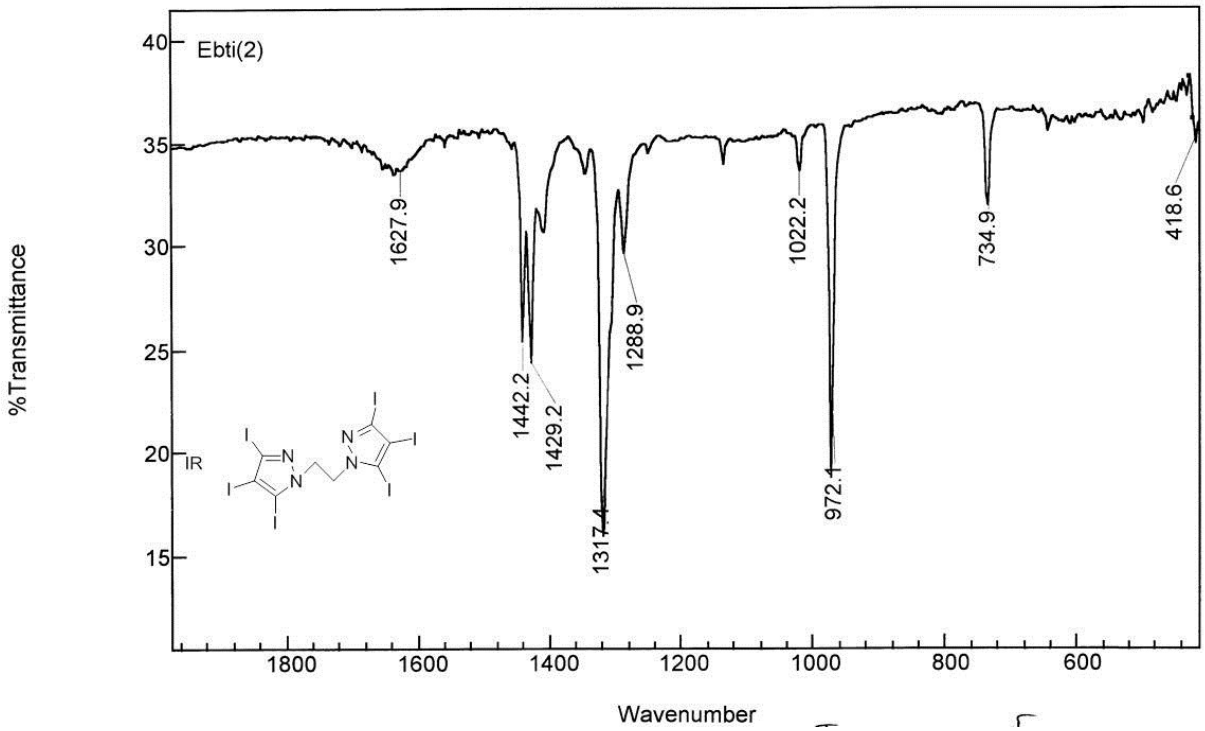
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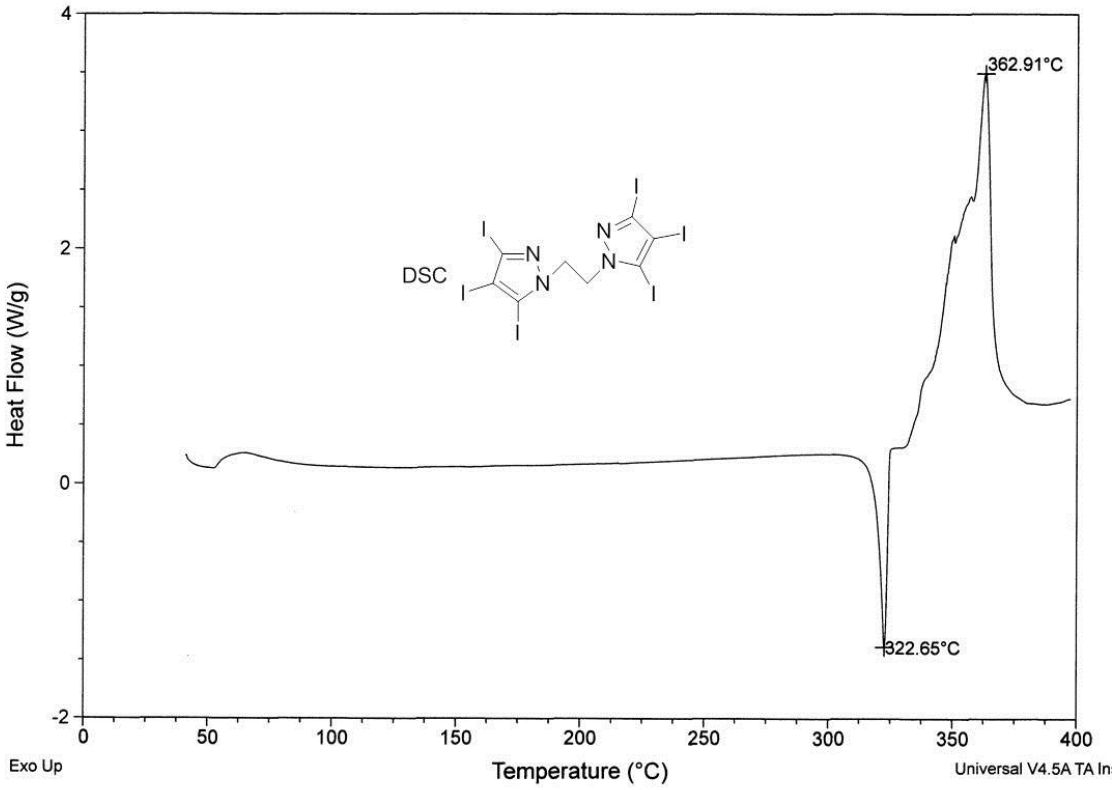
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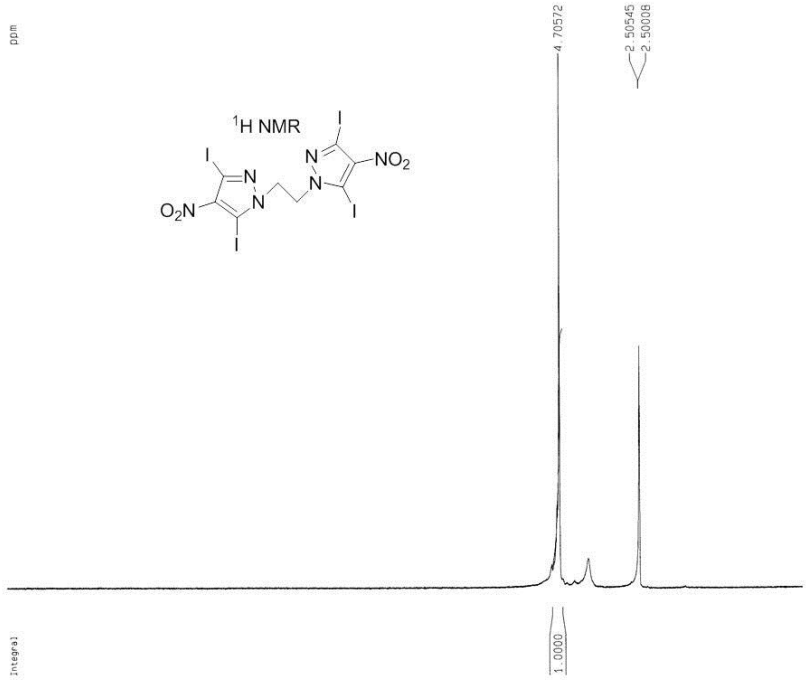
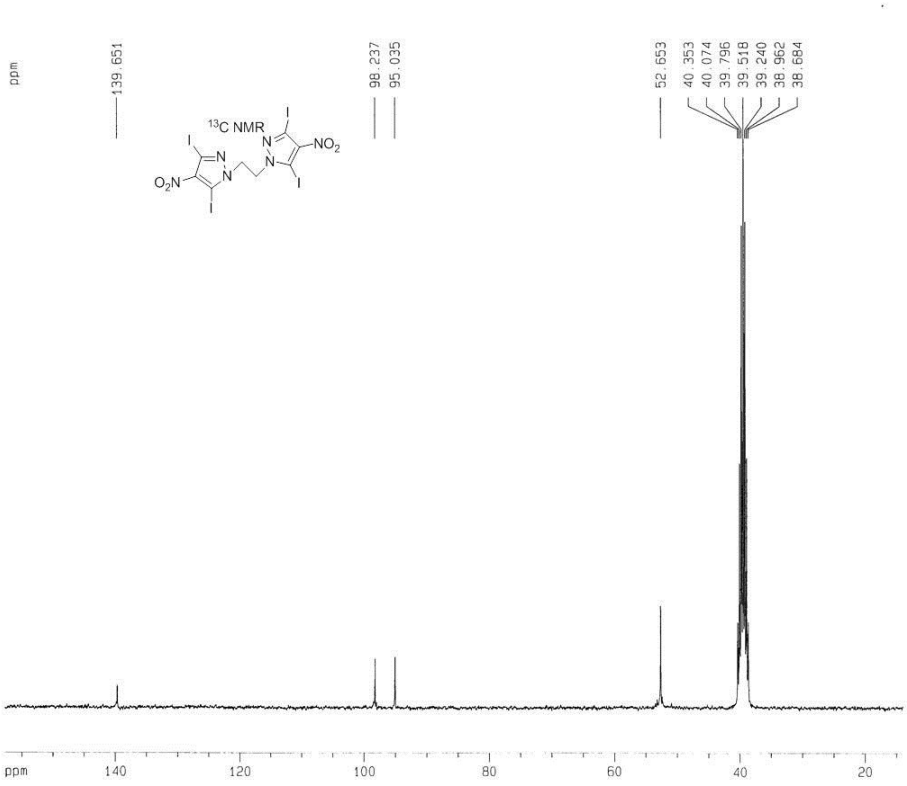
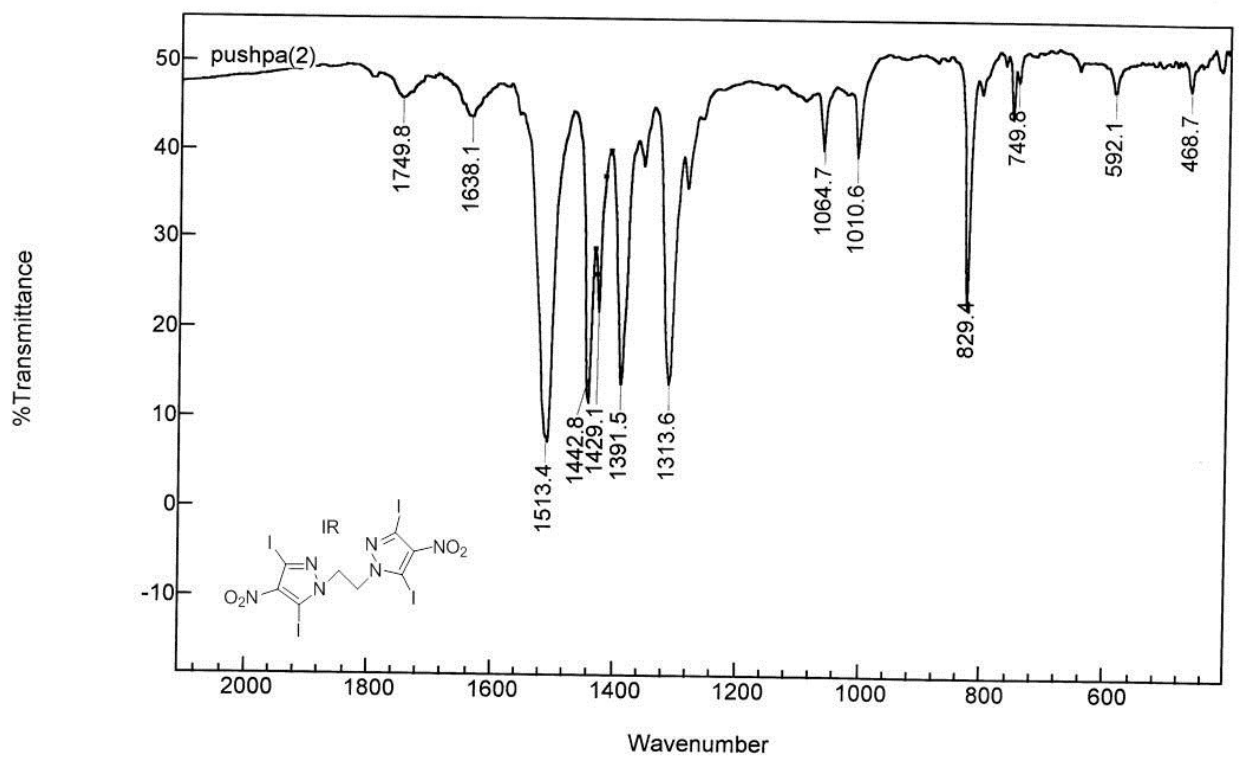
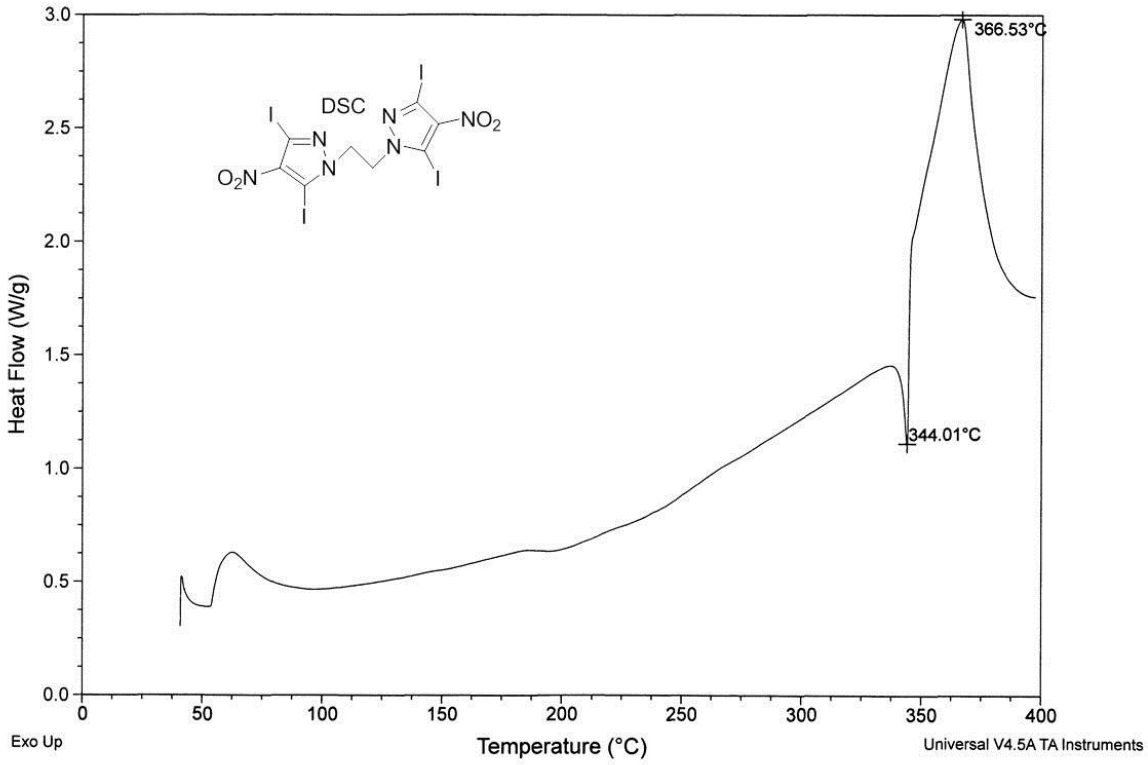


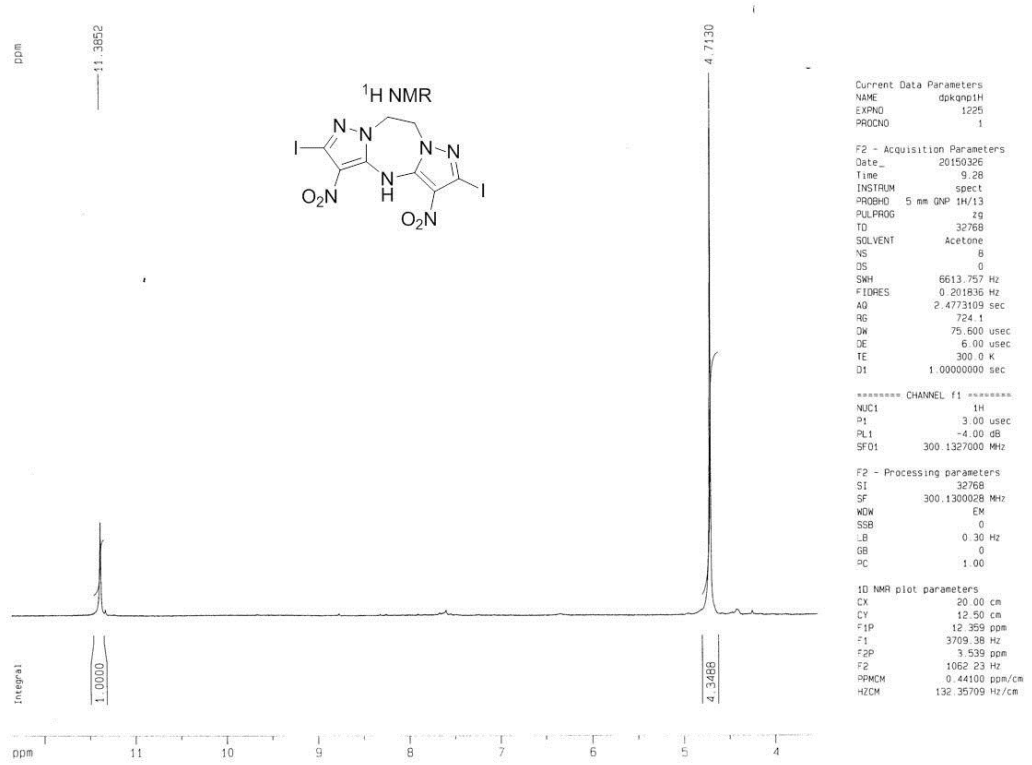

```
Current Data Parameters
NAME                 dpkqnp1H
EXPNO                    1213
PROCNO                      1

F2 - Acquisition Parameters
Date_               20150317
Time                   16.29
INSTRUM                spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zg
TD                      32768
SOLVENT              Acetone
NS                          8
DS                          0
SWH                 6613.757 Hz
FIDRES              0.201836 Hz
AQ                  2.4773109 sec
RG                      645.1
DW                     75.600 usec
DE                      6.00 usec
TE                     300.0 K
D1                1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       3.00 usec
PL1                     -4.00 dB
SFO1              300.1327000 MHz

F2 - Processing parameters
SI                      32768
SF                300.1300022 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.50 cm
F1P                    20.000 ppm
F1                    6002.60 Hz
F2P                    -2.008 ppm
F2                    -602.54 Hz
PPMCM                 1.10038 ppm/cm
HZCM                330.25696 Hz/cm
```

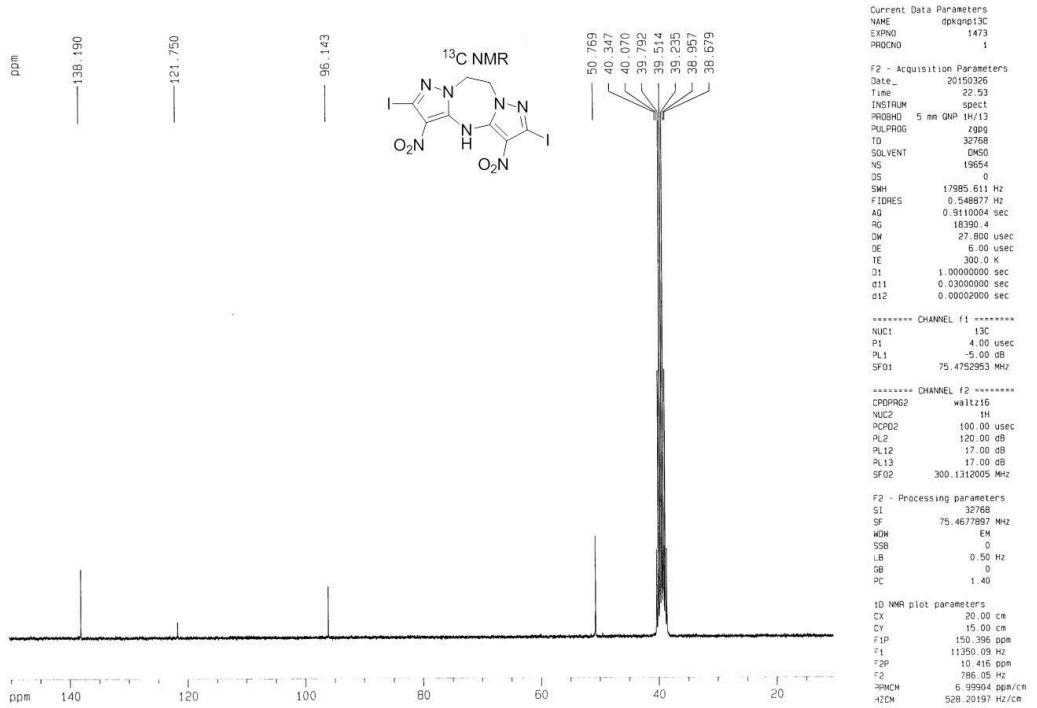


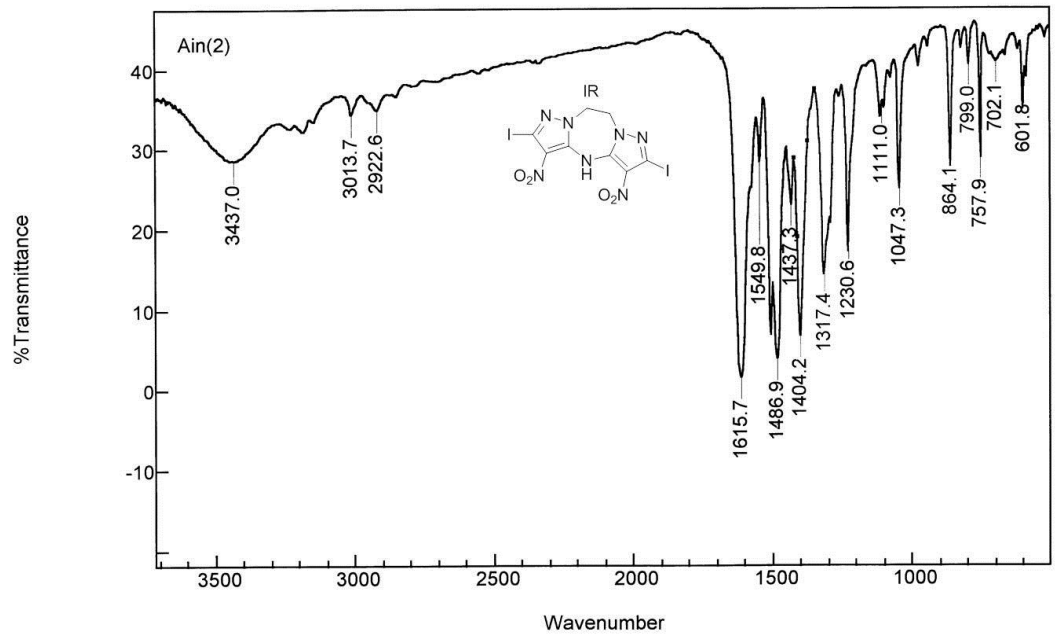

```
Current Data Parameters
NAME                 dpkqnp13C
EXPNO                     1460
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150312
Time                   22.10
INSTRUM                spect
PROBHD   5 mm QNP 1H/13
PULPROG                zgpg
TD                      32768
SOLVENT                CDCl3
NS                       2208
DS                          0
SWH                17985.611 Hz
FIDRES              0.548877 Hz
AQ                  0.9110004 sec
RG                     18390.4
DW                     27.800 usec
DE                      6.00 usec
TE                     300.0 K
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       4.00 usec
PL1                     -5.00 dB
SFO1              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                    120.00 dB
PL12                    17.00 dB
PL13                    17.00 dB
SFO2              300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF                75.4677892 MHz
WDW                        EM
SSB                         0
LB                       3.00 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
CY                      12.50 cm
F1P                   157.787 ppm
F1                  11907.81 Hz
F2P                    13.967 ppm
F2                    1054.04 Hz
PPMCM                7.19100 ppm/cm
HZCM               542.68860 Hz/cm
```

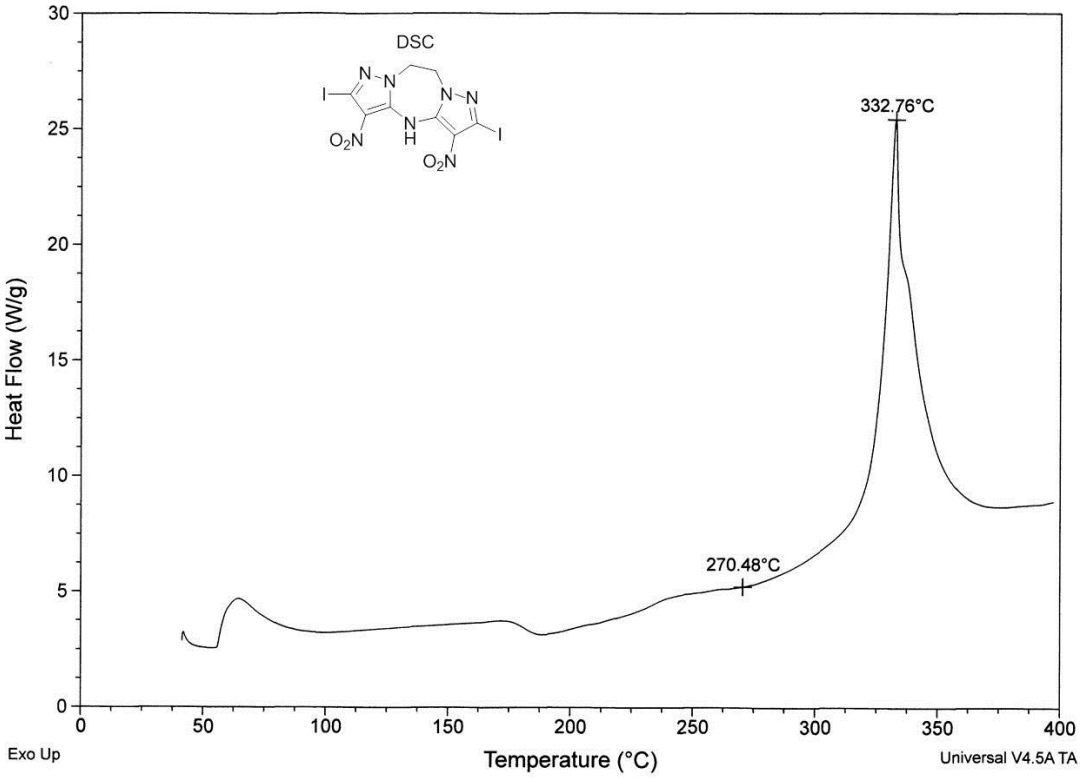

pushpa(2)
%Transmittance
Wavenumber
IR
1749.8
1638.1
1513.4
1442.8
1429.1
1391.5
1313.6
1064.7
1010.6
829.4
749.8
592.1
468.7
50
40
30
20
10
0
-10
2000
1800
1600
1400
1200
1000
800
600
I
N
N
NO2
O2N

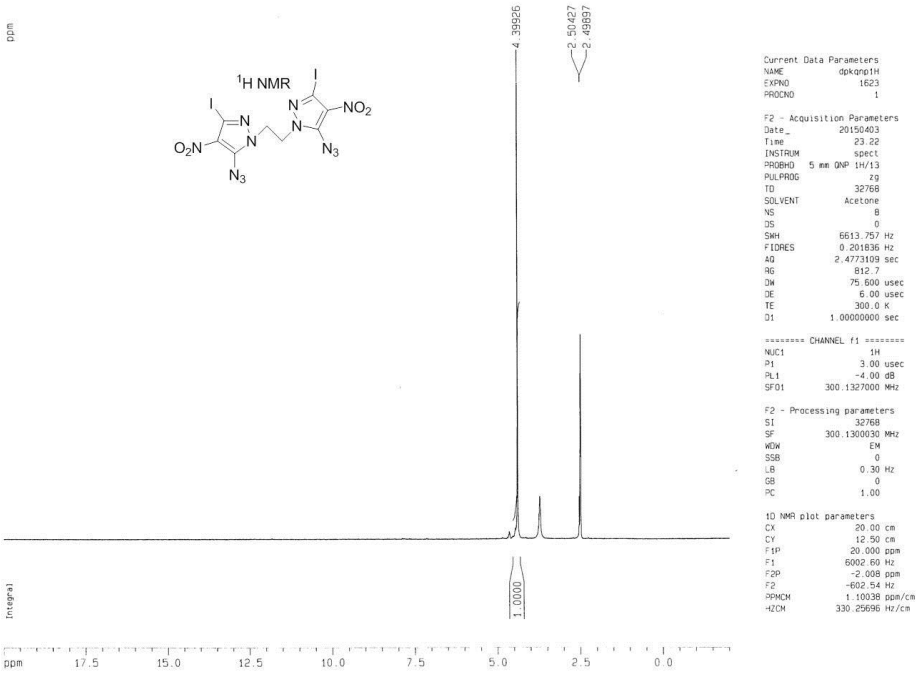

DSC
366.53°C
344.01°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA Instruments

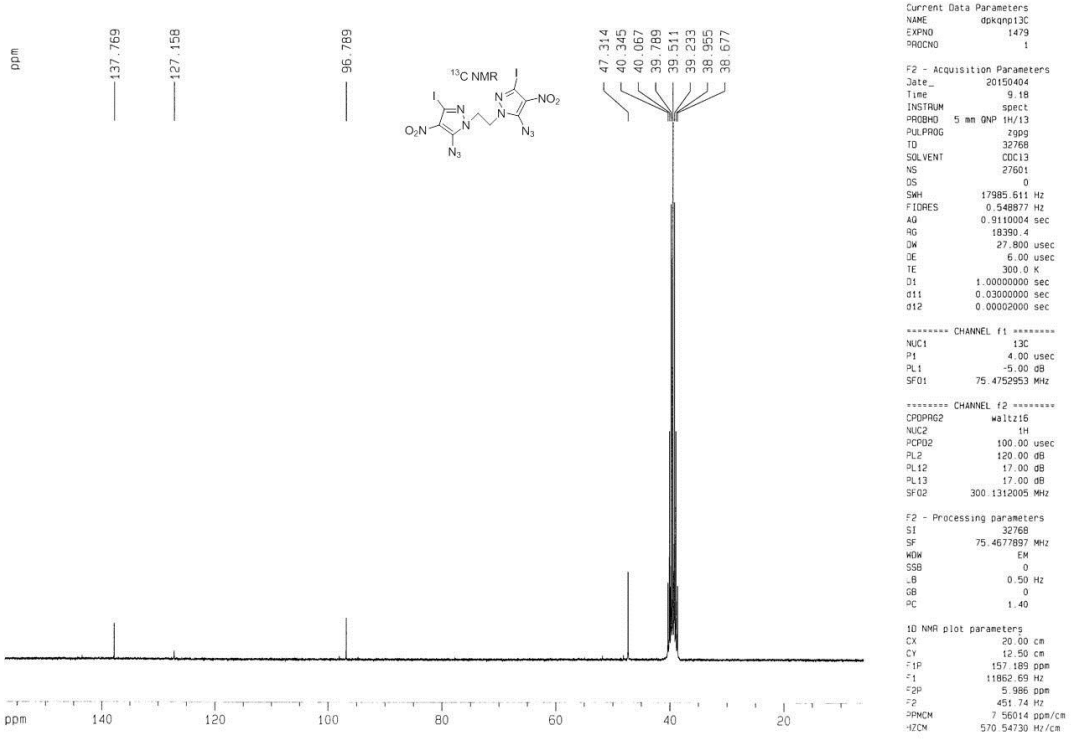

^{1}H NMR
11.3852
4.7130
1.0000
4.3488
Current Data Parameters
NAME dpkqnp1H
EXPNO 1225
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 9.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 724.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 12.359 ppm
F1 3709.38 Hz
F2P 3.539 ppm
F2 1062.23 Hz
PPMCM 0.44100 ppm/cm
HZCM 132.35709 Hz/cm

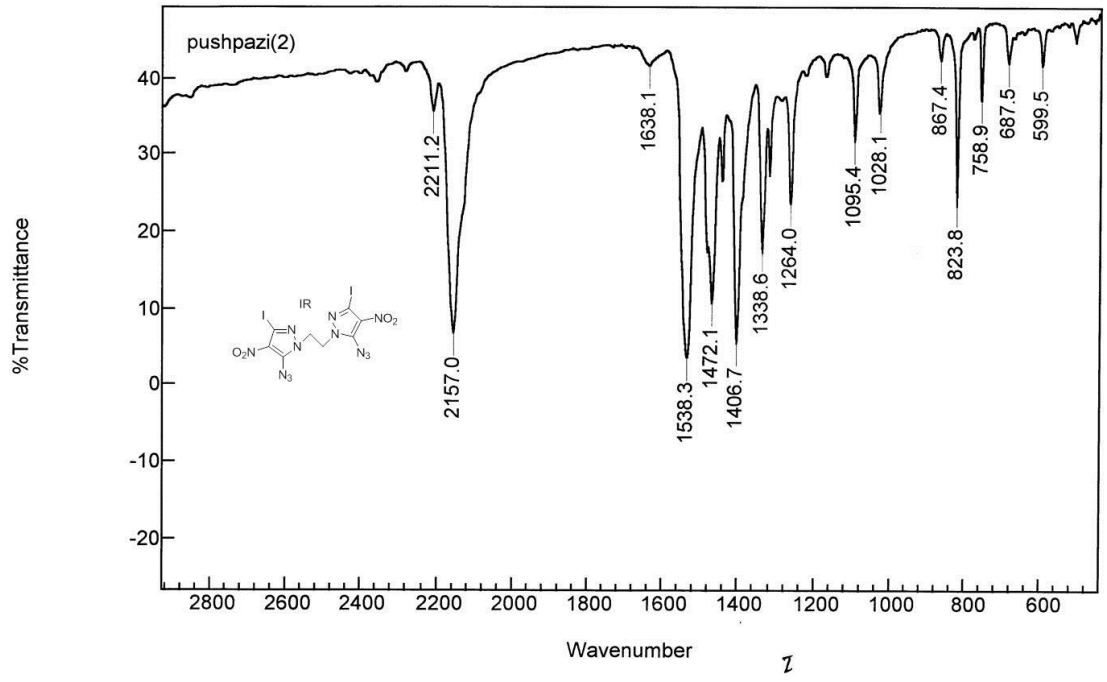

ppm
138.190
121.750
96.143
50.769
40.347
40.070
39.792
39.514
39.235
38.957
38.679
^{13}C NMR
ppm 140 120 100 80 60 40 20
Current Data Parameters
NAME dpkqnpt3C
EXPNO 1473
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150326
Time 22.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 19654
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677897 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 150.396 ppm
F1 11350.09 Hz
F2P 10.416 ppm
F2 786.05 Hz
PPMCM 6.99904 ppm/cm
HZCM 528.20197 Hz/cm

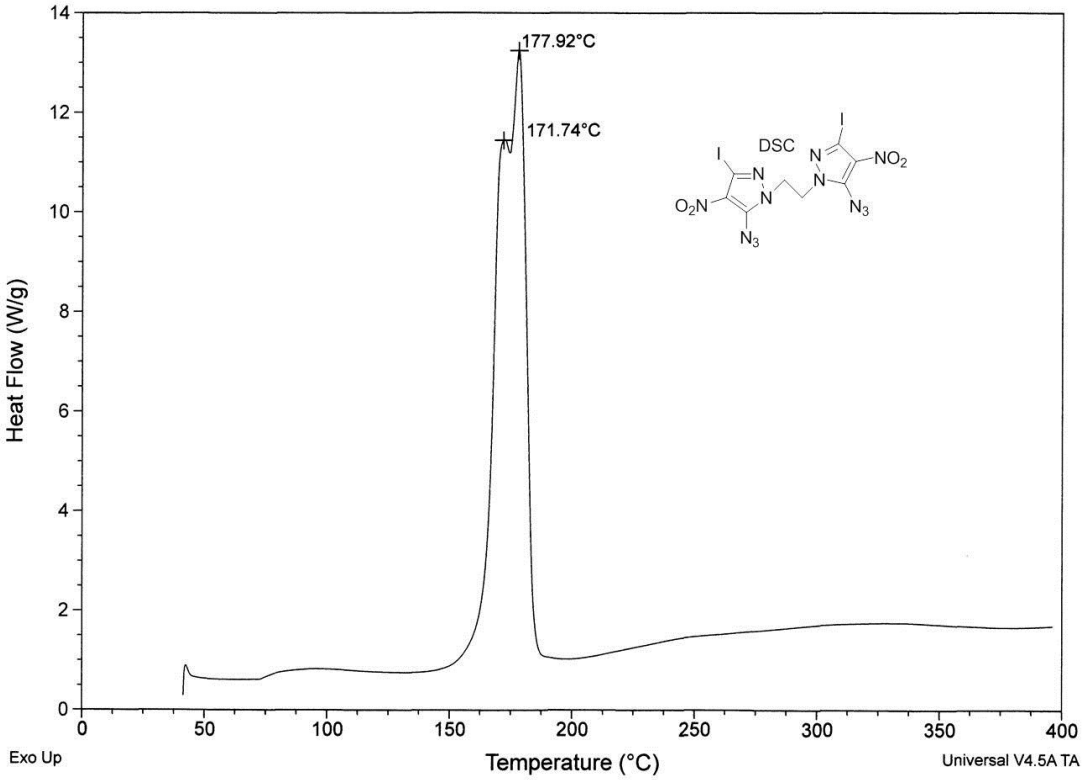

Ain(2)
IR
%Transmittance
Wavenumber
40
30
20
10
0
-10
3500
3000
2500
2000
1500
1000
3437.0
3013.7
2922.6
1615.7
1549.8
1486.9
1437.3
1404.2
1317.4
1230.6
1111.0
1047.3
864.1
799.0
757.9
702.1
601.8

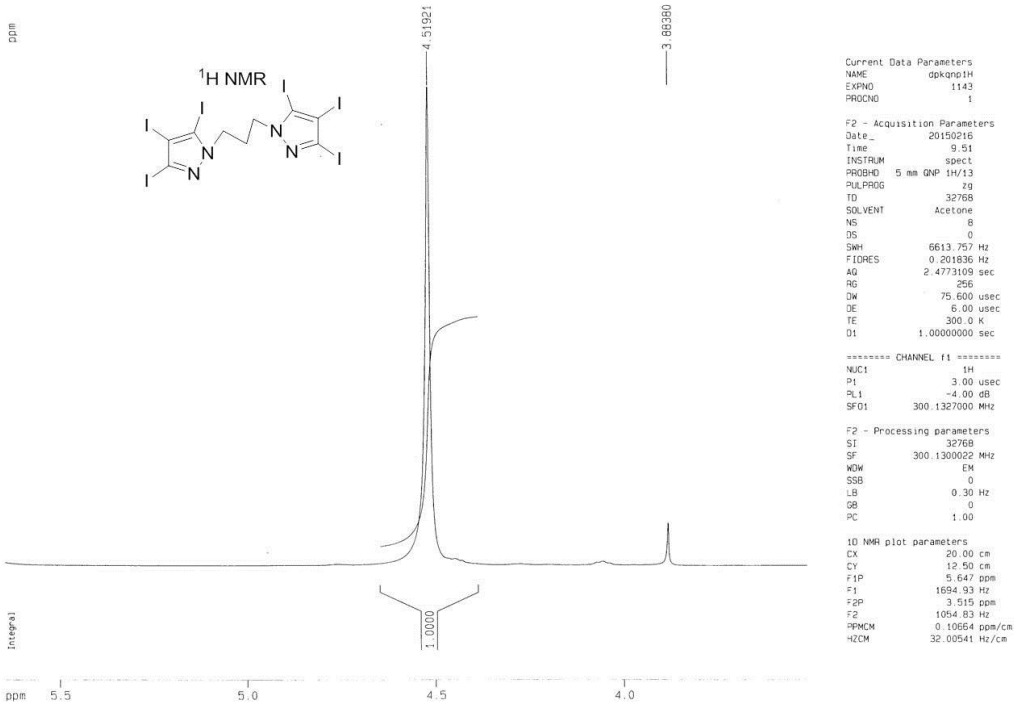

DSC
332.76°C
270.48°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA


^{1}H NMR
4.39926
2.50427
2.49897
1.0000
Current Data Parameters
NAME dpkqnp1H
EXPNO 1623
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150403
Time 23.22
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 812.7
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 20.000 ppm
F1 6002.60 Hz
F2P -2.008 ppm
F2 -602.54 Hz
PPMCM 1.10038 ppm/cm
HZCM 330.25696 Hz/cm

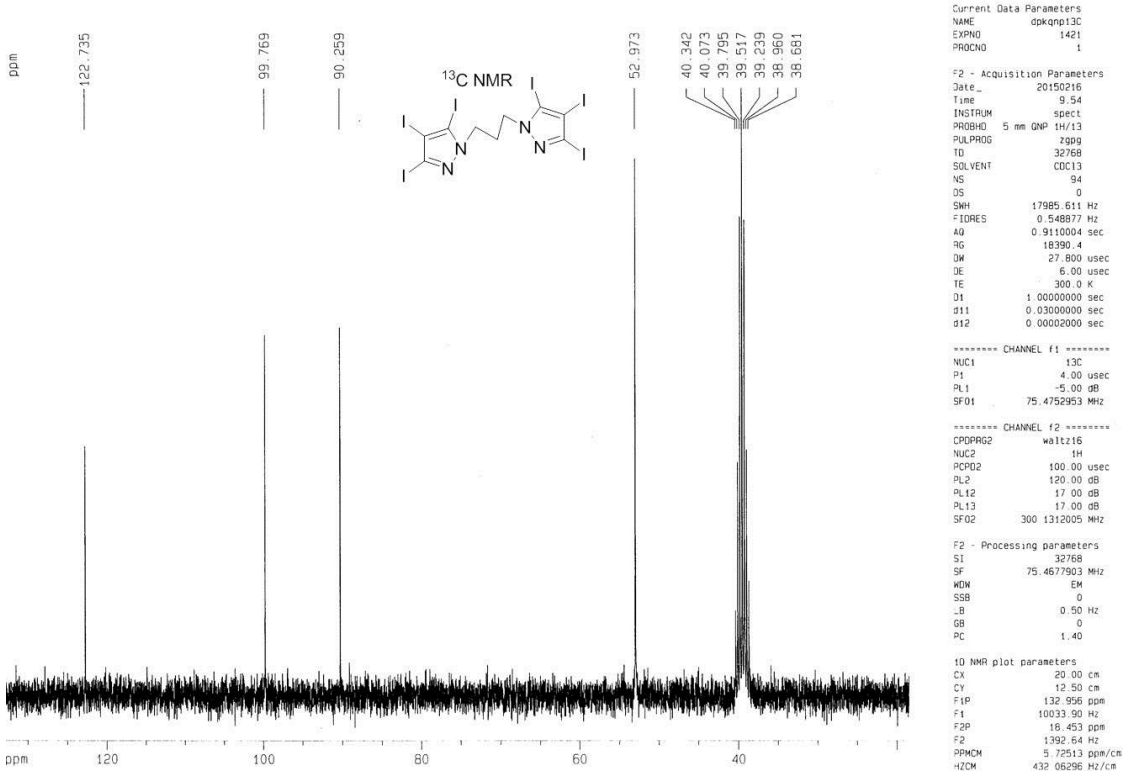

ppm
137.769
127.158
96.789
47.314
40.345
40.067
39.789
39.511
39.233
38.955
38.677
^{13}C NMR
ppm 140 120 100 80 60 40 20
Current Data Parameters
NAME dpkqnp13C
EXPNO 1479
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150404
Time 9.18
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 27601
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677897 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 157.189 ppm
F1 11862.69 Hz
F2P 5.986 ppm
F2 451.74 Hz
PPMCM 7.56014 ppm/cm
HZCM 570.54730 Hz/cm

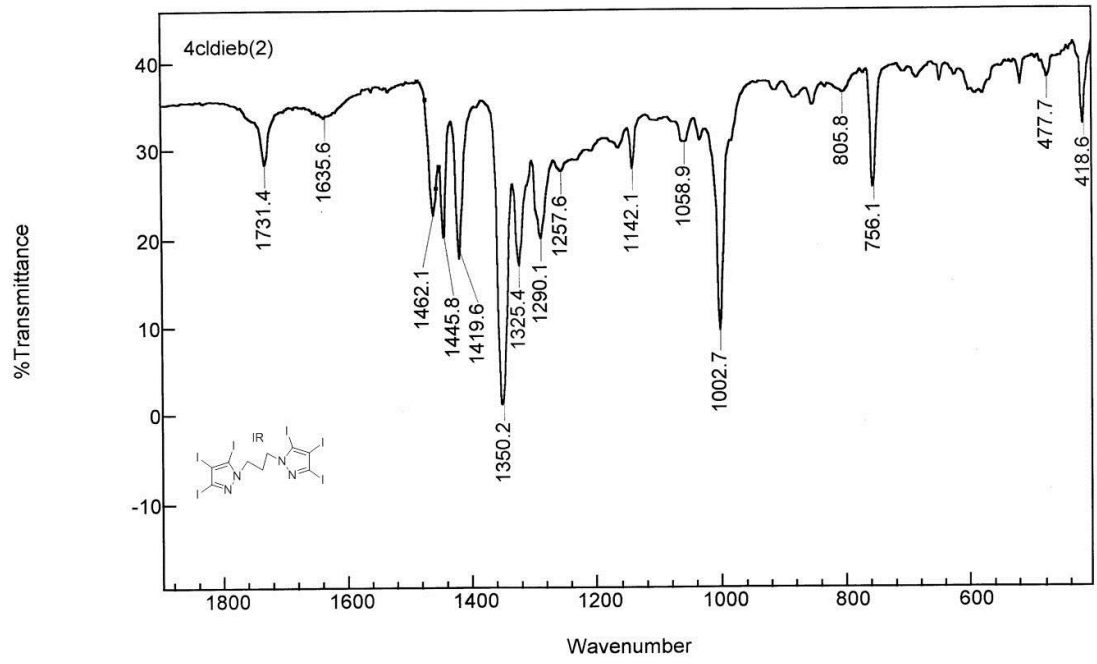

pushpazi(2)
%Transmittance
Wavenumber
IR
2211.2
2157.0
1638.1
1538.3
1472.1
1406.7
1338.6
1264.0
1095.4
1028.1
867.4
823.8
758.9
687.5
599.5
40 30 20 10 0 -10 -20
2800 2600 2400 2200 2000 1800 1600 1400 1200 1000 800 600

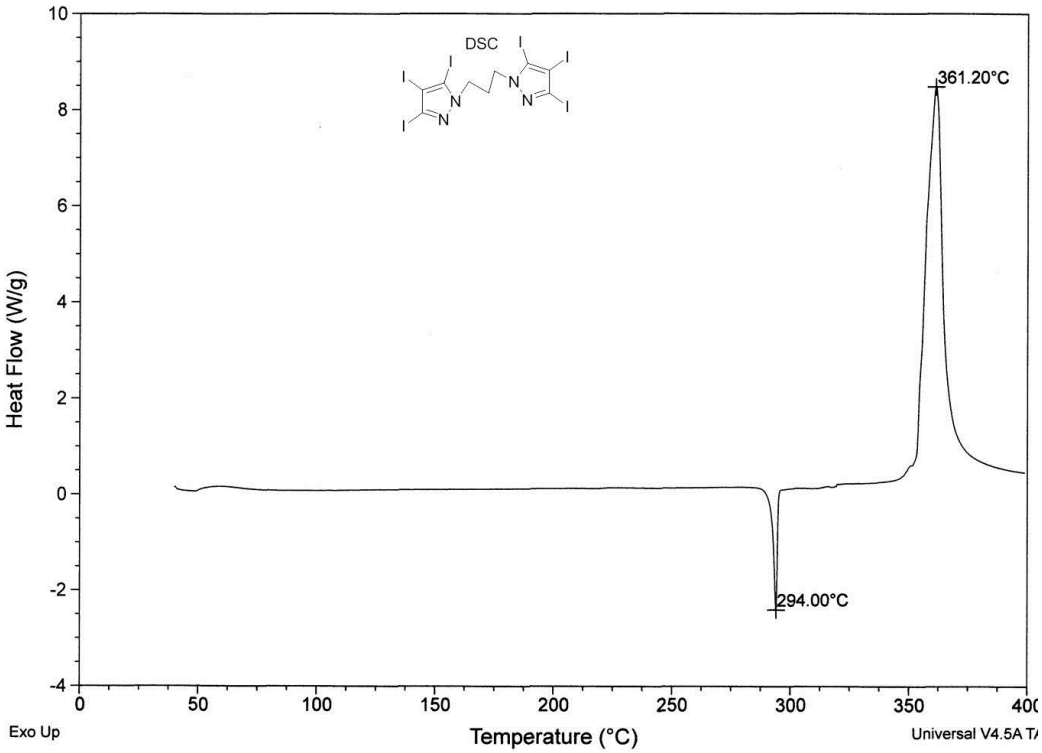


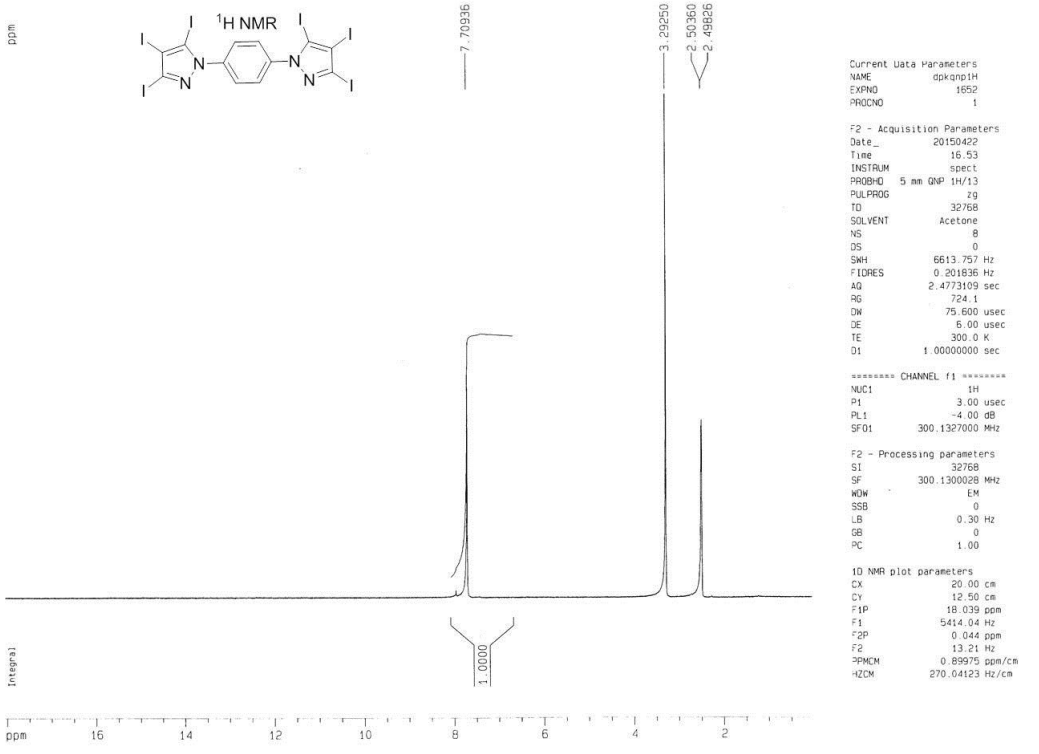


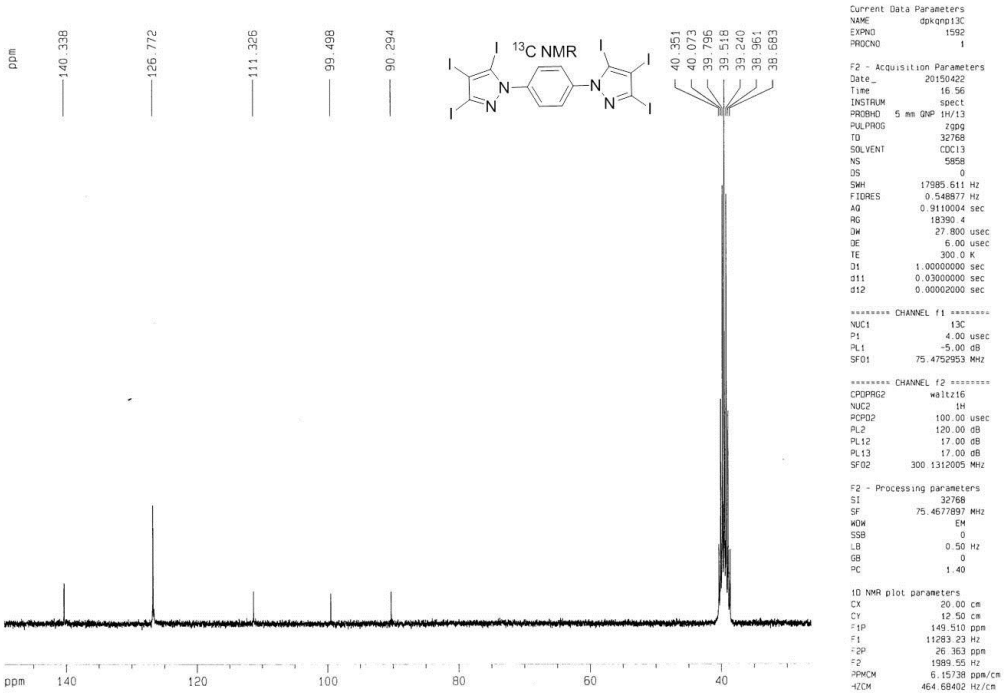

```
Current Data Parameters
NAME                  dpkqnp1H
EXPNO                     1143
PROCNO                       1

F2 - Acquisition Parameters
Date_               20150216
Time                     9.51
INSTRUM                  spect
PROBHD   5 mm QNP 1H/13
PULPROG                    zg
TD                       32768
SOLVENT                Acetone
NS                           8
DS                           0
SWH                 6613.757 Hz
FIDRES              0.201836 Hz
AQ                  2.4773109 sec
RG                         256
DW                   75.600 usec
DE                    6.00 usec
TE                      300.0 K
D1                  1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       3.00 usec
PL1                     -4.00 dB
SFO1             300.1327000 MHz

F2 - Processing parameters
SI                       32768
SF                300.1300022 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       12.50 cm
F1P                      5.647 ppm
F1                     1694.93 Hz
F2P                      3.515 ppm
F2                     1054.83 Hz
PPMCM                 0.10664 ppm/cm
HZCM                 32.00541 Hz/cm
```

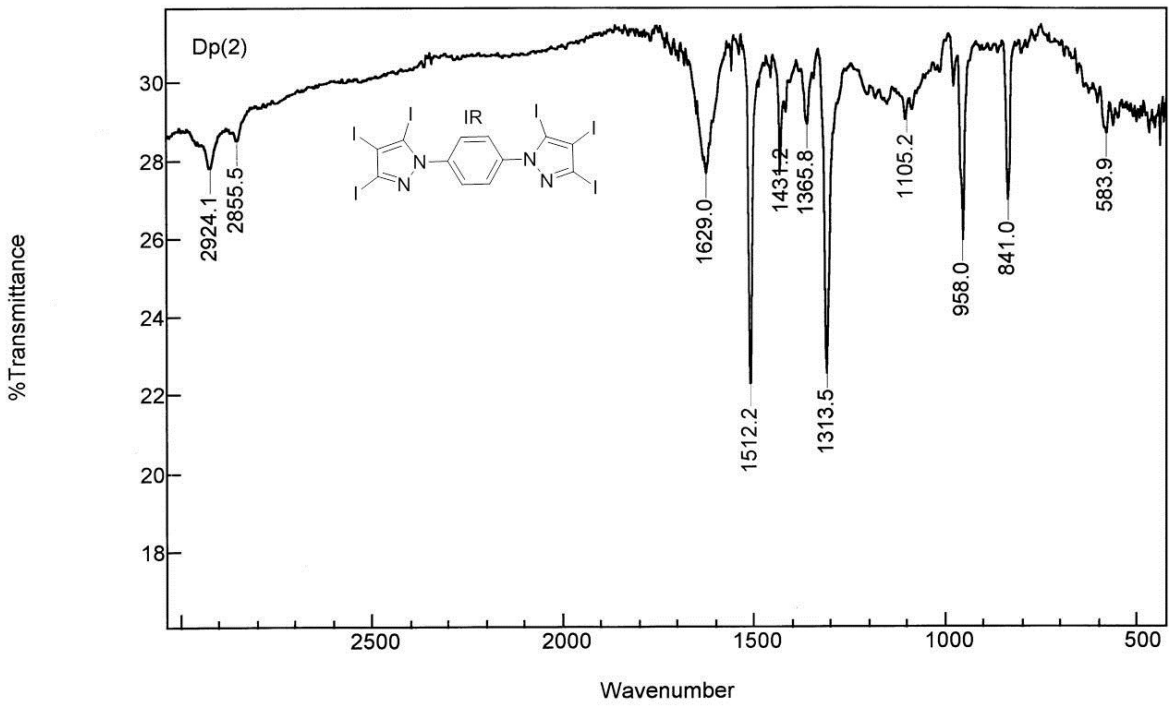

ppm
122.735
99.769
90.259
52.973
40.342
40.073
39.795
39.517
39.239
38.960
38.681
^{13}C NMR
ppm
120
100
80
60
40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1421
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150216
Time 9.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 94
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677903 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 132.956 ppm
F1 10033.90 Hz
F2P 16.453 ppm
F2 1392.64 Hz
PPMCM 5.72513 ppm/cm
HZCM 432.06296 Hz/cm

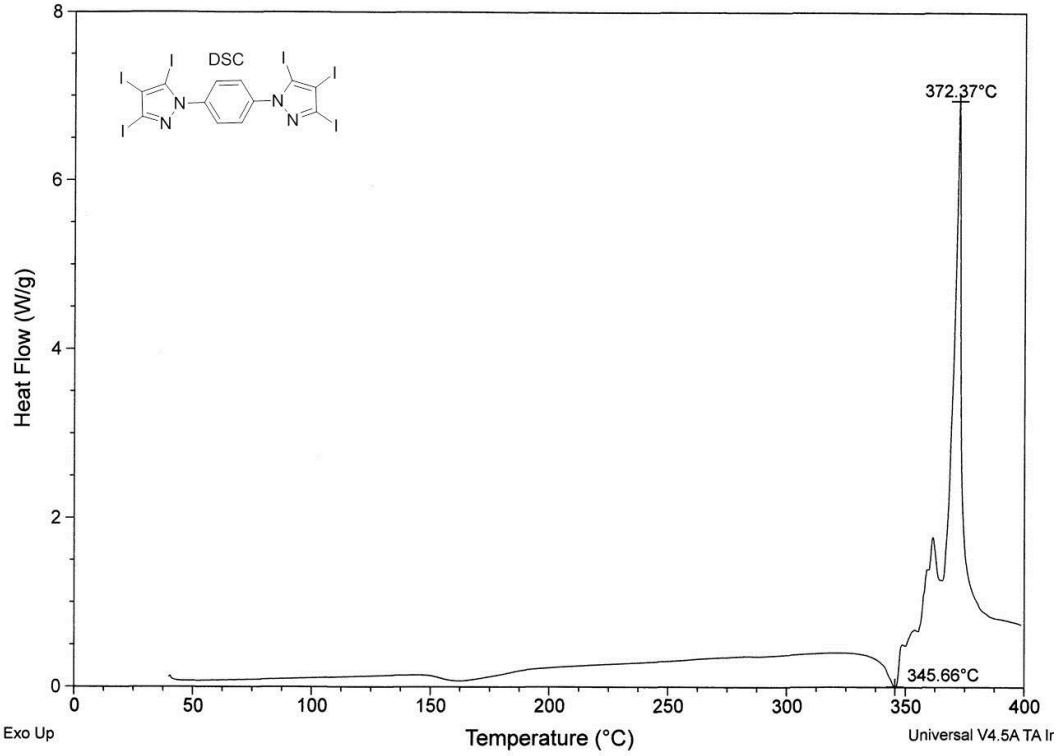

4cldieb(2)
%Transmittance
Wavenumber
40
30
20
10
0
-10
1800
1600
1400
1200
1000
800
600
1731.4
1635.6
1462.1
1445.8
1419.6
1350.2
1325.4
1290.1
1257.6
1142.1
1058.9
1002.7
805.8
756.1
477.7
418.6
IR

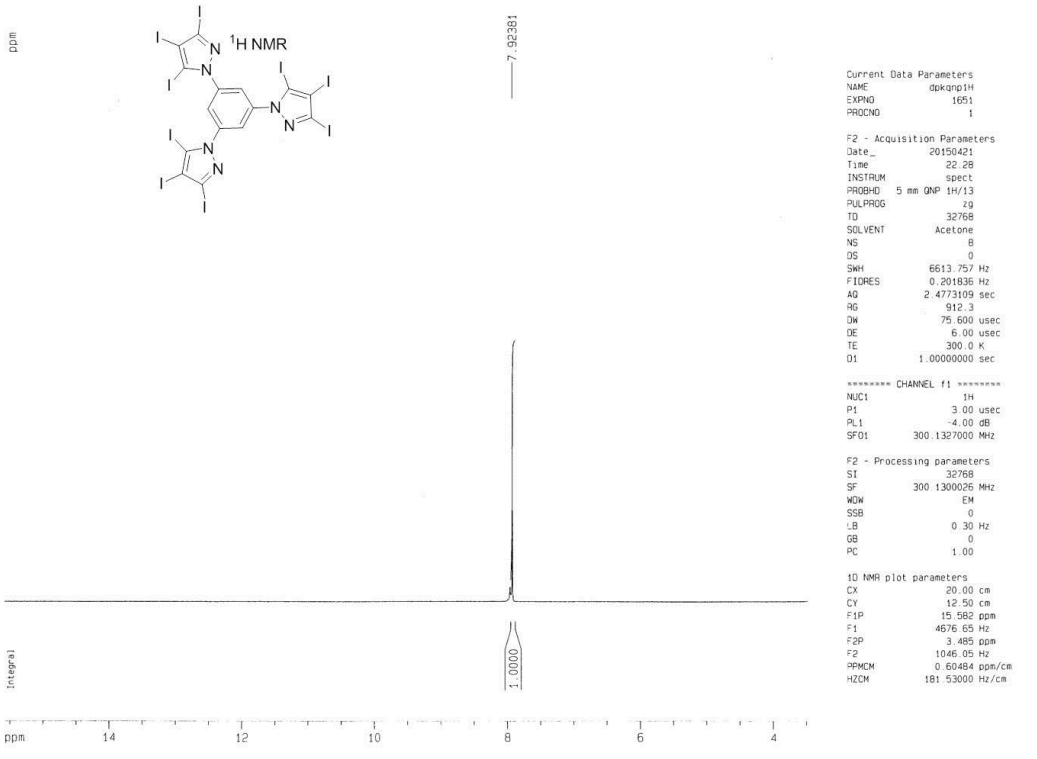

DSC
361.20°C
294.00°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA

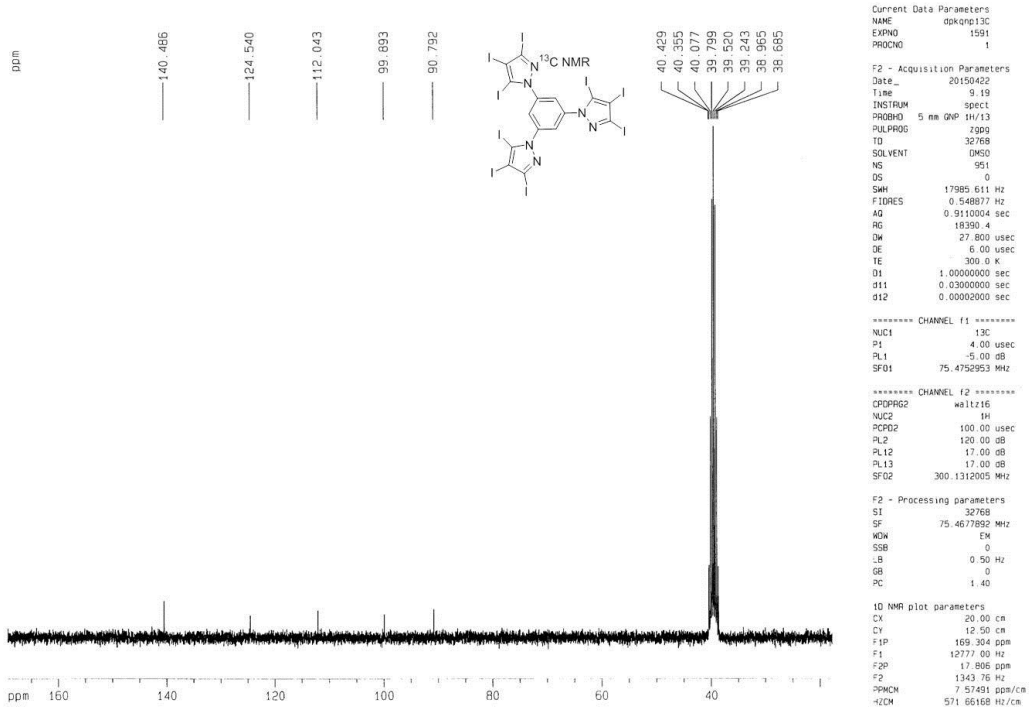

^{1}H NMR
7.70936
3.29250
2.50360
2.49826
ppm
Integral
1.0000
Current Data Parameters
NAME dpkqnp1H
EXPNO 1652
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150422
Time 16.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 724.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 18.039 ppm
F1 5414.04 Hz
F2P 0.044 ppm
F2 13.21 Hz
PPMCM 0.89975 ppm/cm
HZCM 270.04123 Hz/cm

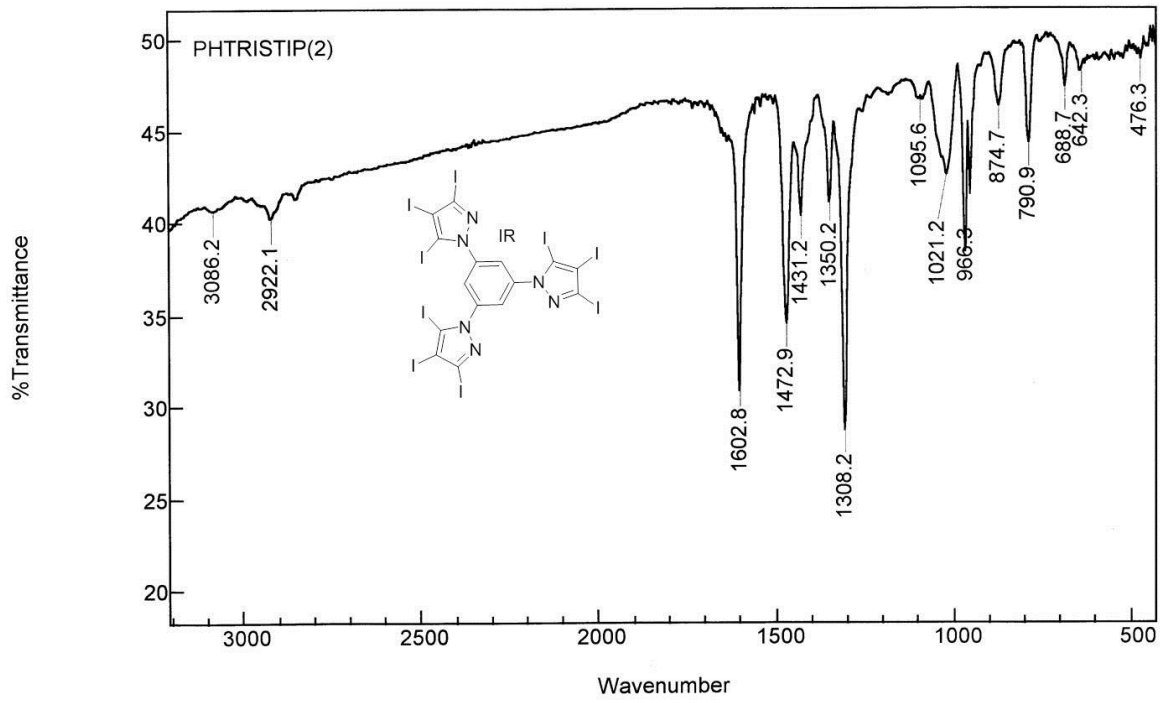

ppm
140.338
126.772
111.326
99.498
90.294
^{13}C NMR
40.351
40.073
39.796
39.518
39.240
38.961
38.683
ppm 140 120 100 80 60 40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1592
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150422
Time 16.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 5858
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677897 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 149.510 ppm
F1 11283.23 Hz
F2P 26.363 ppm
F2 1989.55 Hz
PPMCM 6.15738 ppm/cm
HZCM 464.68402 Hz/cm

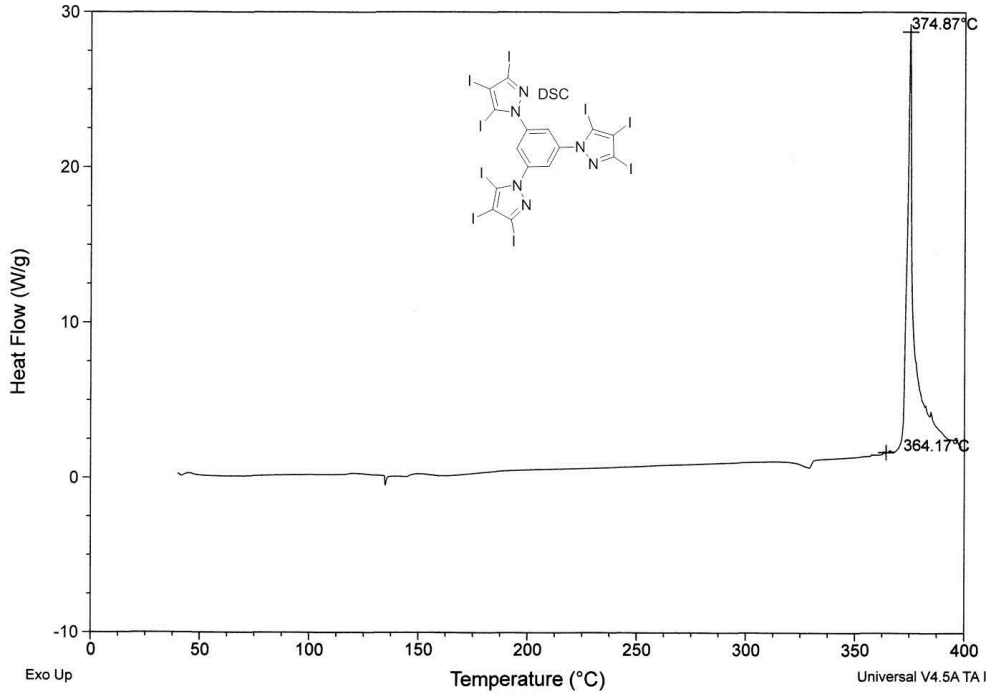

Dp(2)
IR
%Transmittance
30
28
26
24
22
20
18
2924.1
2855.5
1629.0
1512.2
1431.2
1365.8
1313.5
1105.2
958.0
841.0
583.9
2500
2000
1500
1000
500
Wavenumber

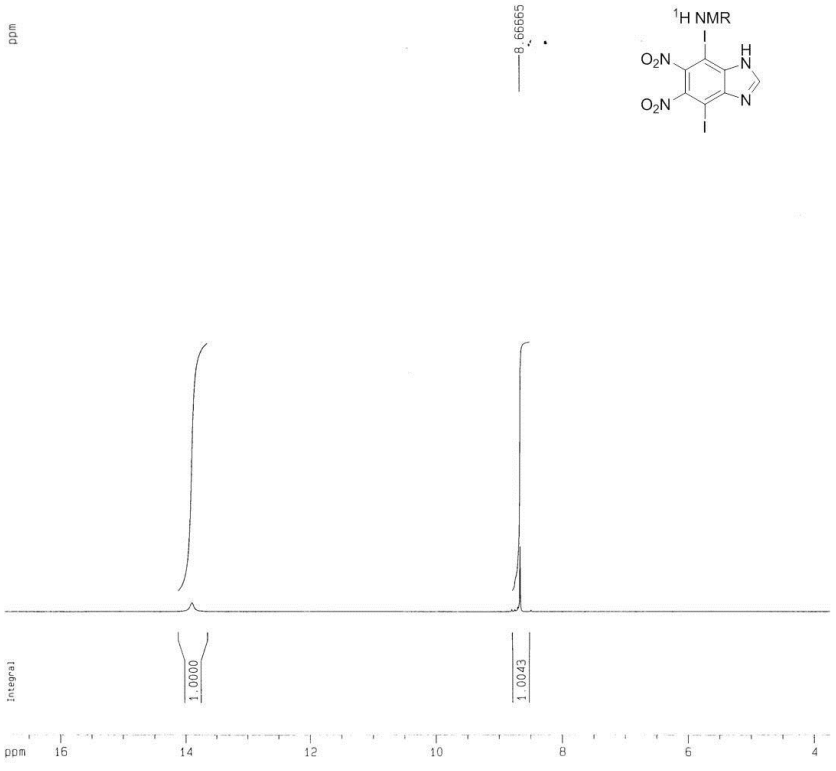

DSC
372.37°C
345.66°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA Ir


^{1}H NMR
7.92381
1.0000
Integral
ppm
Current Data Parameters
NAME dpkqnp1H
EXPNO 1651
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150421
Time 22.28
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 912.3
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 15.582 ppm
F1 4676.65 Hz
F2P 3.485 ppm
F2 1046.05 Hz
PPMCM 0.60484 ppm/cm
HZCM 181.53000 Hz/cm


ppm
140.486
124.540
112.043
99.893
90.792
40.429
40.355
40.077
39.799
39.520
39.243
38.965
38.685
13C NMR
ppm 160 140 120 100 80 60 40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1591
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150422
Time 9.19
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 951
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677892 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 169.304 ppm
F1 12777.00 Hz
F2P 17.806 ppm
F2 1343.76 Hz
PPMCM 7.57491 ppm/cm
HZCM 571.66168 Hz/cm


PHTRISTIP(2)
IR
%Transmittance
Wavenumber
50
45
40
35
30
25
20
3000
2500
2000
1500
1000
500
3086.2
2922.1
1602.8
1472.9
1431.2
1350.2
1308.2
1095.6
1021.2
966.3
874.7
790.9
688.7
642.3
476.3





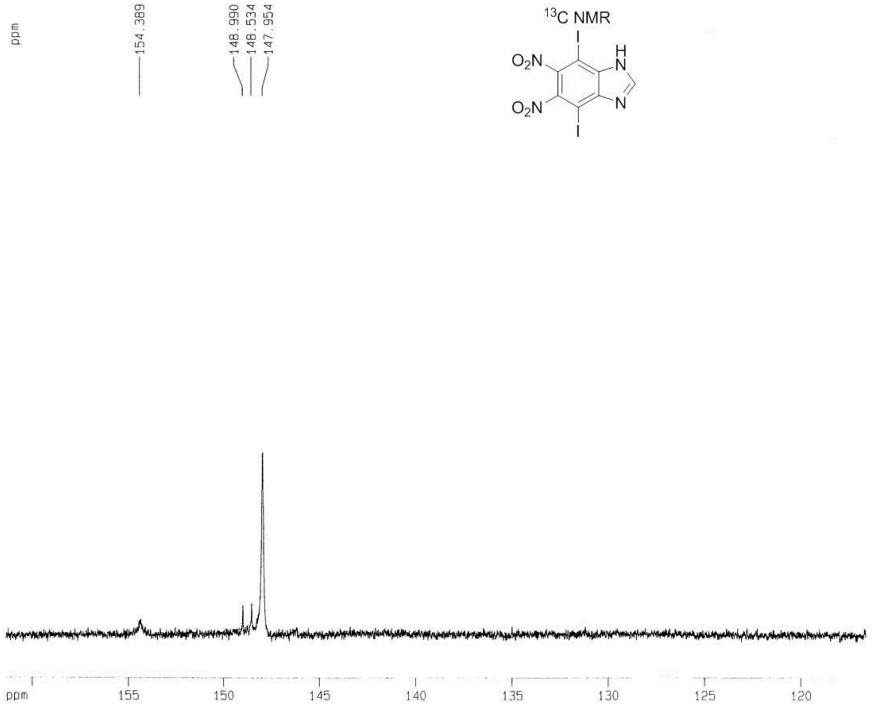
Current Data Parameters
NAME dpkqnp1H
EXPNO 1665
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150508
Time 22.54
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 645.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

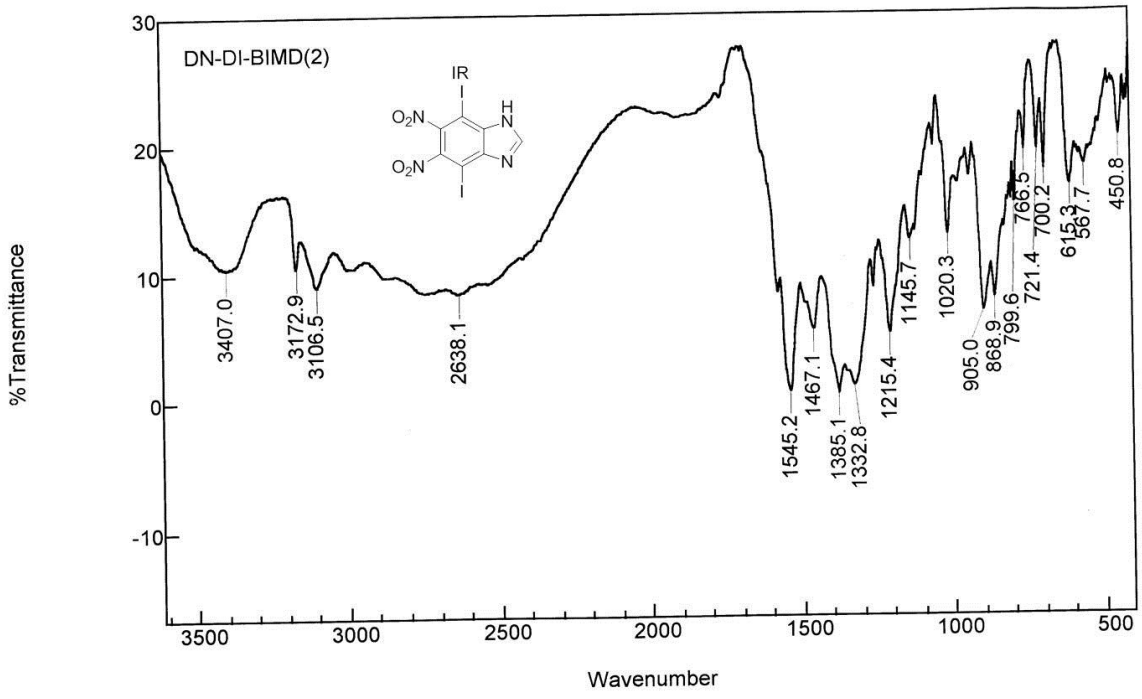
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz

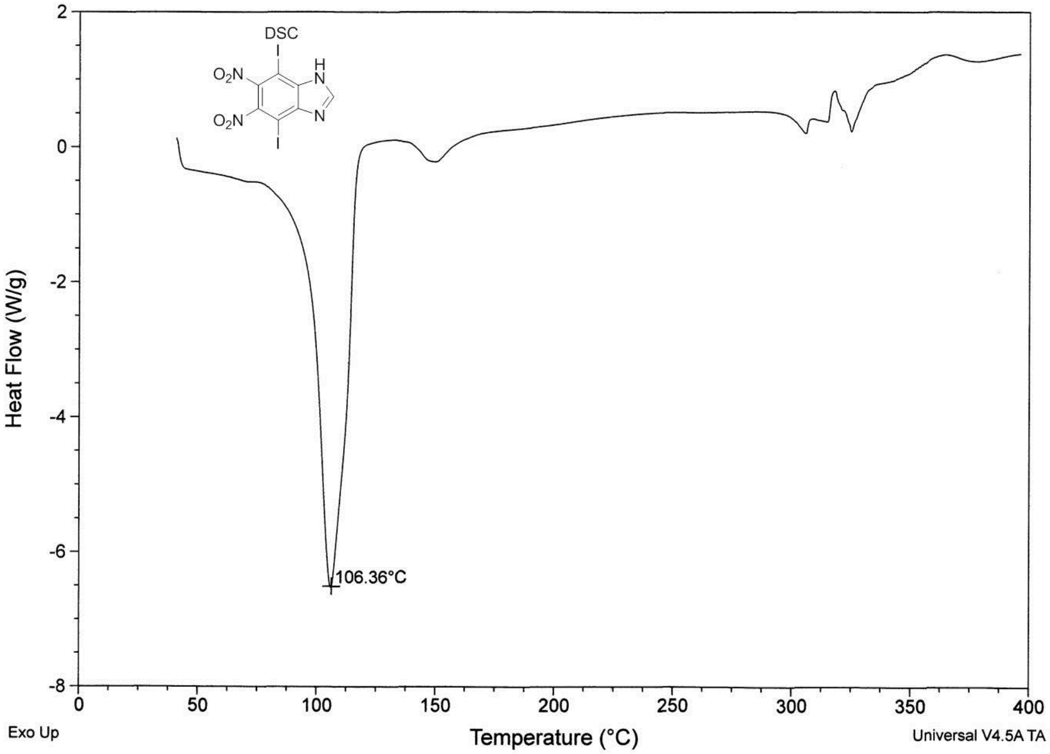
F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

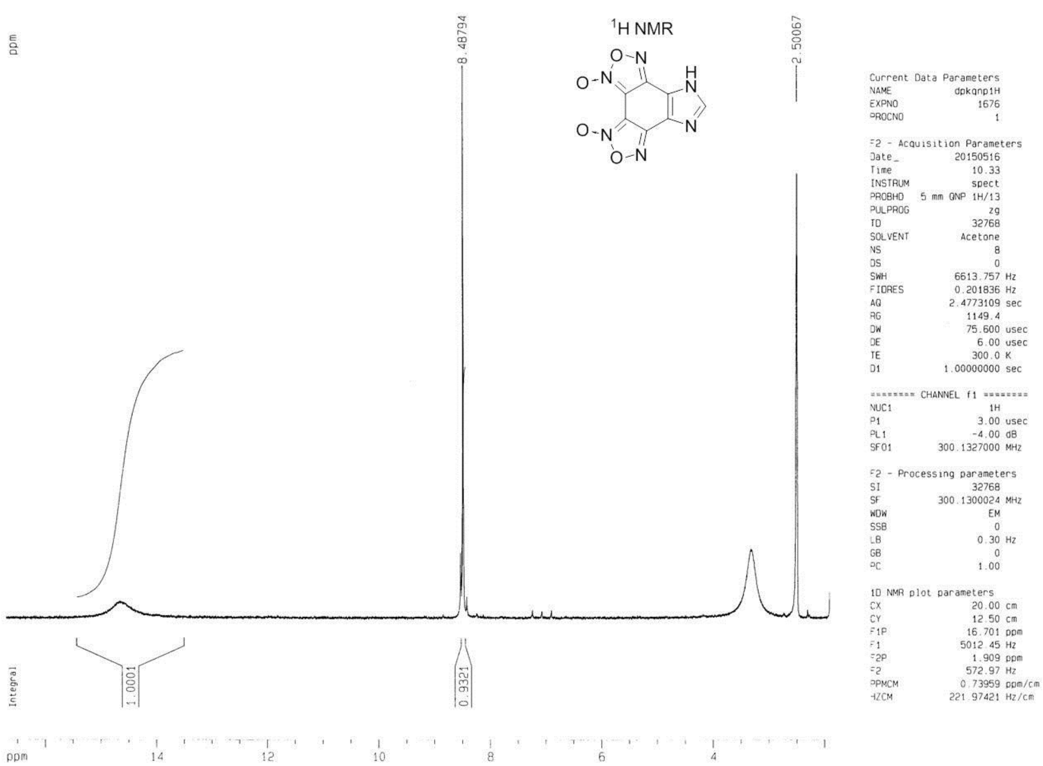
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 16.894 ppm
F1 5070.42 Hz
F2P 3.750 ppm
F2 1125.51 Hz
PPMCM 0.65720 ppm/cm
HZCM 197.24507 Hz/cm

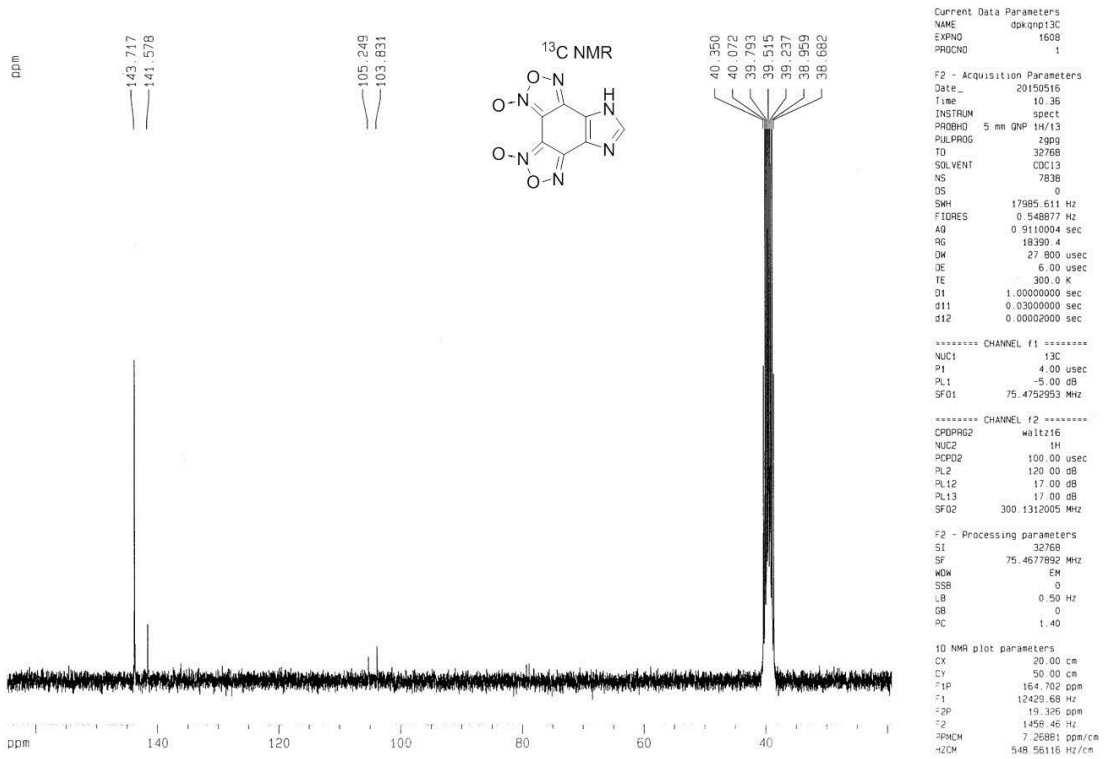


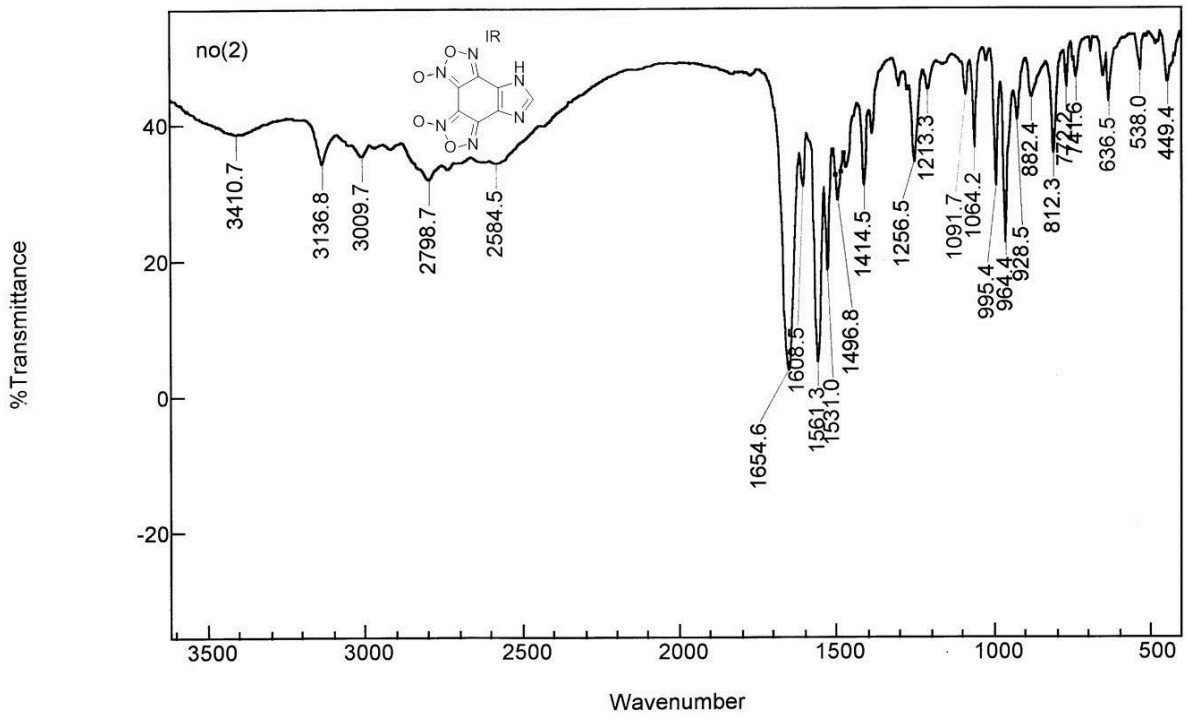

```
Current Data Parameters
NAME            dpkqnp13C
EXPNO                1605
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150509
Time                17.10
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg
TD                 32768
SOLVENT             CDCl3
NS                 32997
DS                     0
SWH           17985.611 Hz
FIDRES         0.548877 Hz
AQ             0.9110004 sec
RG               18390.4
DW                27.800 usec
DE                 6.00 usec
TE                 300.0 K
D1            1.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 4.00 usec
PL1               -5.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             100.00 usec
PL2               120.00 dB
PL12               17.00 dB
PL13               17.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677892 MHz
WDW                   EM
SSB                    0
LB                  0.50 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 20.00 cm
CY                 50.00 cm
F1P              161.360 ppm
F1              12177.48 Hz
F2P              116.615 ppm
F2               8800.69 Hz
PPMCM          2.23724 ppm/cm
HZCM         168.83934 Hz/cm
```

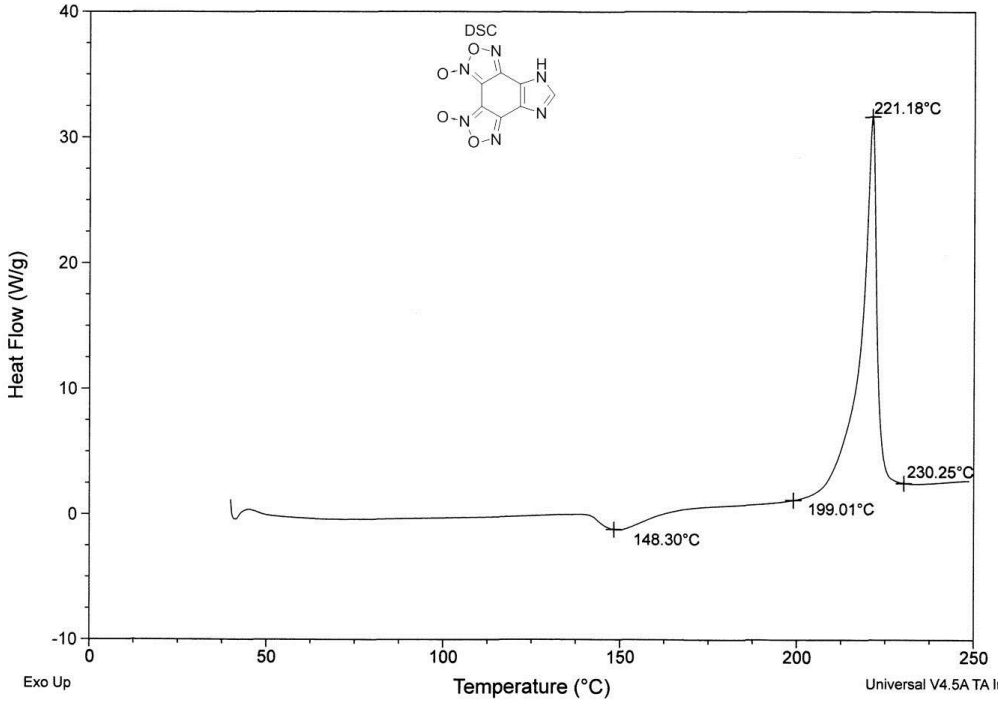


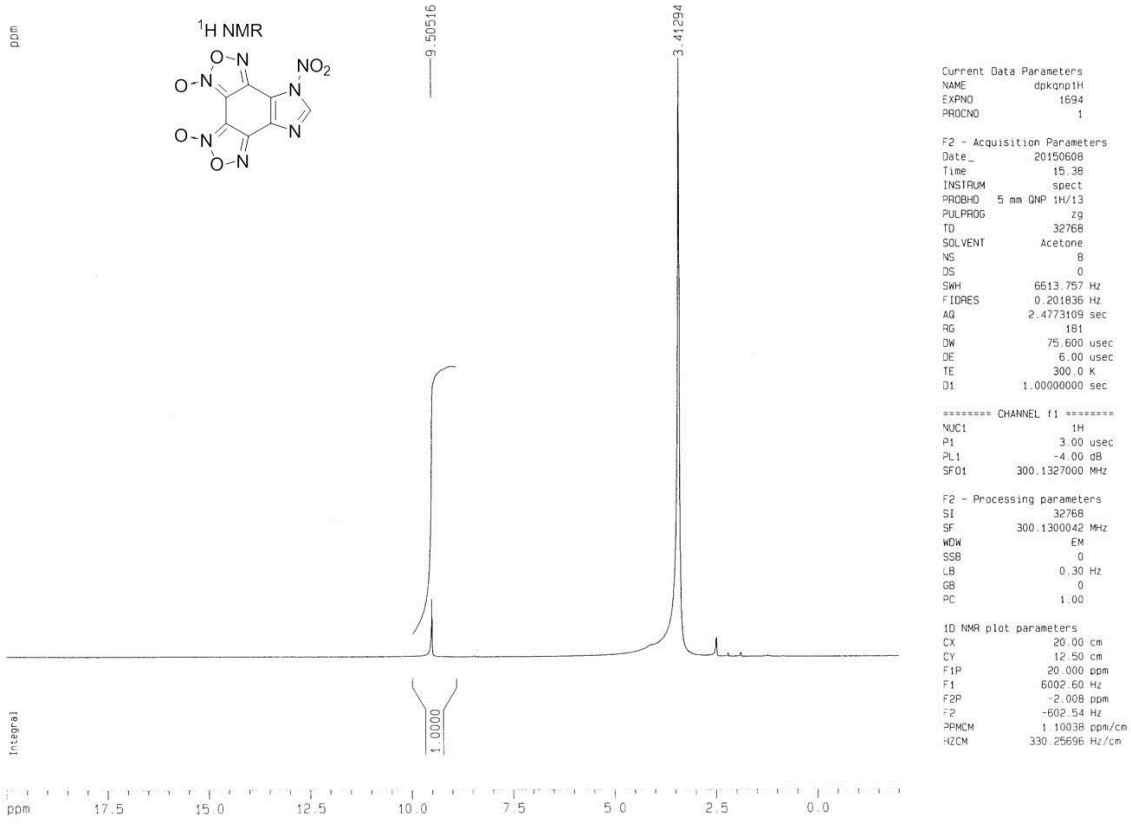

DSC
106.36°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA Ir

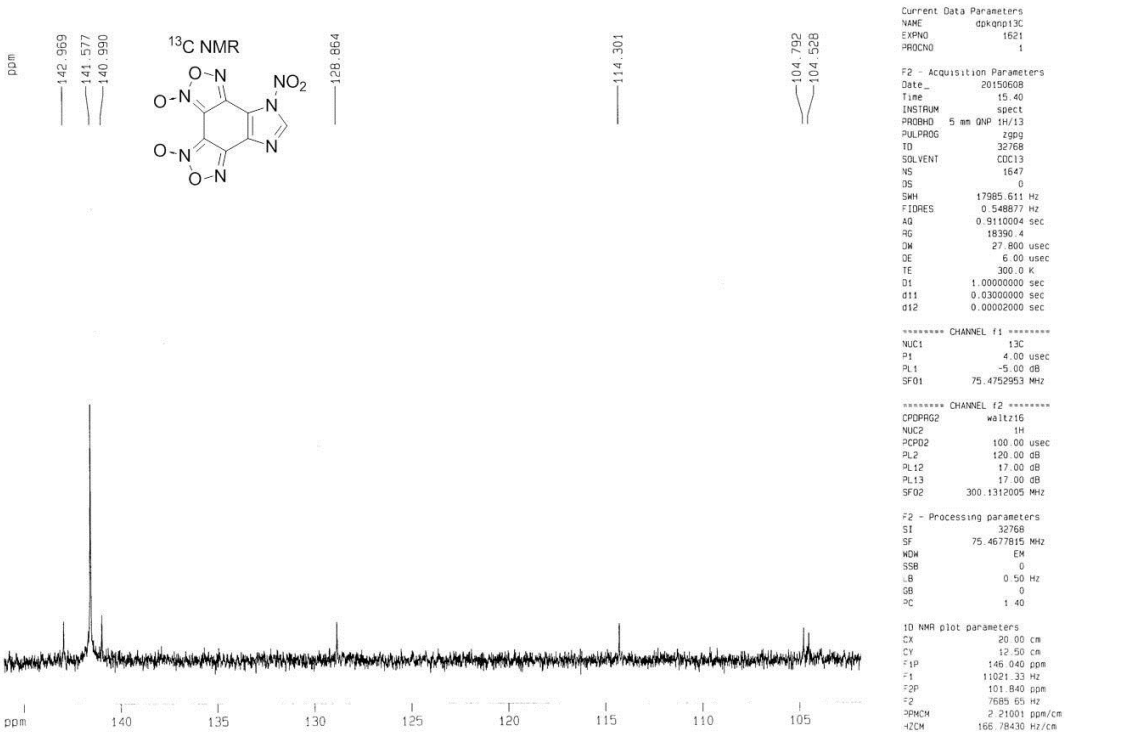

1H NMR
8.48794
2.50067
1.0001
0.9321
Integral
ppm
Current Data Parameters
NAME dpkqnp1H
EXPNO 1676
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150516
Time 10.33
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 1149.4
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 16.701 ppm
F1 5012.45 Hz
F2P 1.909 ppm
F2 572.97 Hz
PPMCM 0.73959 ppm/cm
HZCM 221.97421 Hz/cm

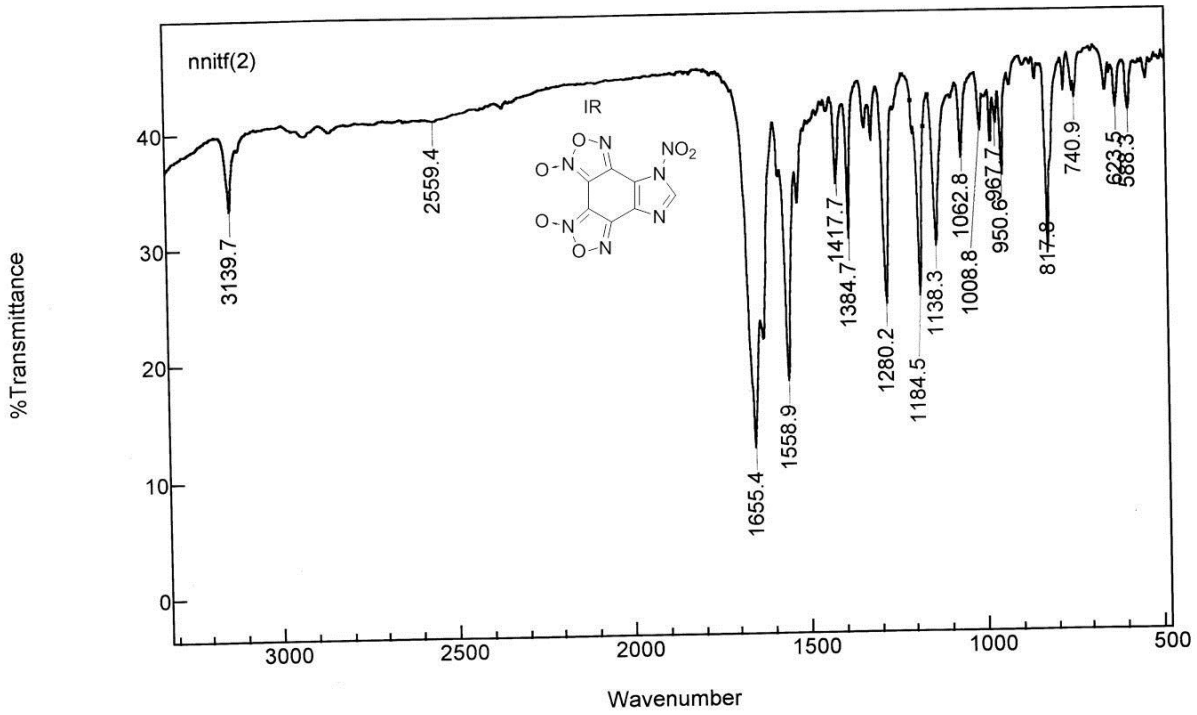

^{13}C NMR
ppm
143.717
141.578
105.249
103.831
40.350
40.072
39.793
39.515
39.237
38.959
38.682
ppm
140
120
100
80
60
40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1608
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150516
Time 10.36
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 7838
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677892 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 50.00 cm
F1P 164.702 ppm
F1 12429.68 Hz
F2P 19.326 ppm
F2 1458.46 Hz
PPMCM 7.26881 ppm/cm
HZCM 548.56116 Hz/cm

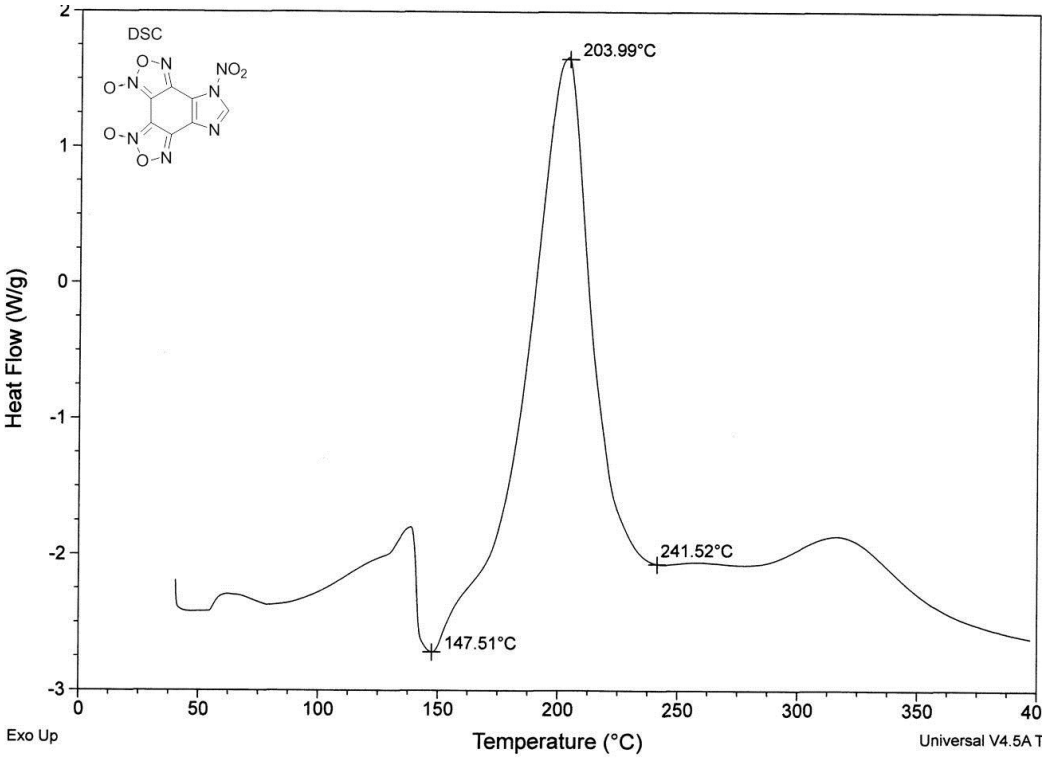

no(2)
IR
%Transmittance
40
20
0
-20
3410.7
3136.8
3009.7
2798.7
2584.5
1654.6
1608.5
1561.3
1531.0
1496.8
1414.5
1256.5
1213.3
1091.7
1064.2
995.4
964.4
928.5
882.4
812.3
772.2
741.6
636.5
538.0
449.4
3500
3000
2500
2000
1500
1000
500
Wavenumber

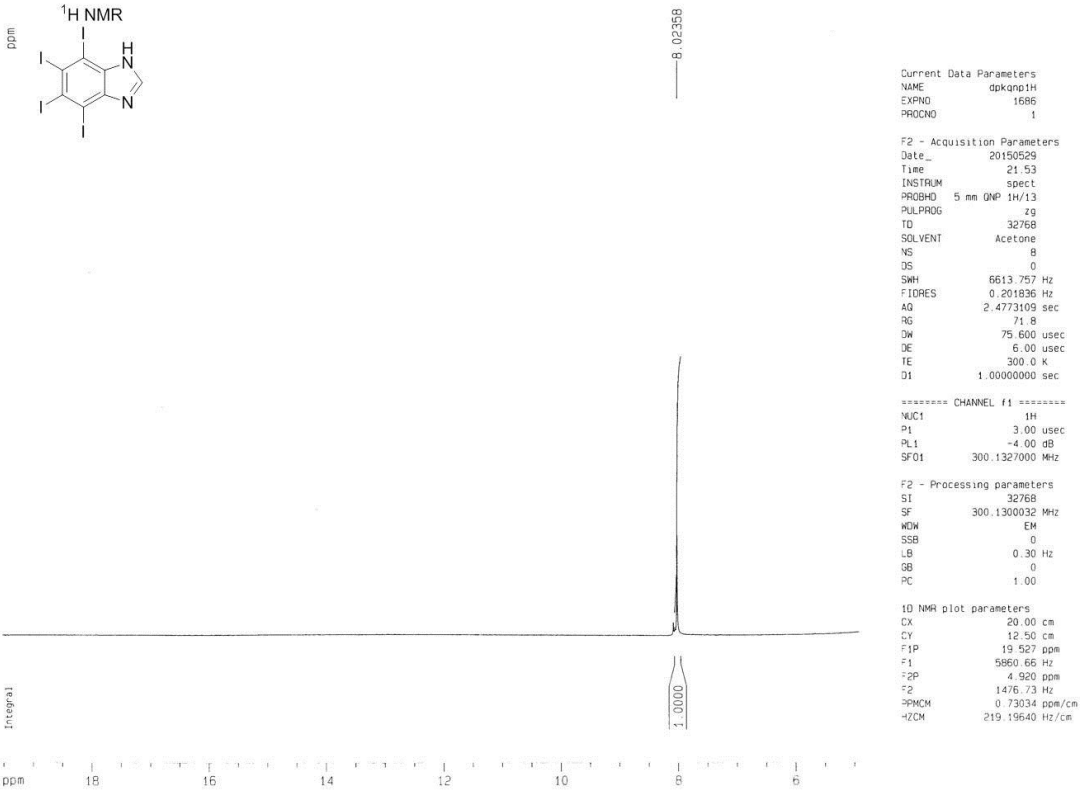

DSC
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA I
221.18°C
230.25°C
199.01°C
148.30°C

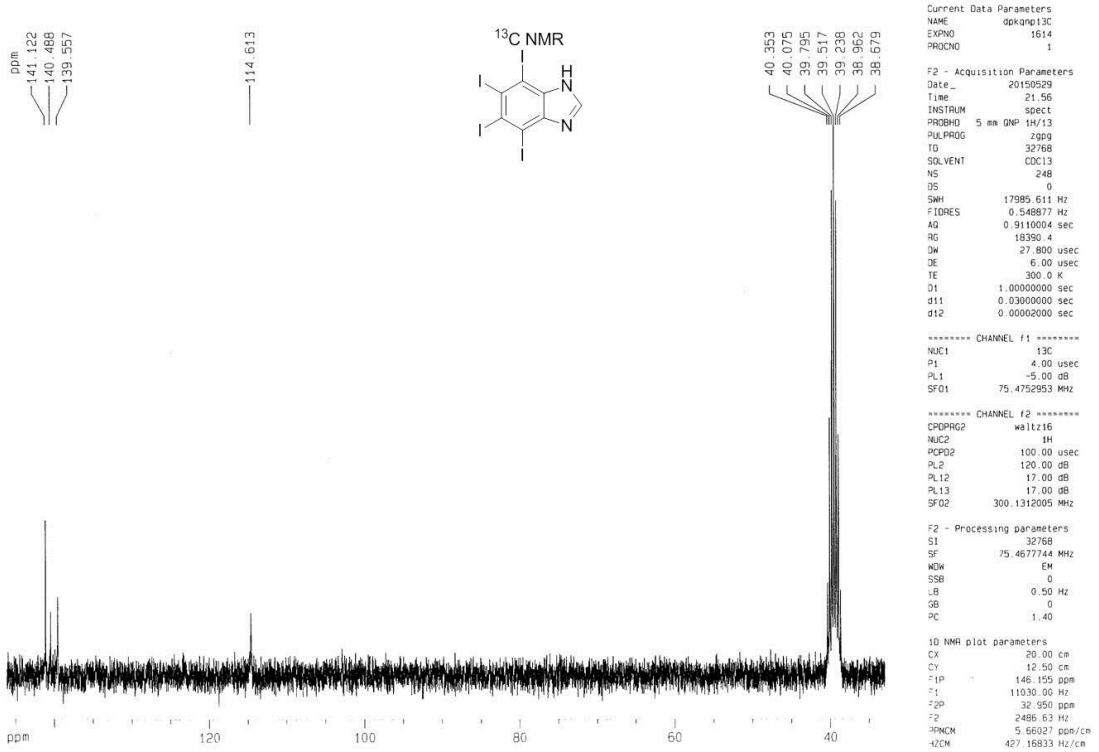

^{1}H NMR
ppm
9.50516
3.41294
Integral
1.0000
Current Data Parameters
NAME dpkqnp1H
EXPNO 1694
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150608
Time 15.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 181
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SF01 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 20.000 ppm
F1 6002.60 Hz
F2P -2.008 ppm
F2 -602.54 Hz
PPMCM 1.10038 ppm/cm
HZCM 330.25696 Hz/cm

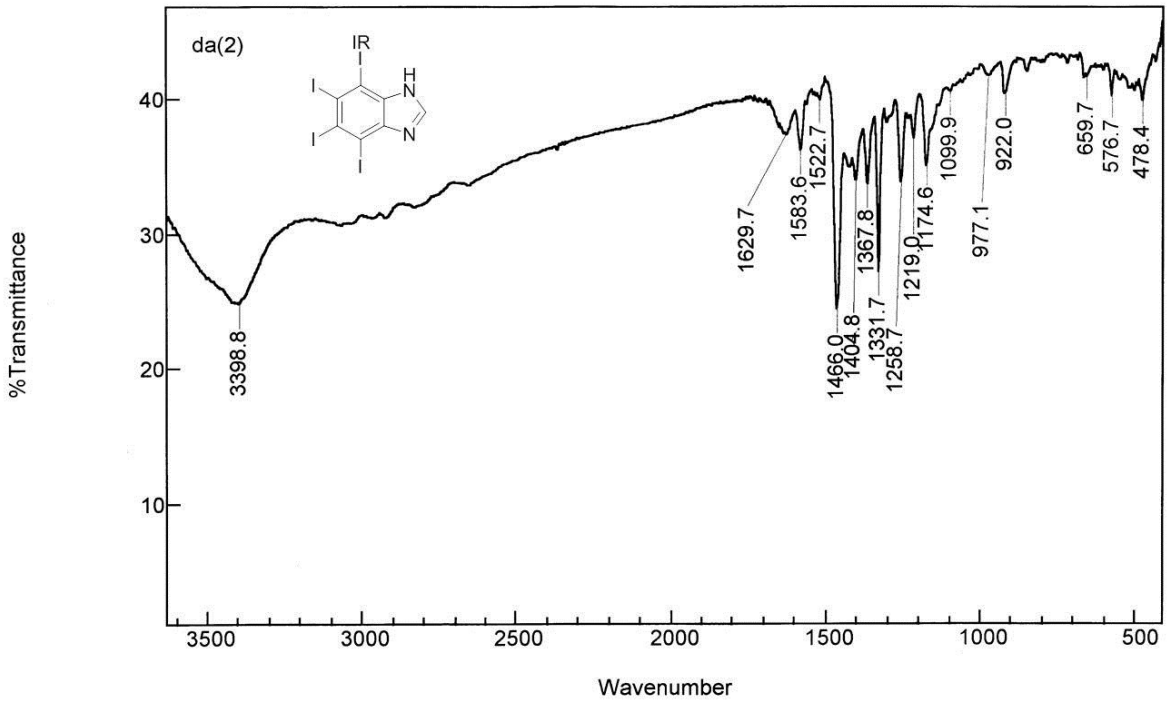

ppm
142.969
141.577
140.990
128.864
114.301
104.792
104.528
^{13}C NMR
NO_2
ppm
140
135
130
125
120
115
110
105
Current Data Parameters
NAME dpkqnp13C
EXPNO 1621
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150608
Time 15.40
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1647
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677815 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 146.040 ppm
F1 11021.33 Hz
F2P 101.840 ppm
F2 7685.65 Hz
PPMCM 2.21001 ppm/cm
HZCM 166.78430 Hz/cm

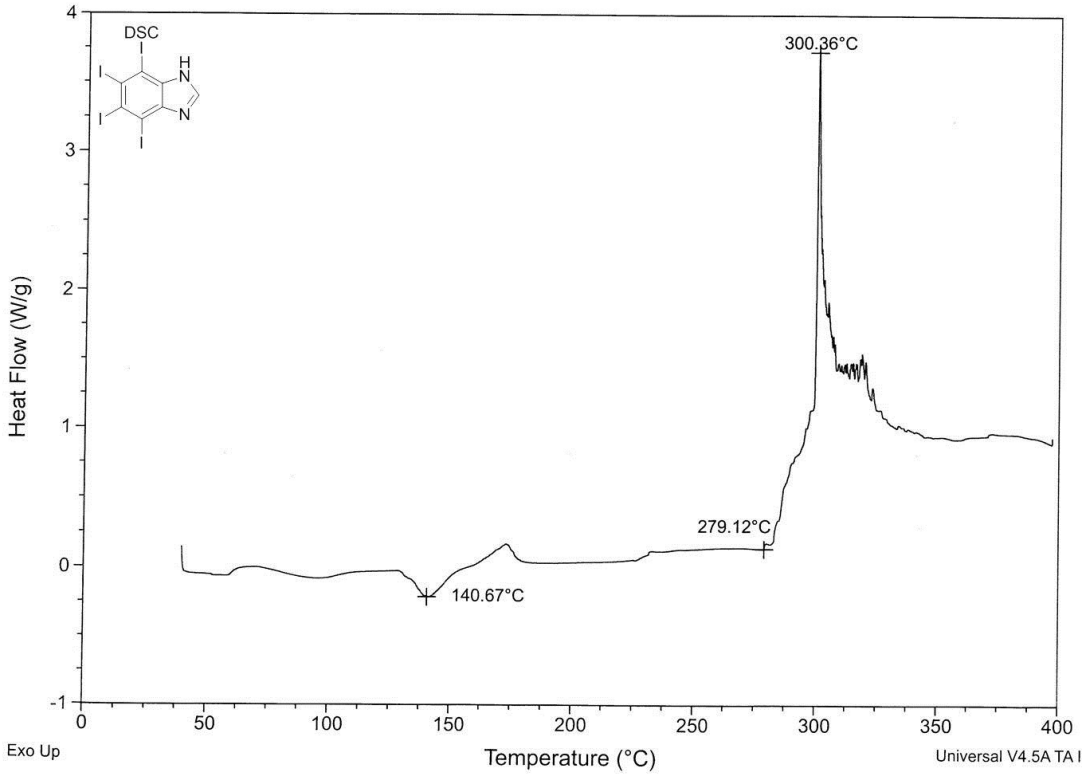

nnitf(2)
IR
NO_2
%Transmittance
Wavenumber
40
30
20
10
0
3000
2500
2000
1500
1000
500
3139.7
2559.4
1655.4
1558.9
1417.7
1384.7
1280.2
1184.5
1138.3
1062.8
1008.8
967.7
950.6
817.8
740.9
623.5
588.3

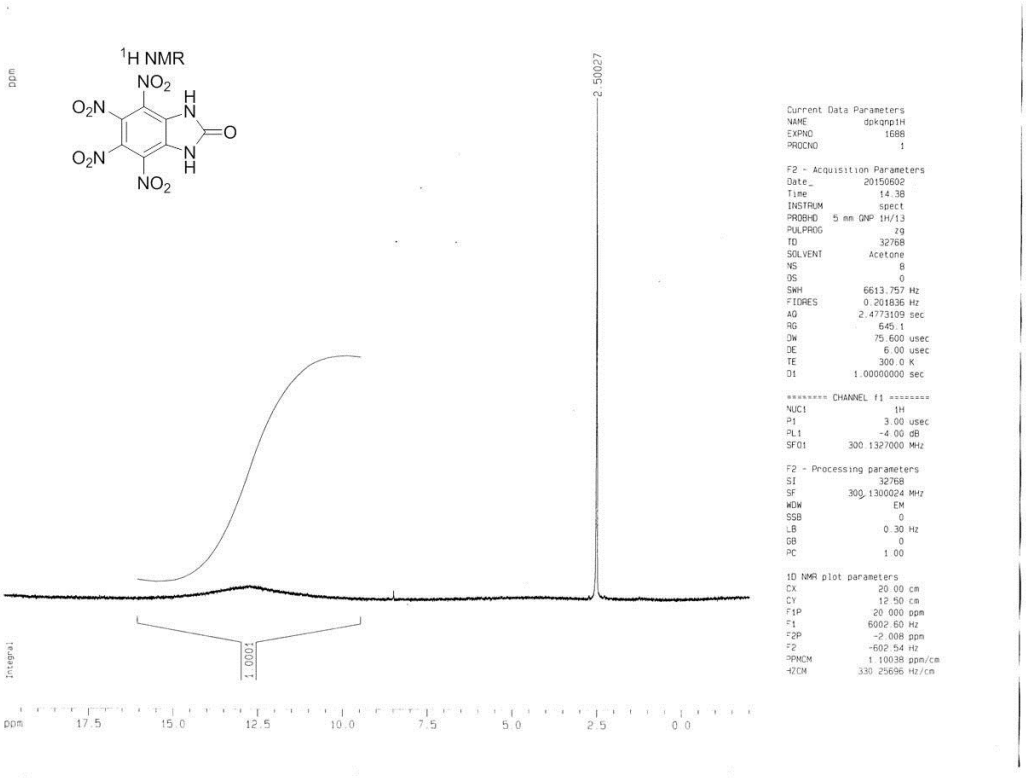

DSC
203.99°C
241.52°C
147.51°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A T

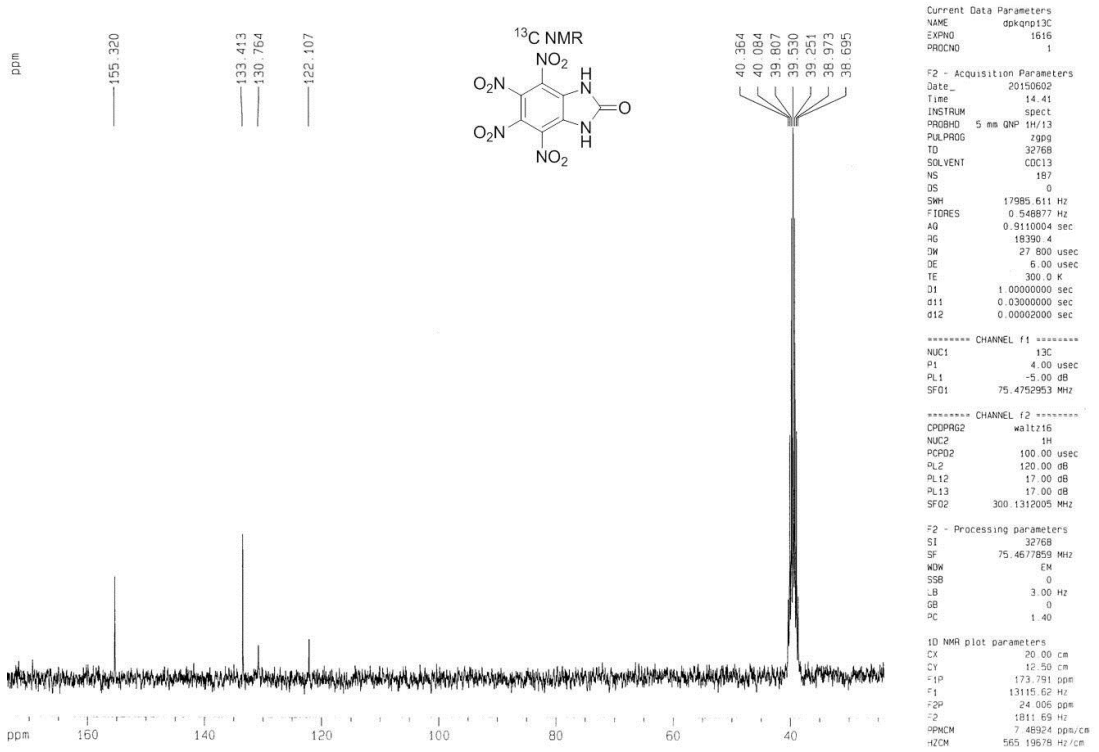

1H NMR
8.02358
1.0000
Integral
ppm
Current Data Parameters
NAME dpkqnp1H
EXPNO 1686
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150529
Time 21.53
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 71.8
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300032 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 19.527 ppm
F1 5860.66 Hz
F2P 4.920 ppm
F2 1476.73 Hz
PPMCM 0.73034 ppm/cm
HZCM 219.19640 Hz/cm

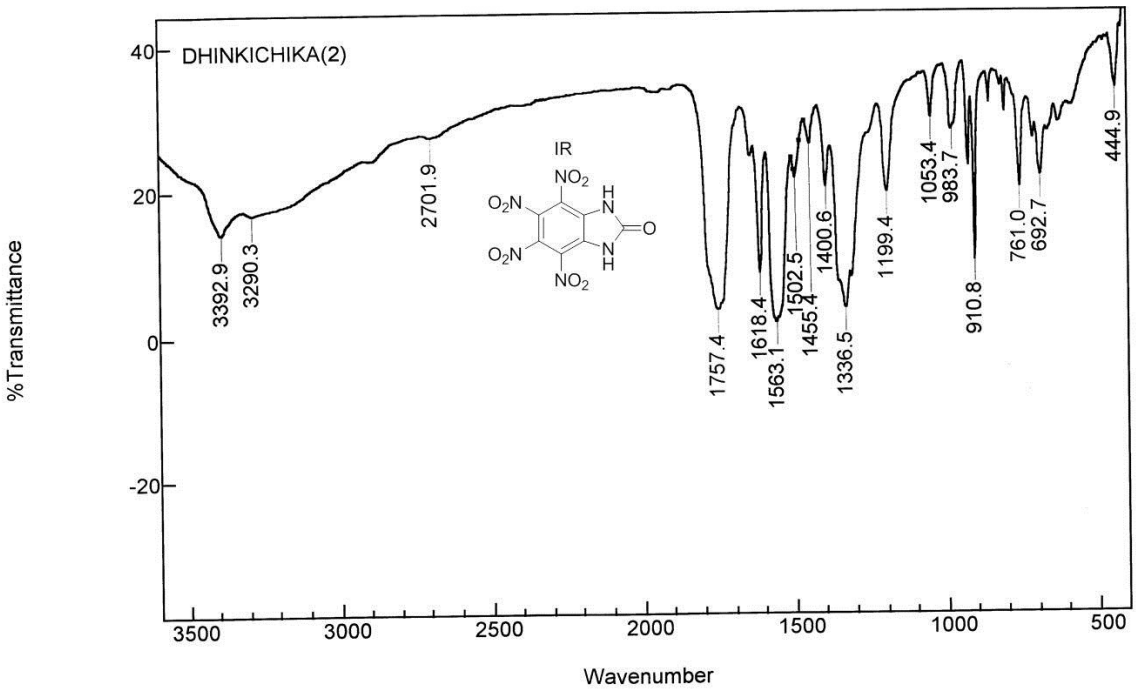

ppm
141.122
140.488
139.557
114.613
40.353
40.075
39.795
39.517
39.238
38.962
38.679
13C NMR
ppm
120
100
80
60
40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1614
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150529
Time 21.56
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 248
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677744 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 146.155 ppm
F1 11030.00 Hz
F2P 32.950 ppm
F2 2486.63 Hz
PPMCM 5.66027 ppm/cm
HZCM 427.16833 Hz/cm

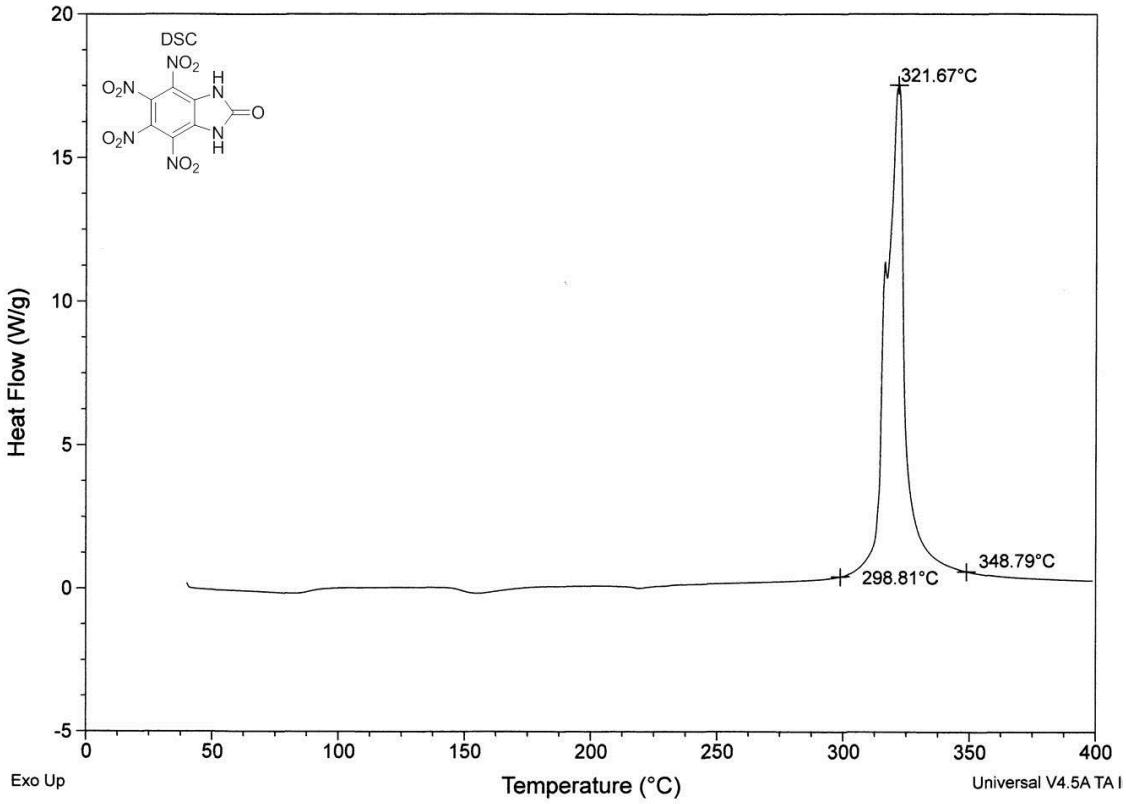

da(2)
IR
%Transmittance
40
30
20
10
3500
3000
2500
2000
1500
1000
500
Wavenumber
3398.8
1629.7
1583.6
1522.7
1466.0
1404.8
1367.8
1331.7
1258.7
1219.0
1174.6
1099.9
977.1
922.0
659.7
576.7
478.4


DSC
300.36°C
279.12°C
140.67°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA I


1H NMR
2.50027
1.0001
Integral
ppm
Current Data Parameters
NAME dpkqnp1H
EXPNO 1688
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150602
Time 14.38
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIGRES 0.201836 Hz
AQ 2.4773109 sec
RG 645.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 20.000 ppm
F1 6002.60 Hz
F2P -2.008 ppm
F2 -602.54 Hz
PPMCM 1.10038 ppm/cm
HZCM 330.25696 Hz/cm


^{13}C NMR
ppm
155.320
133.413
130.764
122.107
40.364
40.084
39.807
39.530
39.251
38.973
38.695
ppm 160 140 120 100 80 60 40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1616
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150602
Time 14.41
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 187
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677859 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 173.791 ppm
F1 13115.62 Hz
F2P 24.006 ppm
F2 1811.69 Hz
PPMCM 7.48924 ppm/cm
HZCM 565.19678 Hz/cm


DHINKICHIKA(2)
IR
%Transmittance
Wavenumber
40
20
0
-20
3500
3000
2500
2000
1500
1000
500
3392.9
3290.3
2701.9
1757.4
1618.4
1563.1
1502.5
1455.4
1400.6
1336.5
1199.4
1053.4
983.7
910.8
761.0
692.7
444.9


DSC
321.67°C
348.79°C
298.81°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA I