# Supporting Information

## A Convenient Three-Component Reaction Leading to the Synthesis of Polysubstituted Cyclohexene Derivatives

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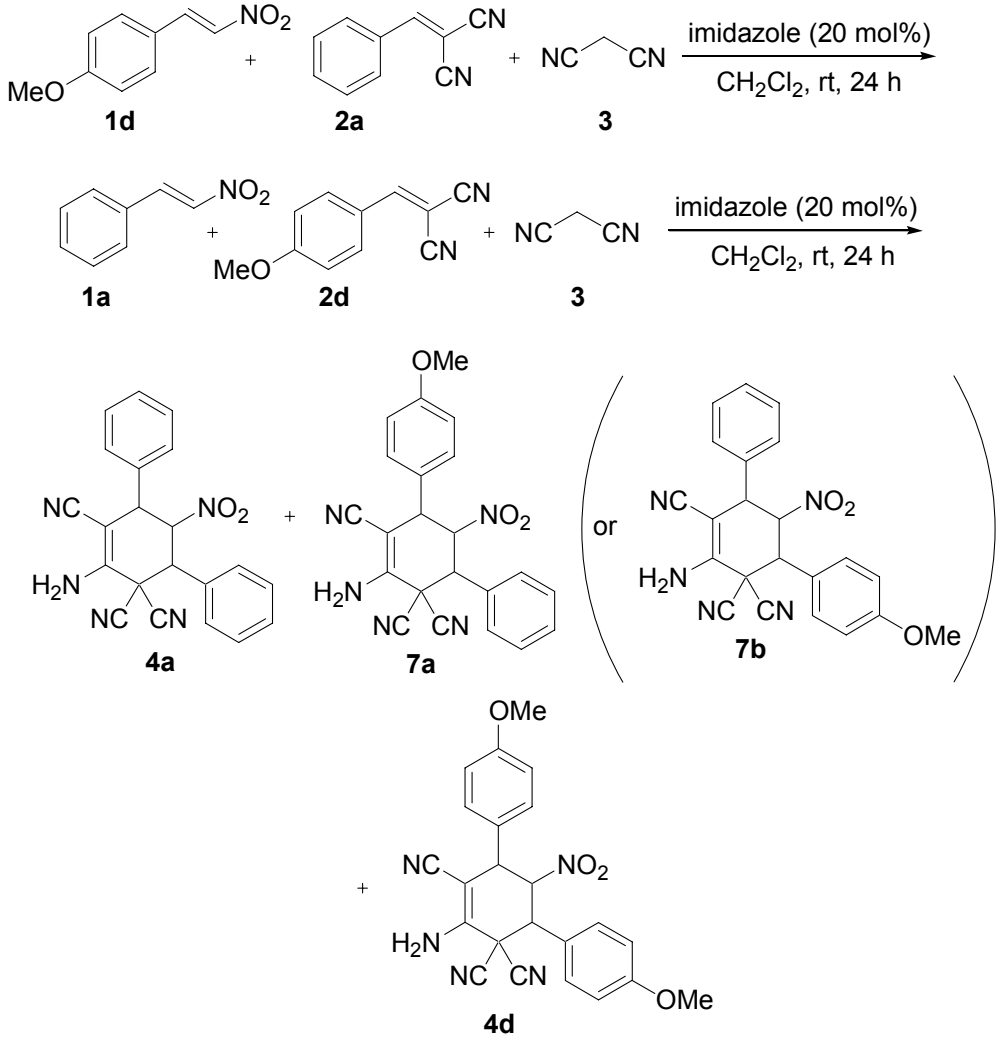
***RECEIVED DATE (to be automatically inserted after your manuscript is accepted if required according to the journal that you are submitting your paper to)***

***Content***

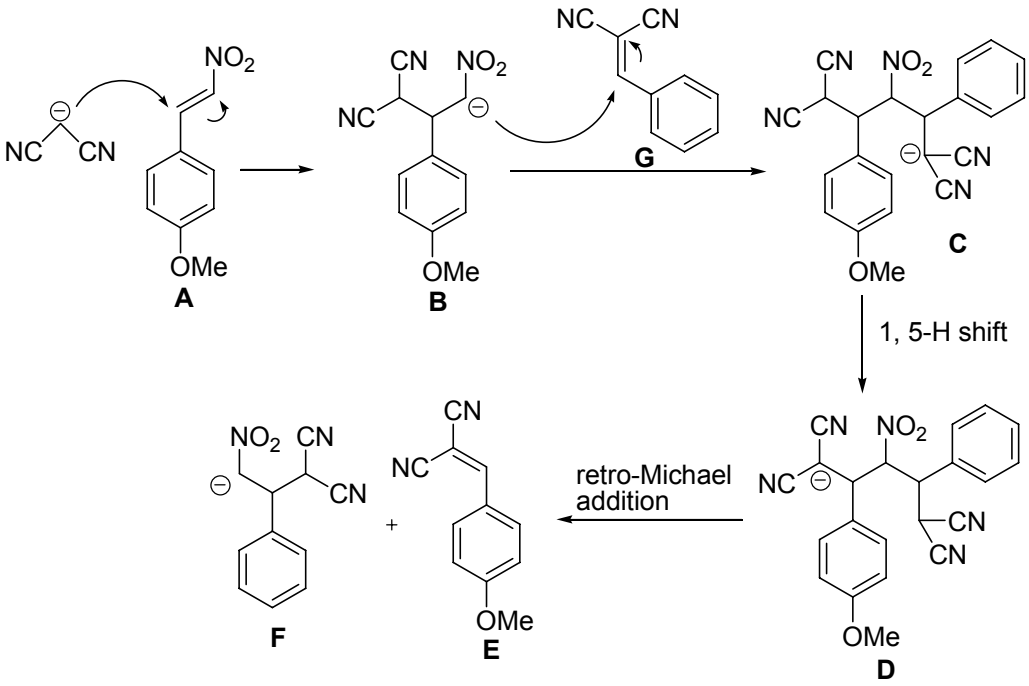
**Mechanistic investigation by cross-over experiments**

Under these optimized reaction conditions, we also examined the three-component reaction in which the substituents on the benzene rings of nitroalkene **1** and arylmethylidenemalononitrile **2** are different. Unfortunately, complex product mixtures were formed on the basis of $^1$H NMR spectroscopic investigation under identical conditions. The three-component reaction of nitroalkene **1d**, arylmethylidenemalononitrile **2a** and malononitrile **3** was conducted to give the mixture of compounds **4a**, **7a** (or **7b**) and **4d**. Also we could get compounds **7a** (or **7b**) and **4d** from the reaction of **1a**, **2d** and **3** (Scheme 1).




**Scheme 1** The three-component reaction in which the substitution groups on the benzene rings of nitroalkene and arylidenemalononitrile were different.

According to our understanding of the mechanism, the aromatic group exchange is due to 1,5-H shift in intermediate **C** and subsequent retro-Michael addition (Scheme 2). The anionic intermediates **B** and **F** could undergo nucleophilic attack to either arylmethylidenemalononitrile **E** or **G** to give different products.

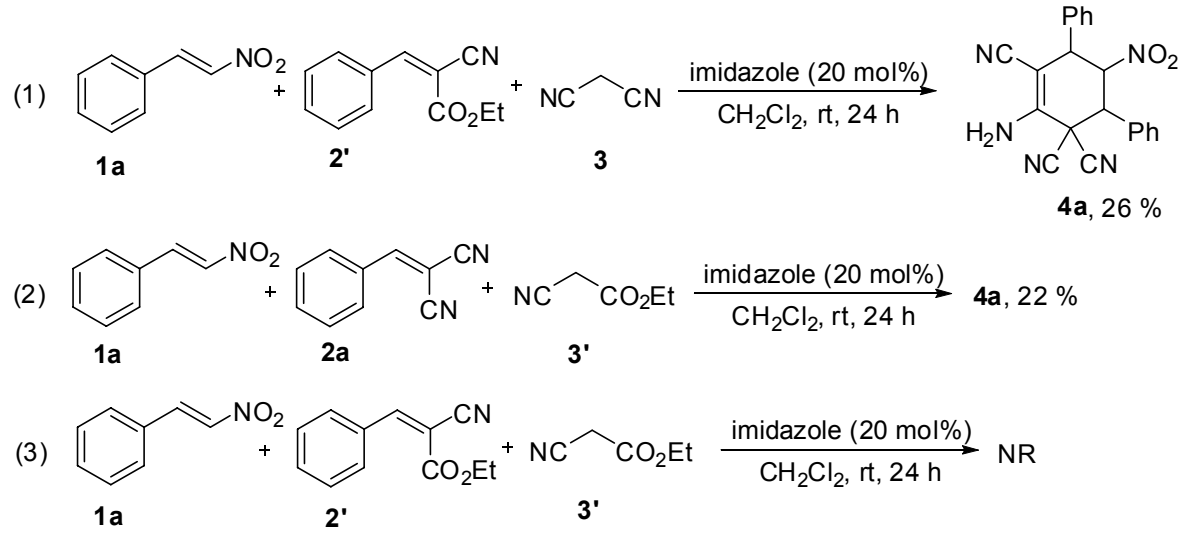



**Scheme 2** The mechanism of the aromatic group exchange process

To investigate the reaction mechanism, some other cross-over experiments were conducted. For example, we carried out the reaction of nitroalkene **1a**, arylmethylidenemalononitrile **2'** and malononitrile **3** under the standard conditions. To our surprise, we only obtained product **4a** in 26 % yield, which did not contain $CO_2Et$ group (Scheme 3, eq 1). The similar result was also obtained in the reaction of **1a**, **2a** and cyanoacetic acid ethyl ester **3'** (Scheme 3, eq 2). However, the reaction did not take place in the absence of both arylmethylidenemalononitrile and malononitrile (Scheme 3, eq 3).

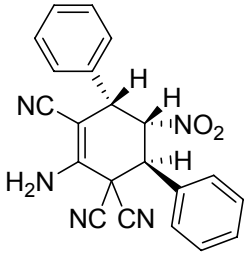
Through the results shown in Schemes 1 and 3, we could conclude that the malononitrile or its derivative arylmethylidenemalononitrile is very important in this three-component

reaction. The aromatic groups between nitroalkene **1** and arylmethylidenemalononitrile **2** exchange processes exist during the reaction. Moreover, malononitrile also can exchange between arylmethylidenemalononitrile **2** and **3** during the reaction.

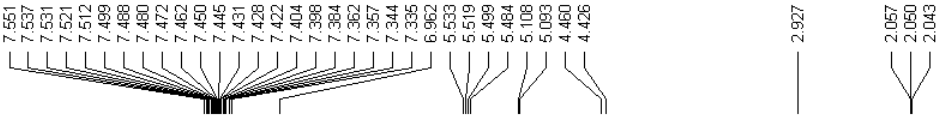


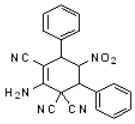

**Scheme 3** Some other cross-over experiments

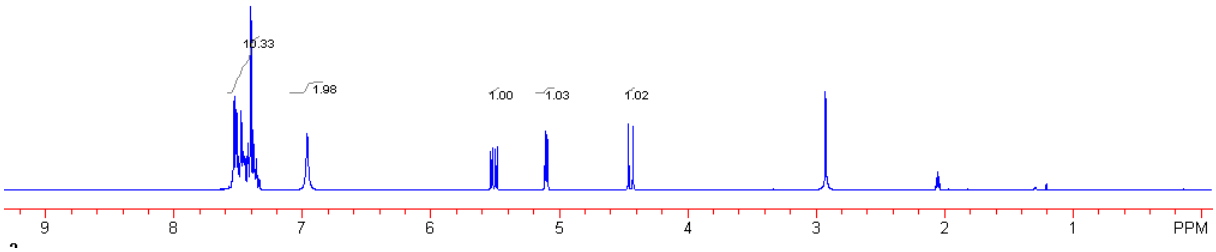
## Spectroscopic data of the reaction products

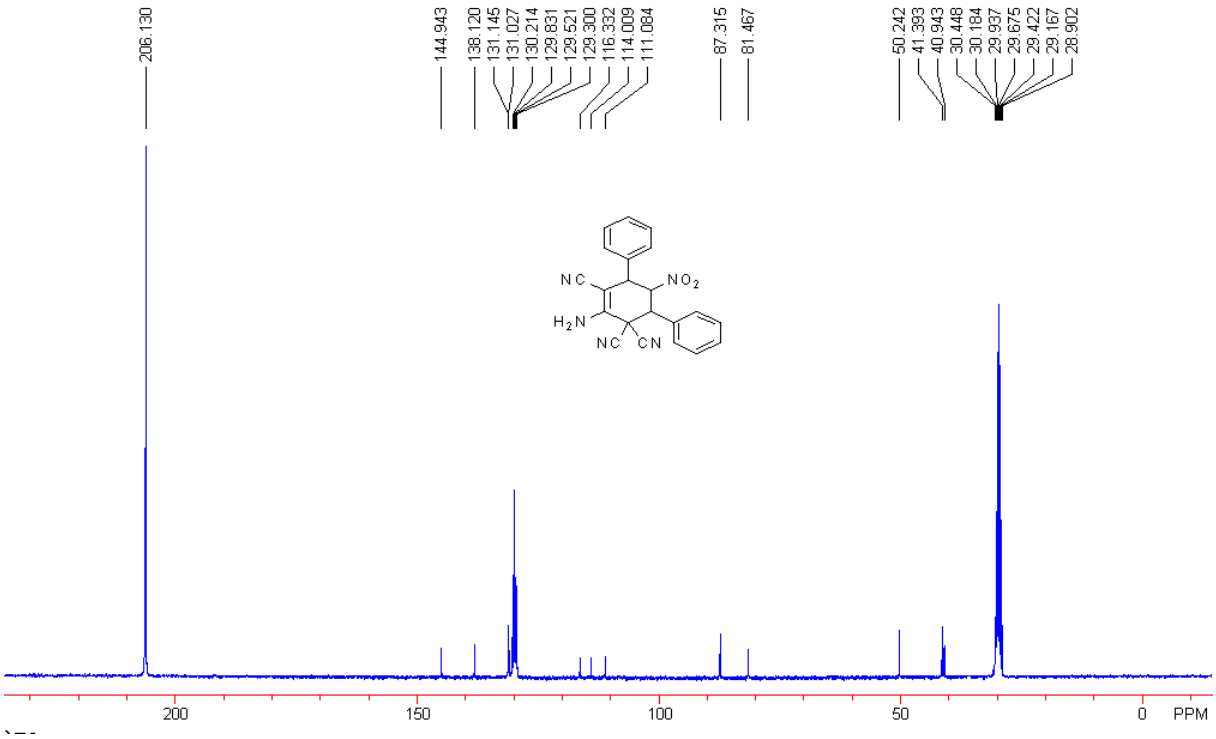



**4a-1**

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131.145
131.027
130.214
129.831
129.521
129.300
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114.009
111.084
87.315
81.467
50.242
41.393
40.943
30.448
30.184
29.937
29.675
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29.167
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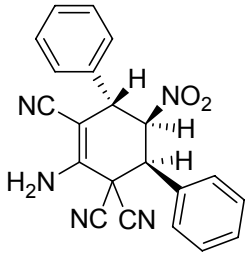
NC
NO2
H2N
NC
CN
200
150
100
50
0
PPM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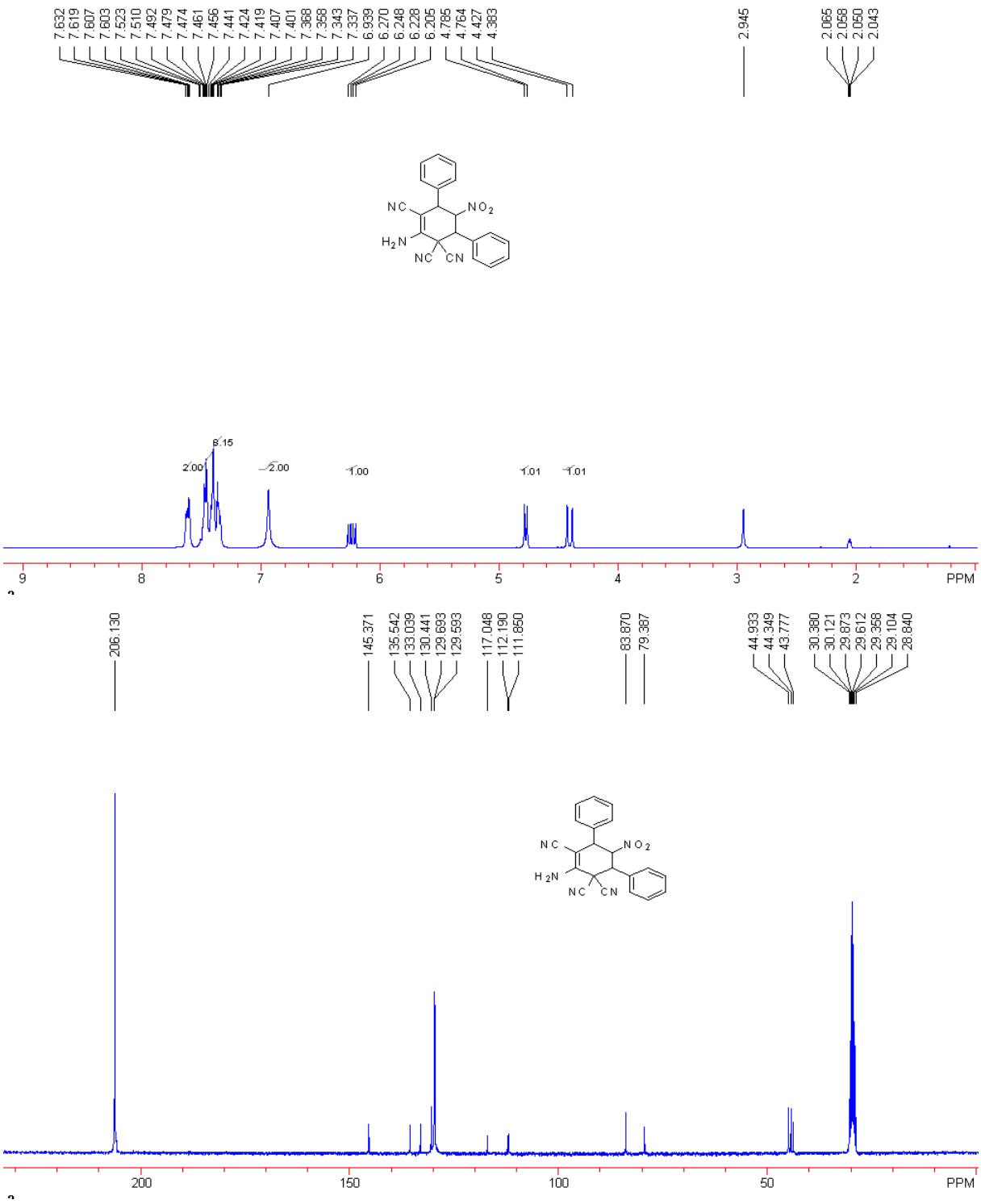
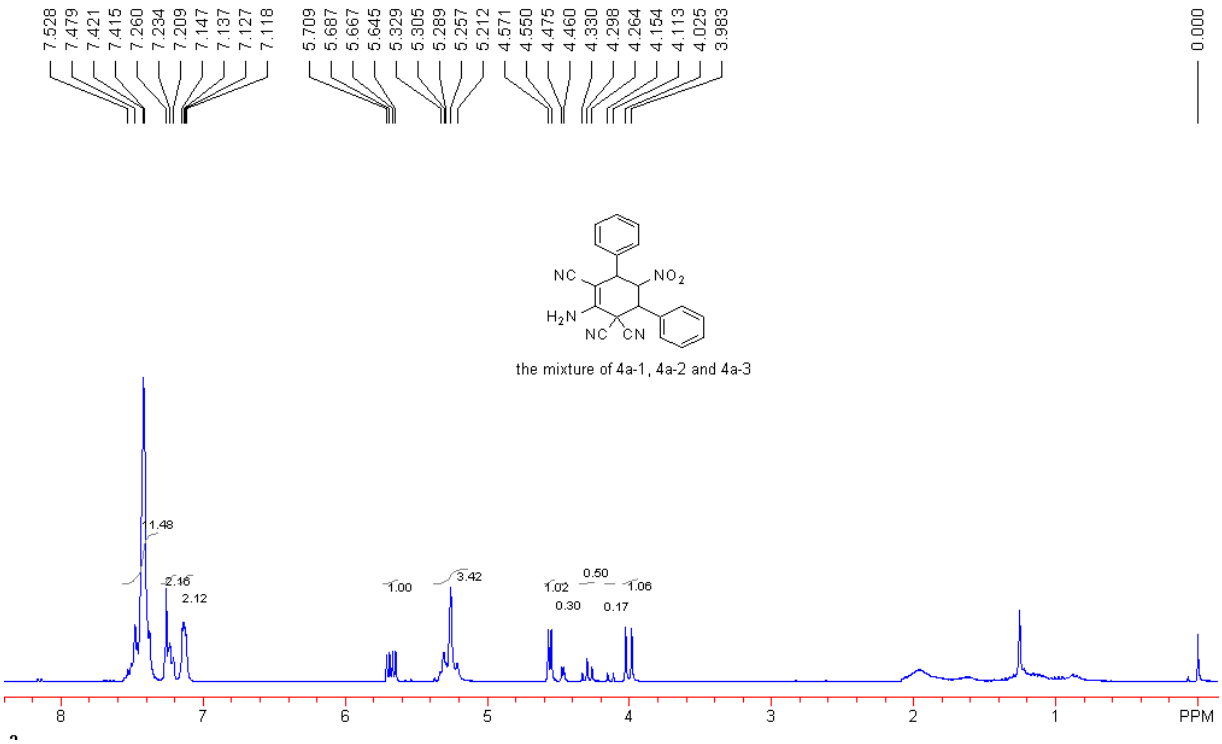
NC
NO2
H
H
H2N
NC
CN

**4a-2**




A mixture of compounds **4a-1**, **4a-2** and **4a-3** for the determination of the product distribution.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7.127
7.118
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5.687
5.667
5.645
5.329
5.305
5.289
5.257
5.212
4.571
4.550
4.475
4.460
4.330
4.298
4.264
4.154
4.113
4.025
3.983
0.000
NC
NO2
H2N
NC CN
the mixture of 4a-1, 4a-2 and 4a-3
1.48
2.16
2.12
1.00
3.42
1.02
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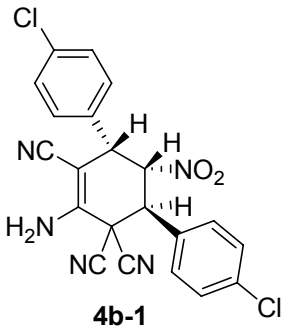
1.06
0.30
0.17
8
7
6
5
4
3
2
1
PPM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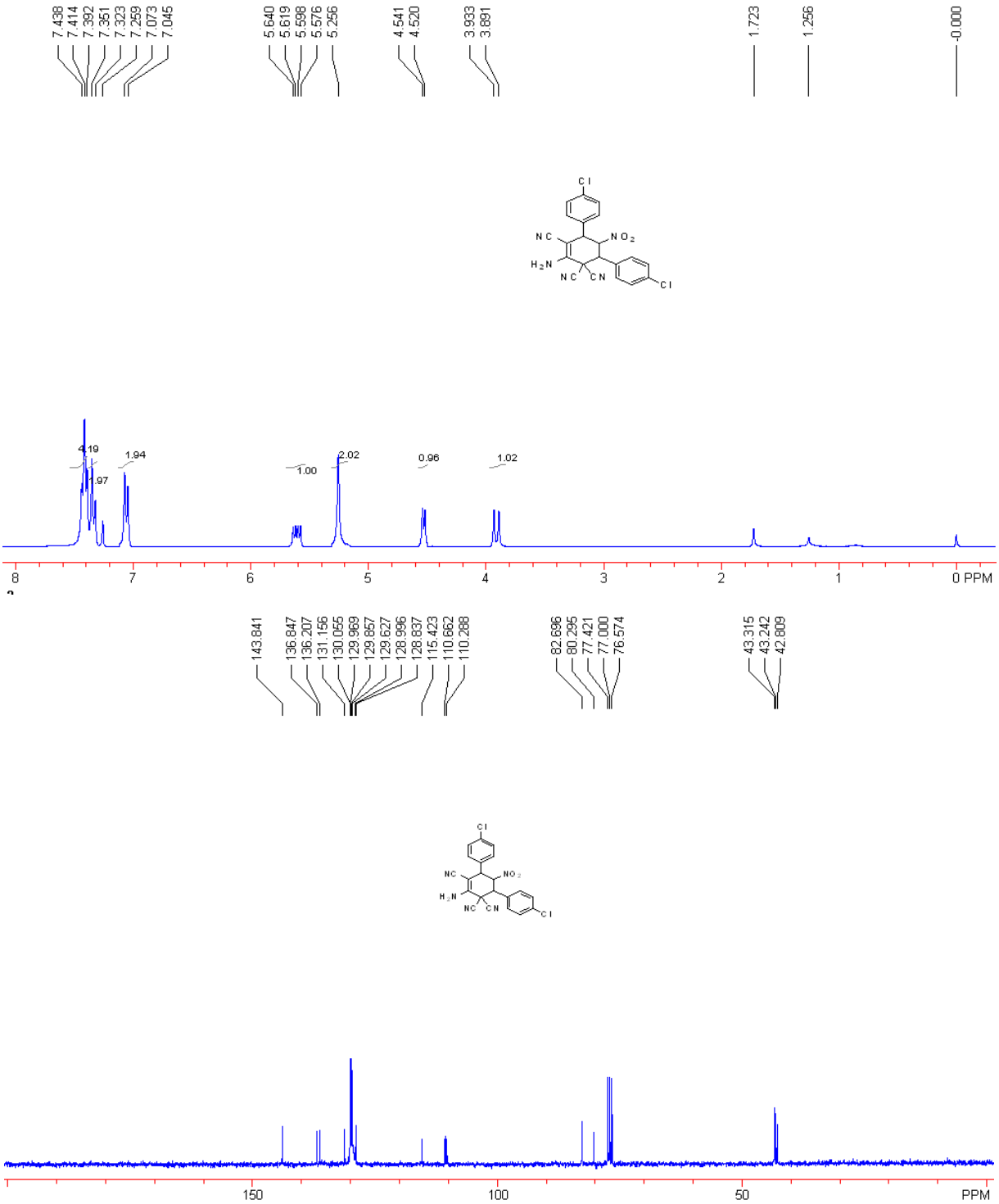
H
NO2
H
H2N
NC CN
Cl

**4b-1**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5.256
4.541
4.520
3.933
3.891
1.723
1.256
-0.000
Cl
NC
NO2
H2N
NC
CN
Cl
4.19
1.94
1.97
1.00
2.02
0.96
1.02
8
7
6
5
4
3
2
1
0 PPM
143.841
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136.207
131.156
130.055
129.969
129.857
129.627
128.996
128.837
115.423
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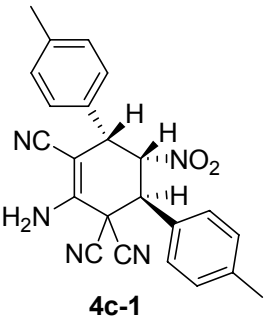
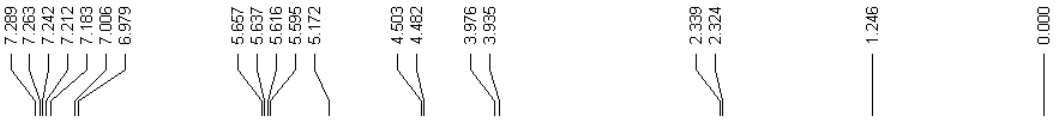
150
100
50
PPM


H
NC
H
NO2
H2N
H
NC CN

**4c-1**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5.657
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3.935
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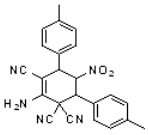
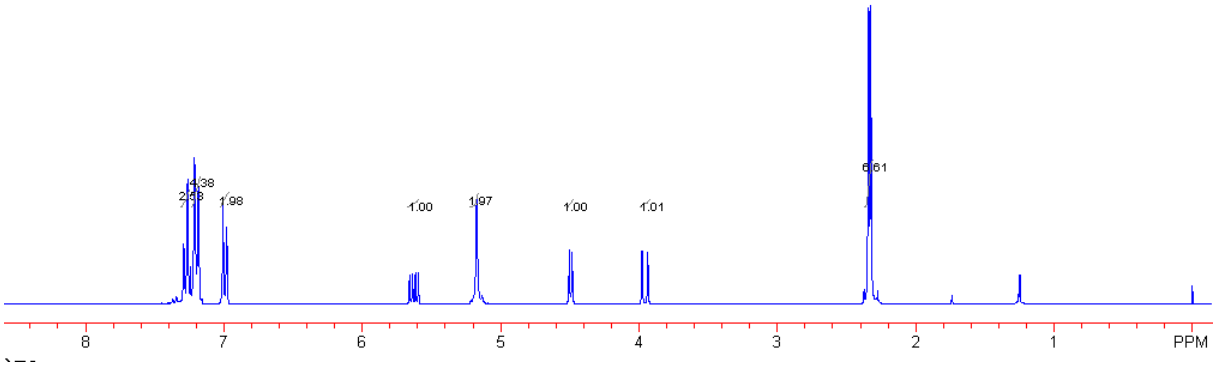
0.000

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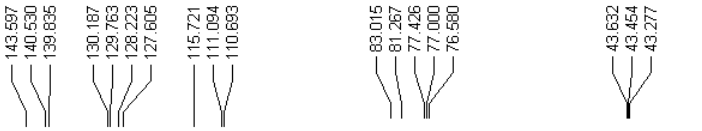
8
7
6
5
4
3
2
1
PPM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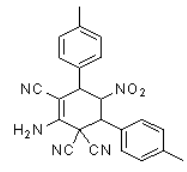
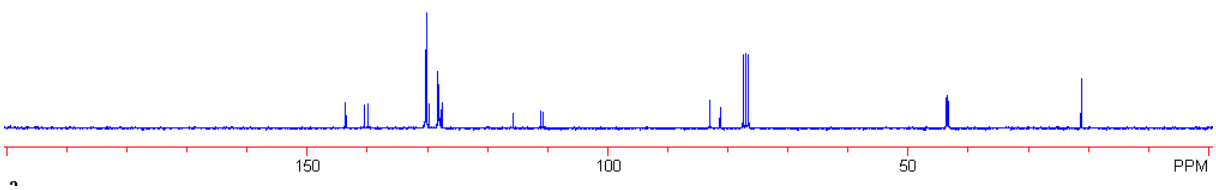
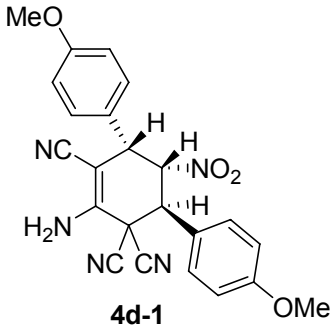
43.454
43.277
21.120




150
100
50
PPM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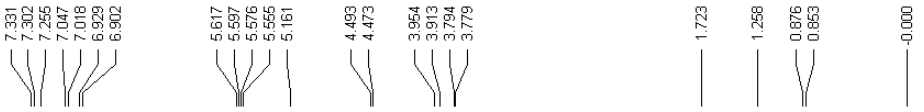
NC
H
NO2
H
H2N
NC CN
OMe

**4d-1**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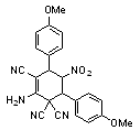
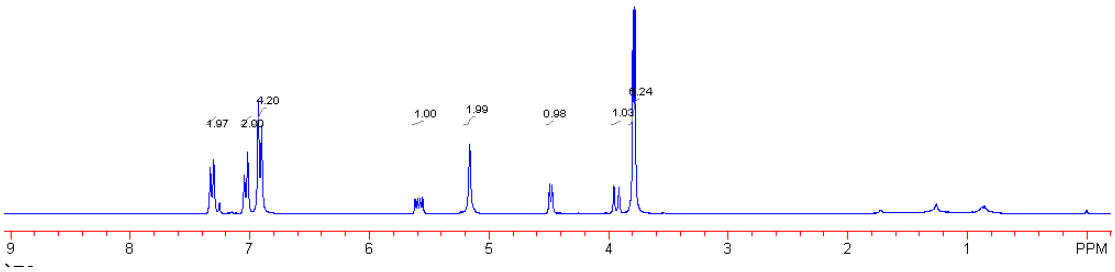
-0.000

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7
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5
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3
2
1
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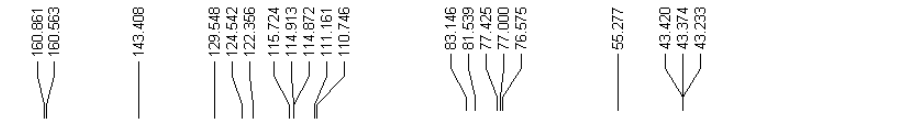
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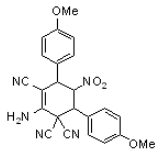

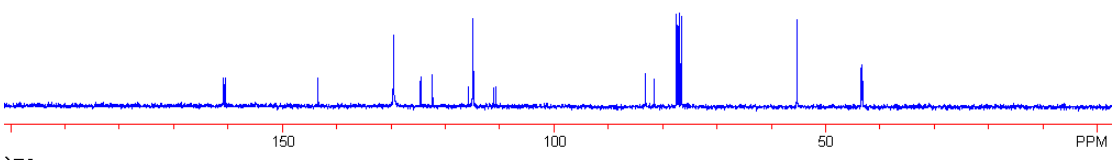
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50
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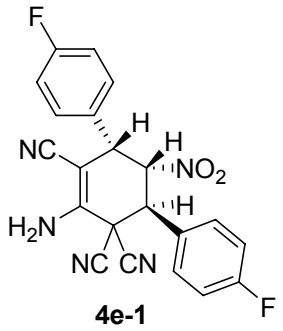
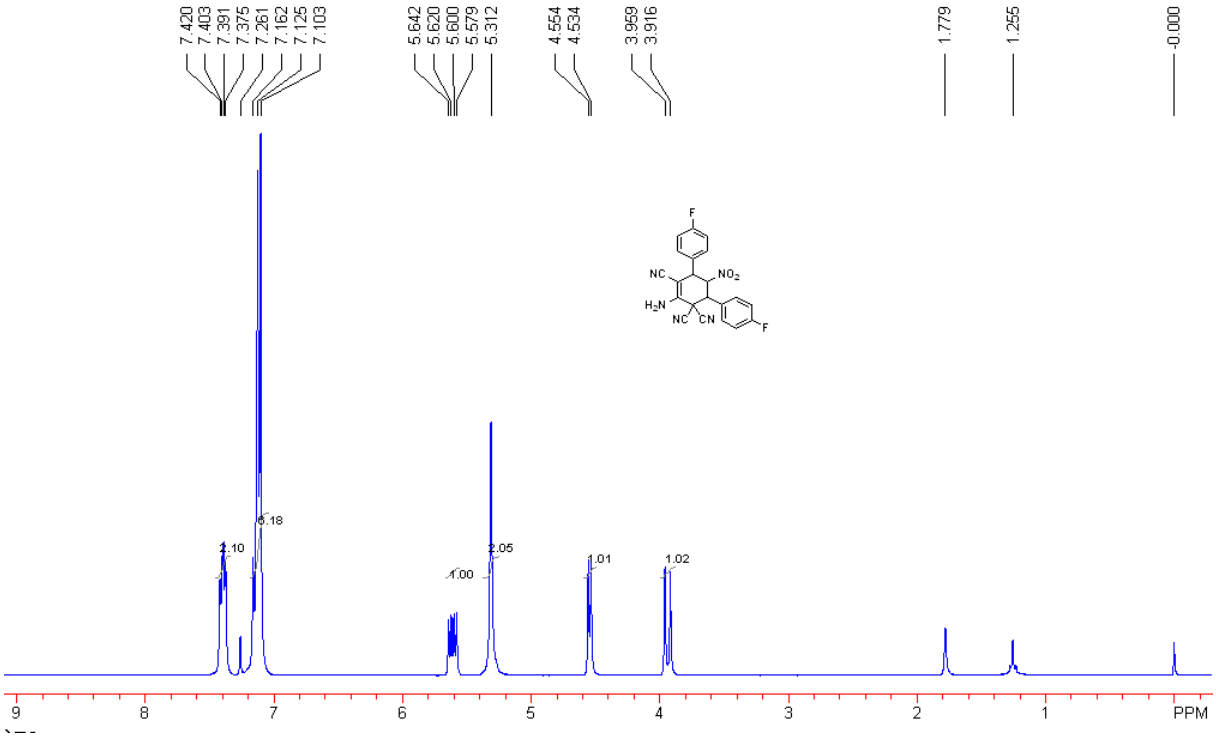

F
H
H
NC
NO2
H2N
H
NC CN
F

**4e-1**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4.554
4.534
3.959
3.916
1.779
1.255
0.000
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1.02
9
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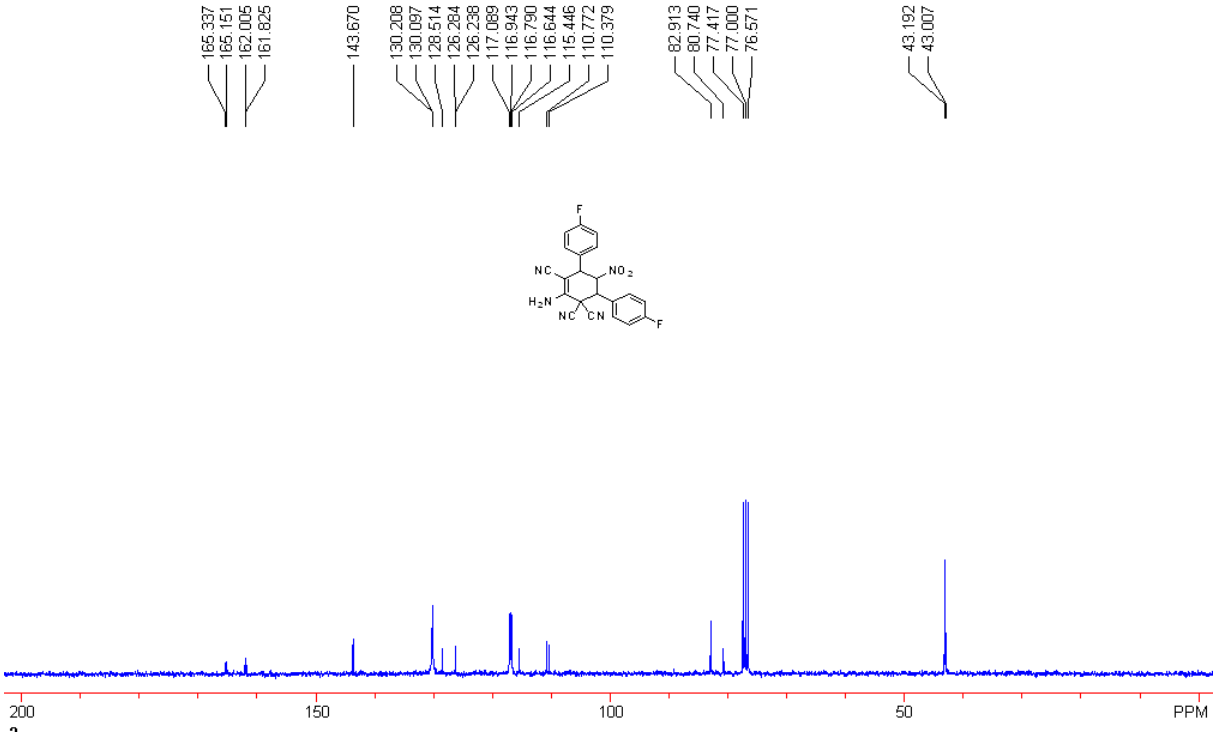
7
6
5
4
3
2
1
PPM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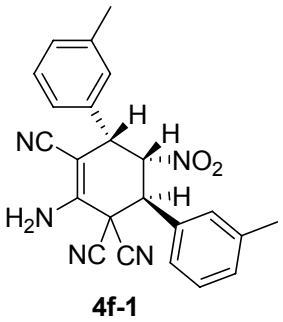
50
PPM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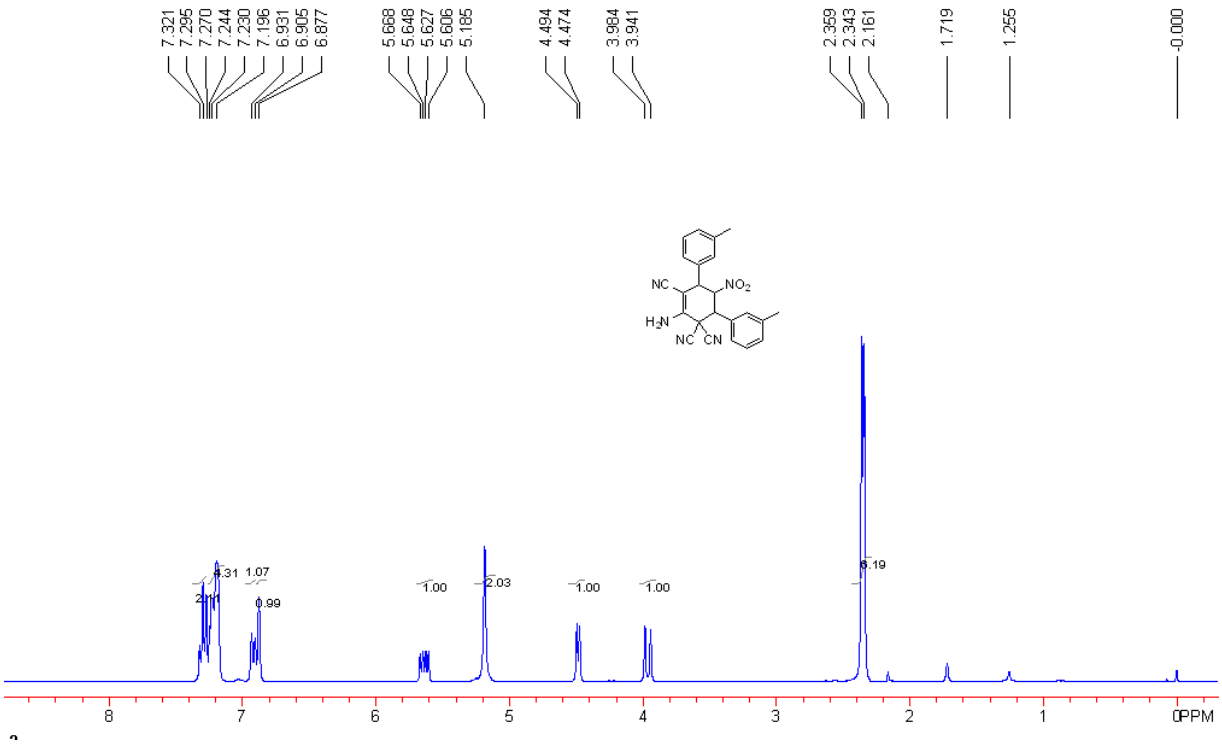
NO2
H
H2N
NC CN

**4f-1**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5.606
5.185
4.494
4.474
3.984
3.941
2.359
2.343
2.161
1.719
1.255
-0.000
NC
NO2
H2N
NC CN
2.11
4.31
1.07
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6
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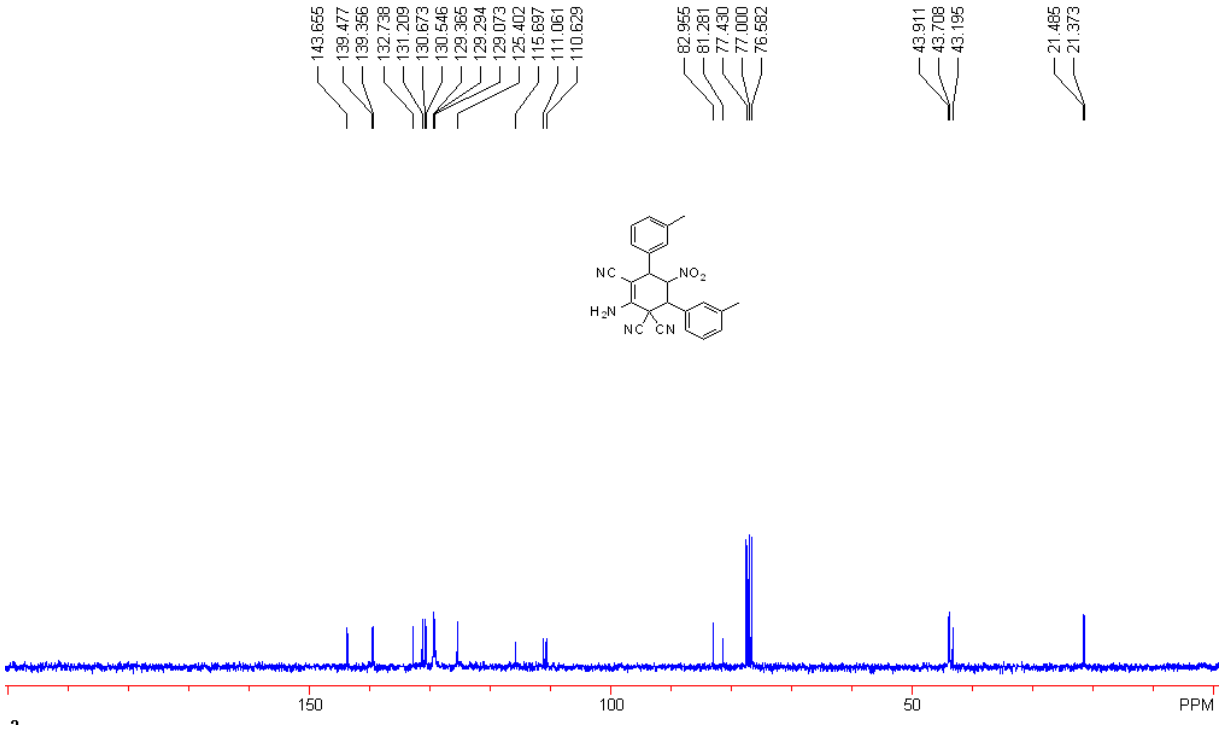
4
3
2
1
0PPM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111.061
110.629
82.955
81.281
77.430
77.000
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43.708
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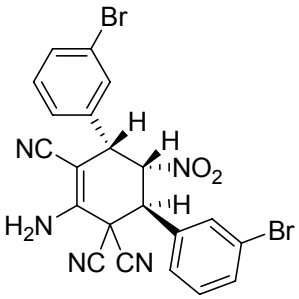
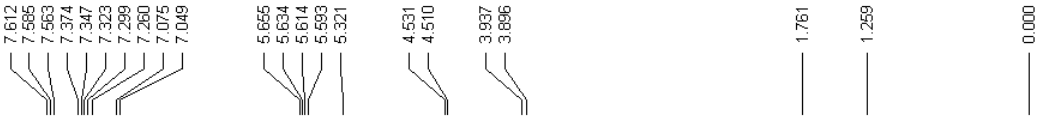
21.373
NC
NO2
H2N
NC CN
150
100
50
PPM


Br
H
NC
H
NO2
H
H2N
Br
NC CN

**4g-1**


7.612
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7.563
7.374
7.347
7.323
7.299
7.260
7.075
7.049
5.655
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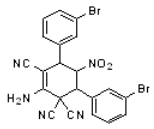
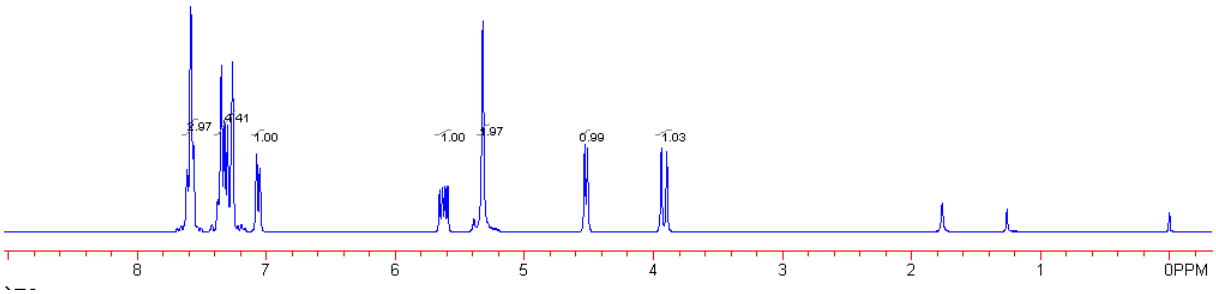
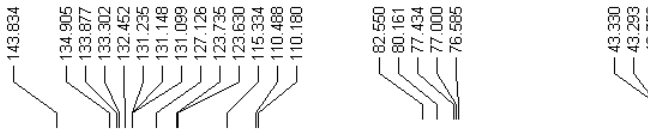



2.97
4.41
1.00
1.00
1.97
0.99
1.03
8
7
6
5
4
3
2
1
0PPM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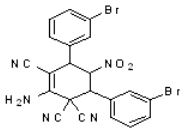
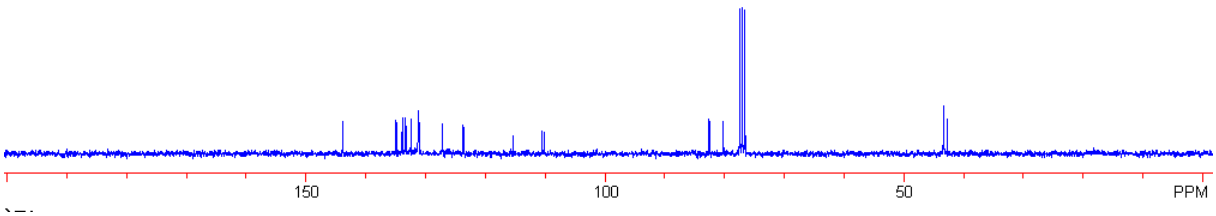
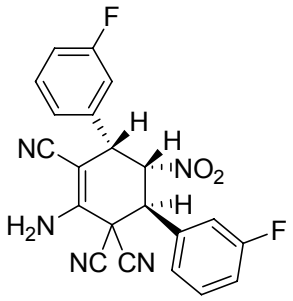
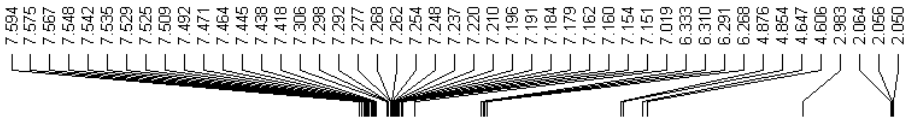
134.905
133.877
133.302
132.452
131.235
131.148
131.099
127.126
123.735
123.630
115.334
110.488
110.180
82.550
80.161
77.434
77.000
76.585
43.330
43.293
42.752




150
100
50
PPM


F
H
NC
H
NO2
H2N
H
F
NC CN

**4h-1**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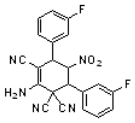
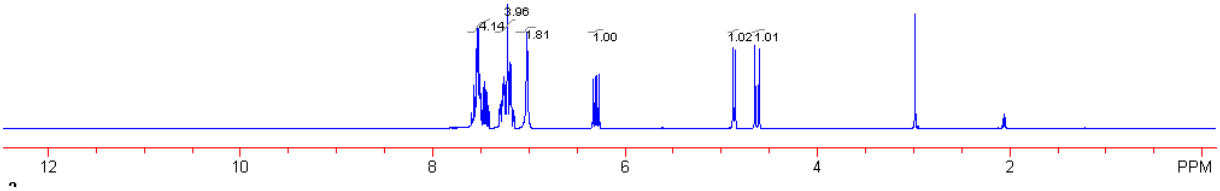
7.567
7.548
7.542
7.535
7.529
7.525
7.509
7.492
7.471
7.464
7.445
7.438
7.418
7.306
7.298
7.292
7.277
7.268
7.262
7.254
7.248
7.237
7.220
7.210
7.196
7.191
7.184
7.179
7.162
7.160
7.154
7.151
7.019
6.333
6.310
6.291
6.268
4.876
4.854
4.647
4.606
2.983
2.064
2.056
2.050

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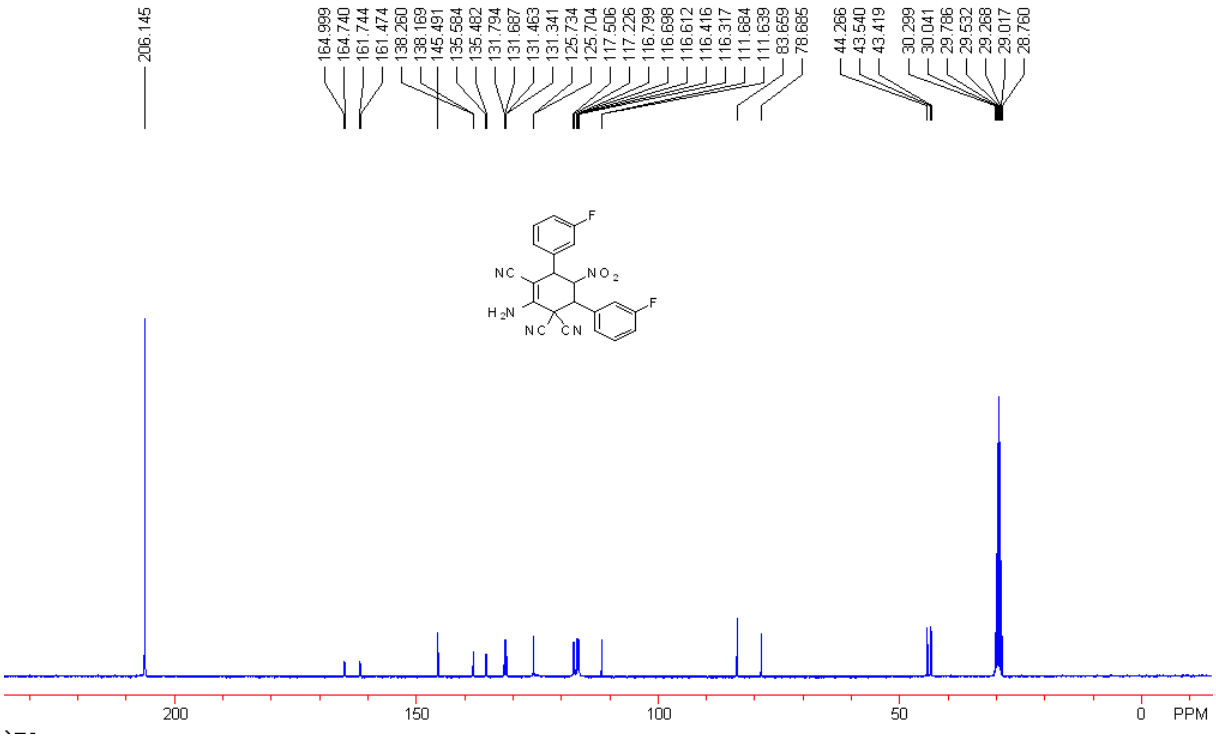
4.14
1.81
1.00
1.02
1.01
12
10
8
6
4
2
PPM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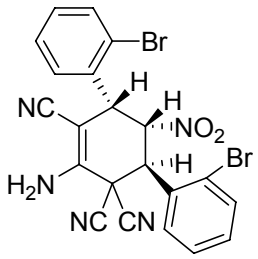
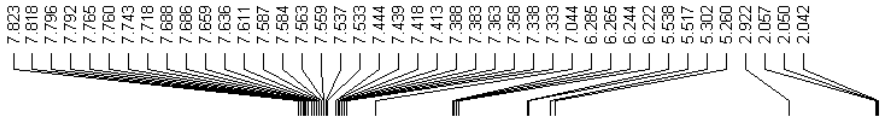
164.999
164.740
161.744
161.474
138.260
138.169
145.491
135.584
135.462
131.794
131.687
131.463
131.341
125.734
125.704
117.506
117.226
116.799
116.698
116.612
116.416
116.317
111.684
111.639
83.659
78.685
44.266
43.540
43.419
30.299
30.041
29.786
29.532
29.268
29.017
28.760
F
NC
NO2
H2N
NC
CN
F
200
150
100
50
0
PPM


Br
H
NC
H
NO2
H
Br
H2N
NC
CN

**4i-1**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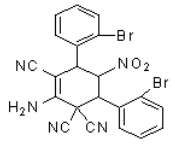
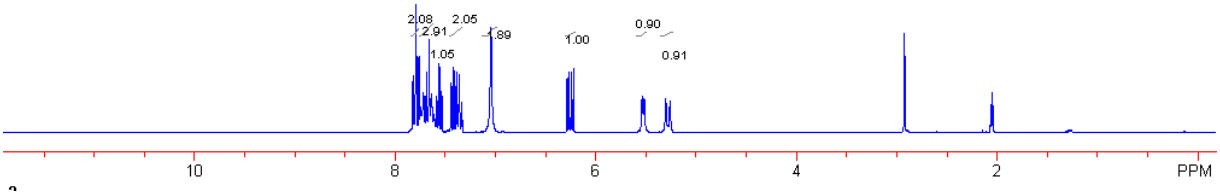
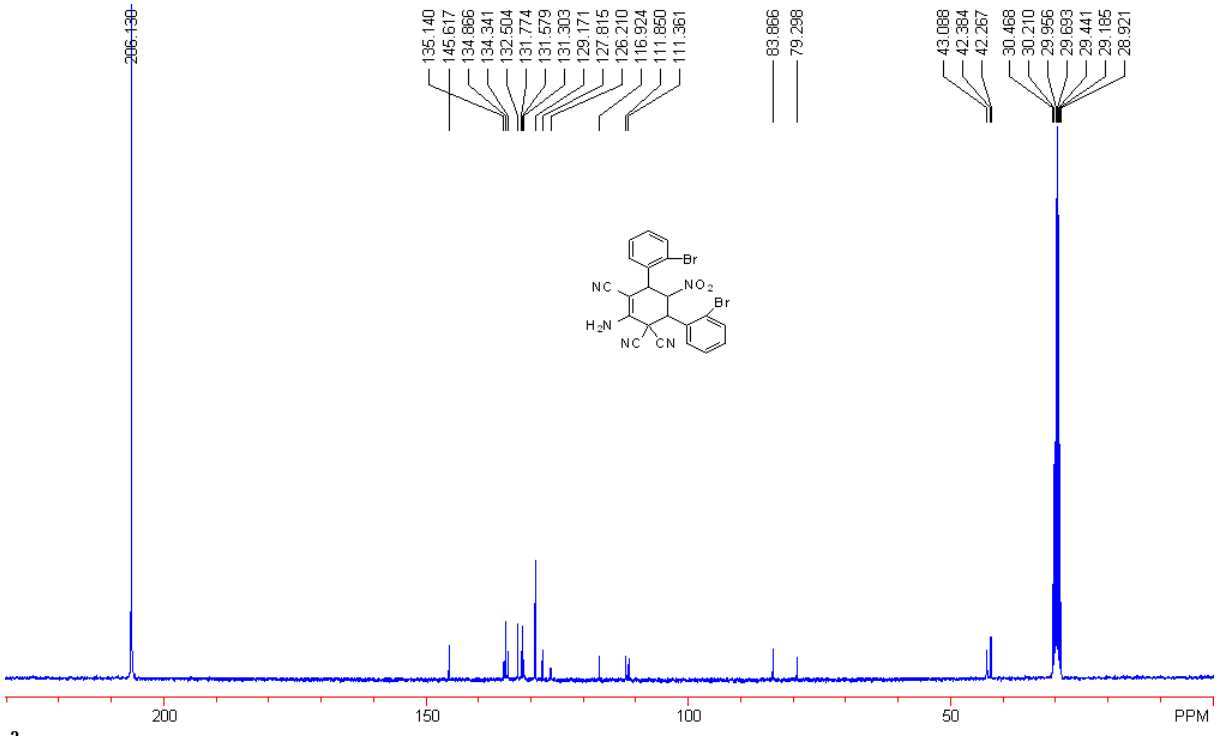
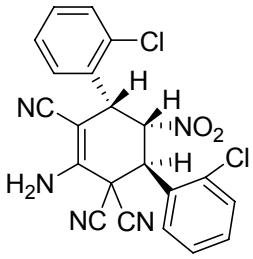
7.796
7.792
7.765
7.760
7.743
7.718
7.688
7.686
7.659
7.636
7.611
7.587
7.584
7.563
7.559
7.537
7.533
7.444
7.439
7.418
7.413
7.388
7.383
7.363
7.358
7.338
7.333
7.044
6.285
6.265
6.244
6.222
5.538
5.517
5.302
5.260
2.922
2.057
2.050
2.042

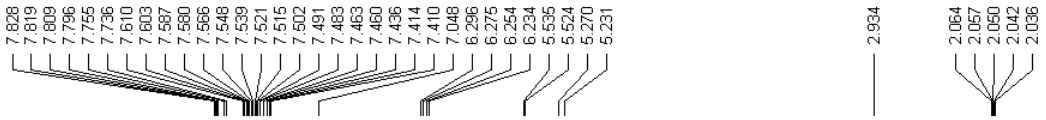

Br
NC
NO2
Br
H2N
NC
CN

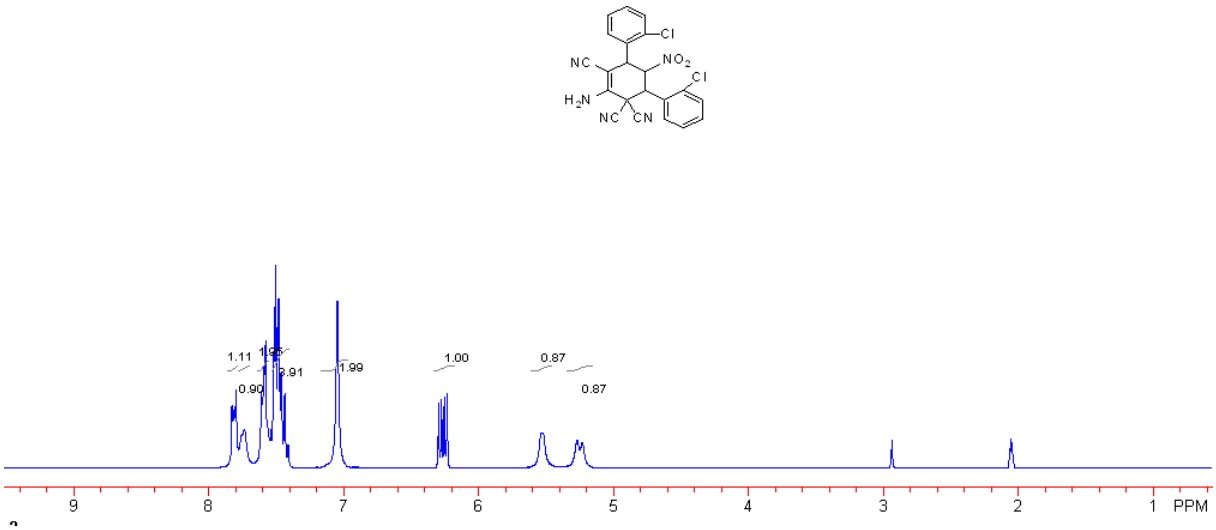

2.08
2.91
2.05
1.05
1.89
1.00
0.90
0.91
10
8
6
4
2
PPM

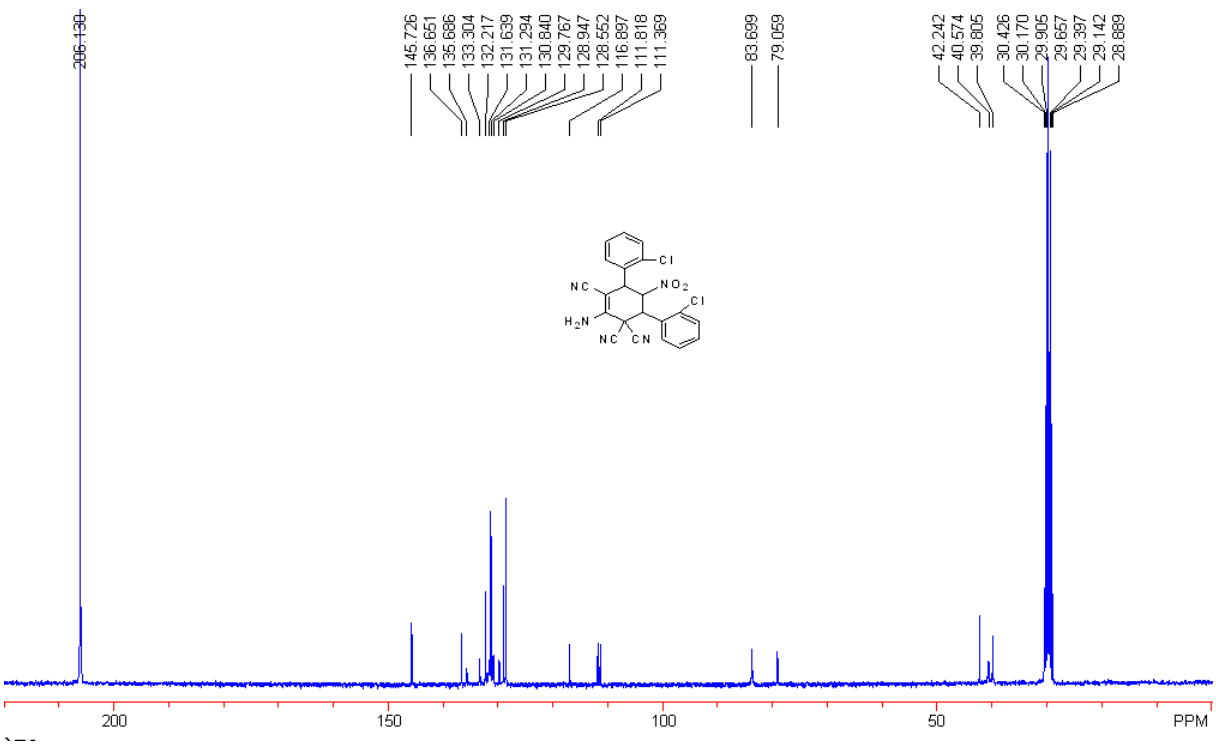

206.130
135.140
145.617
134.866
134.341
132.504
131.774
131.579
131.303
129.171
127.815
126.210
116.924
111.850
111.361
83.866
79.298
43.088
42.384
42.267
30.468
30.210
29.956
29.693
29.441
29.185
28.921
Br
NC
NO2
Br
H2N
NC
CN
200
150
100
50
PPM

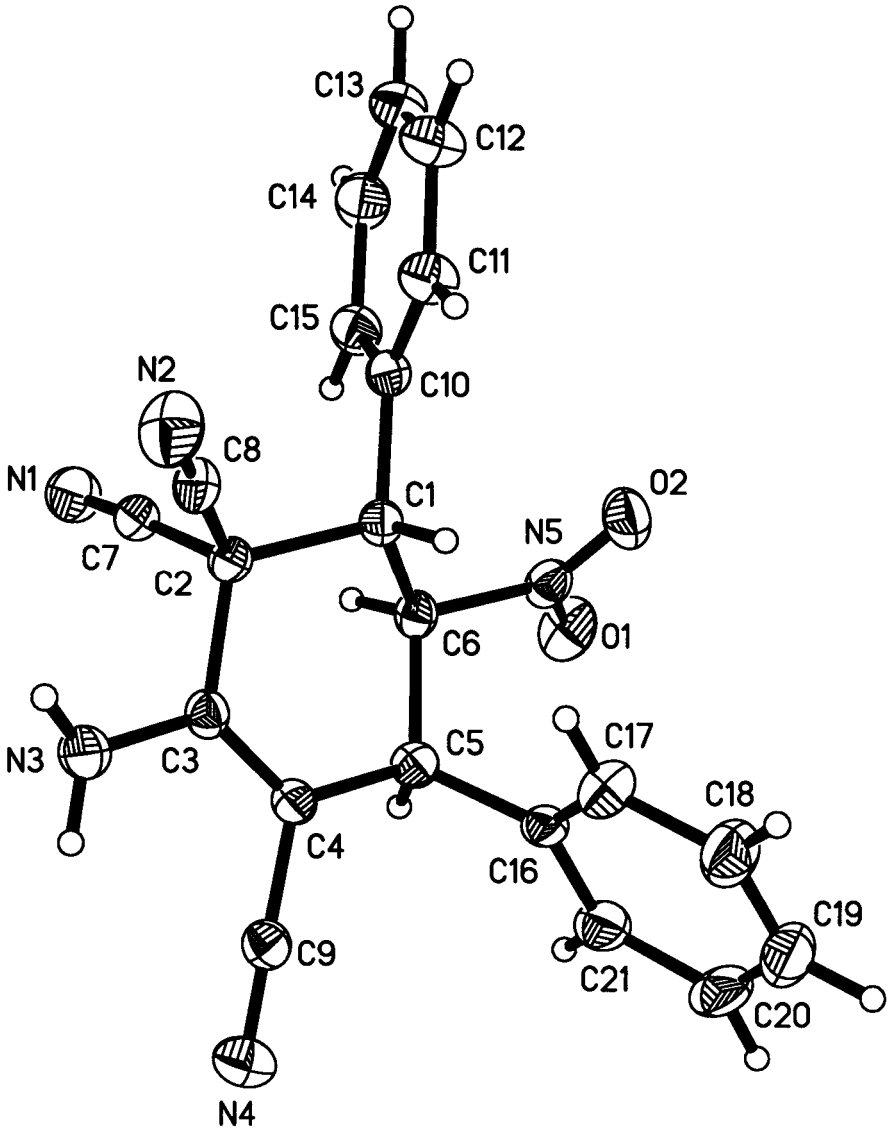

Cl
H
NC
H
NO2
H
Cl
H2N
NC
CN

**4j-1**


7.828
7.819
7.809
7.796
7.755
7.736
7.610
7.603
7.587
7.580
7.566
7.548
7.539
7.521
7.515
7.502
7.491
7.483
7.463
7.460
7.436
7.414
7.410
7.048
6.296
6.275
6.254
6.234
5.535
5.524
5.270
5.231
2.934
2.064
2.057
2.050
2.042
2.036


1.11
1.95
0.90
2.91
1.99
1.00
0.87
0.87
9
8
7
6
5
4
3
2
1
PPM


206.130
145.726
136.651
135.686
133.304
132.217
131.639
131.294
130.840
129.767
128.947
128.552
116.897
111.818
111.369
83.699
79.059
42.242
40.574
39.805
30.426
30.170
29.905
29.657
29.397
29.142
28.889
200
150
100
50
PPM




The crystal data of compound **4a-1** have been deposited in CCDC with number 688760. Empirical Formula: $C_{21}H_{16}N_5O_{2.33}$; Formula Weight: 375.72; Crystal size: 0.469 x 0.411 x 0.347; Crystal Color, Habit: colorless, prismatic; Crystal System: Rhombohedral; Lattice Type: Primitive; Lattice Parameters: a = 23.2536(10)Å, b = 23.2536(10)Å, c = 17.7700(11)Å, $\alpha$ = 90°, $\beta$ = 90°, $\gamma$ = 120°, V = 8321.4(7)Å$^3$; Space group: R-3; Z = 18; $D_{calc}$ = 1.350 g/cm$^3$; $F_{000}$ = 3522; R1 = 0.0514, wR2 = 0.1330. Diffractometer: Rigaku AFC7R.

Table 1. Crystal data and structure refinement for cd28234.

| | |
|---|---|
| Identification code | cd28234 |
| Empirical formula | C21 H16 N5 O2.33 |
| Formula weight | 375.72 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Rhombohedral, R-3 |
| Unit cell dimensions | a = 23.2536(10) A alpha = 90 deg.<br>b = 23.2536(10) A beta = 90 deg.<br>c = 17.7700(11) A gamma = 120 deg. |
| Volume | 8321.4(7) A^3 |
| Z, Calculated density | 18, 1.350 Mg/m^3 |
| Absorption coefficient | 0.092 mm^-1 |
| F(000) | 3522 |
| Crystal size | 0.469 x 0.411 x 0.347 mm |
| Theta range for data collection | 1.53 to 27.00 deg. |
| Limiting indices | -28<=h<=29, -25<=k<=29, -19<=l<=22 |
| Reflections collected / unique | 16528 / 4041 [R(int) = 0.0765] |
| Completeness to theta = 27.00 | 100.0 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 1.00000 and 0.75474 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4041 / 3 / 267 |
| Goodness-of-fit on F^2 | 1.020 |
| Final R indices [I>2sigma(I)] | R1 = 0.0514, wR2 = 0.1330 |
| R indices (all data) | R1 = 0.0744, wR2 = 0.1418 |
| Largest diff. peak and hole | 0.735 and -0.309 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd28234.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| N(1) | -201(1) | 2526(1) | 1388(1) | 56(1) |
| N(2) | -675(1) | 2670(1) | -966(1) | 65(1) |
| N(3) | -733(1) | 3637(1) | 462(1) | 55(1) |
| N(4) | 119(1) | 5301(1) | 1062(1) | 55(1) |
| N(5) | 1975(1) | 4296(1) | 430(1) | 44(1) |
| O(1) | 2348(1) | 4571(1) | 956(1) | 64(1) |
| O(2) | 2153(1) | 4239(1) | -192(1) | 62(1) |
| C(1) | 814(1) | 3547(1) | -28(1) | 35(1) |
| C(2) | 68(1) | 3281(1) | 202(1) | 34(1) |
| C(3) | -79(1) | 3826(1) | 432(1) | 35(1) |
| C(4) | 416(1) | 4420(1) | 649(1) | 35(1) |
| C(5) | 1146(1) | 4634(1) | 697(1) | 37(1) |
| C(6) | 1243(1) | 4030(1) | 584(1) | 36(1) |
| C(7) | -104(1) | 2829(1) | 855(1) | 38(1) |
| C(8) | -354(1) | 2919(1) | -453(1) | 40(1) |
| C(9) | 250(1) | 4909(1) | 879(1) | 40(1) |
| C(10) | 929(1) | 2963(1) | -172(1) | 38(1) |
| C(11) | 856(1) | 2718(1) | -893(1) | 52(1) |
| C(12) | 935(1) | 2177(1) | -1049(2) | 66(1) |
| C(13) | 1096(1) | 1884(1) | -485(2) | 65(1) |
| C(14) | 1180(1) | 2126(1) | 231(1) | 61(1) |
| C(15) | 1093(1) | 2662(1) | 398(1) | 48(1) |
| C(16) | 1552(1) | 5233(1) | 191(1) | 40(1) |
| C(17) | 1493(1) | 5206(1) | -583(1) | 56(1) |
| C(18) | 1856(1) | 5762(1) | -1014(2) | 71(1) |
| C(19) | 2269(1) | 6358(1) | -699(2) | 79(1) |
| C(20) | 2323(1) | 6406(1) | 68(2) | 79(1) |
| C(21) | 1968(1) | 5842(1) | 520(1) | 59(1) |
| O(3) | 10000 | 10000 | 9509(7) | 165(7) |

Table 3. Bond lengths [A] and angles [deg] for cd28234.

| | |
|---|---|
| N(1)-C(7) | 1.133(2) |
| N(2)-C(8) | 1.136(2) |
| N(3)-C(3) | 1.356(2) |
| N(3)-H(3A) | 0.814(15) |
| N(3)-H(3B) | 0.863(16) |
| N(4)-C(9) | 1.142(2) |
| N(5)-O(2) | 1.211(2) |
| N(5)-O(1) | 1.215(2) |
| N(5)-C(6) | 1.517(2) |
| C(1)-C(6) | 1.523(2) |
| C(1)-C(10) | 1.531(2) |
| C(1)-C(2) | 1.576(2) |
| C(1)-H(1) | 0.9800 |
| C(2)-C(7) | 1.481(2) |
| C(2)-C(8) | 1.483(2) |
| C(2)-C(3) | 1.524(2) |
| C(3)-C(4) | 1.339(2) |
| C(4)-C(9) | 1.431(2) |
| C(4)-C(5) | 1.513(2) |
| C(5)-C(16) | 1.525(2) |
| C(5)-C(6) | 1.544(2) |
| C(5)-H(5) | 0.9800 |
| C(6)-H(6) | 0.9800 |
| C(10)-C(11) | 1.378(3) |
| C(10)-C(15) | 1.388(3) |
| C(11)-C(12) | 1.386(3) |
| C(11)-H(11) | 0.9300 |
| C(12)-C(13) | 1.367(3) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.365(3) |
| C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.391(3) |
| C(14)-H(14) | 0.9300 |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.381(3) |
| C(16)-C(21) | 1.382(3) |
| C(17)-C(18) | 1.370(3) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(19) | 1.353(4) |
| C(18)-H(18) | 0.9300 |
| C(19)-C(20) | 1.368(4) |
| C(19)-H(19) | 0.9300 |
| C(20)-C(21) | 1.402(3) |
| C(20)-H(20) | 0.9300 |
| C(21)-H(21) | 0.9300 |
| O(3)-O(3)#1 | 1.75(3) |
| O(3)-H(3C) | 1.086(17) |

| | |
|---|---|
| C(3)-N(3)-H(3A) | 119.8(15) |
| C(3)-N(3)-H(3B) | 115.2(15) |
| H(3A)-N(3)-H(3B) | 120(2) |
| O(2)-N(5)-O(1) | 124.57(16) |
| O(2)-N(5)-C(6) | 119.57(15) |
| O(1)-N(5)-C(6) | 115.84(17) |
| C(6)-C(1)-C(10) | 115.68(14) |
| C(6)-C(1)-C(2) | 106.89(13) |
| C(10)-C(1)-C(2) | 109.95(13) |
| C(6)-C(1)-H(1) | 108.0 |
| C(10)-C(1)-H(1) | 108.0 |
| C(2)-C(1)-H(1) | 108.0 |
| C(7)-C(2)-C(8) | 110.15(14) |
| C(7)-C(2)-C(3) | 106.65(13) |
| C(8)-C(2)-C(3) | 108.81(14) |
| C(7)-C(2)-C(1) | 109.60(13) |
| C(8)-C(2)-C(1) | 107.78(14) |
| C(3)-C(2)-C(1) | 113.84(13) |
| C(4)-C(3)-N(3) | 124.58(17) |
| C(4)-C(3)-C(2) | 120.06(14) |

| | |
|---|---|
| N(3)-C(3)-C(2) | 115.08(16) |
| C(3)-C(4)-C(9) | 117.98(15) |
| C(3)-C(4)-C(5) | 126.84(15) |
| C(9)-C(4)-C(5) | 115.16(15) |
| C(4)-C(5)-C(16) | 110.34(14) |
| C(4)-C(5)-C(6) | 110.09(13) |
| C(16)-C(5)-C(6) | 116.63(14) |
| C(4)-C(5)-H(5) | 106.4 |
| C(16)-C(5)-H(5) | 106.4 |
| C(6)-C(5)-H(5) | 106.4 |
| N(5)-C(6)-C(1) | 111.10(14) |
| N(5)-C(6)-C(5) | 107.34(13) |
| C(1)-C(6)-C(5) | 115.13(13) |
| N(5)-C(6)-H(6) | 107.7 |
| C(1)-C(6)-H(6) | 107.7 |
| C(5)-C(6)-H(6) | 107.7 |
| N(1)-C(7)-C(2) | 174.4(2) |
| N(2)-C(8)-C(2) | 176.7(2) |
| N(4)-C(9)-C(4) | 179.9(3) |
| C(11)-C(10)-C(15) | 118.51(17) |
| C(11)-C(10)-C(1) | 118.83(16) |
| C(15)-C(10)-C(1) | 122.65(17) |
| C(10)-C(11)-C(12) | 121.1(2) |
| C(10)-C(11)-H(11) | 119.5 |
| C(12)-C(11)-H(11) | 119.5 |
| C(13)-C(12)-C(11) | 120.0(2) |
| C(13)-C(12)-H(12) | 120.0 |
| C(11)-C(12)-H(12) | 120.0 |
| C(14)-C(13)-C(12) | 119.6(2) |
| C(14)-C(13)-H(13) | 120.2 |
| C(12)-C(13)-H(13) | 120.2 |
| C(13)-C(14)-C(15) | 120.9(2) |
| C(13)-C(14)-H(14) | 119.5 |
| C(15)-C(14)-H(14) | 119.5 |
| C(10)-C(15)-C(14) | 119.8(2) |
| C(10)-C(15)-H(15) | 120.1 |
| C(14)-C(15)-H(15) | 120.1 |
| C(17)-C(16)-C(21) | 118.13(19) |
| C(17)-C(16)-C(5) | 122.96(16) |
| C(21)-C(16)-C(5) | 118.80(18) |
| C(18)-C(17)-C(16) | 120.9(2) |
| C(18)-C(17)-H(17) | 119.6 |
| C(16)-C(17)-H(17) | 119.6 |
| C(19)-C(18)-C(17) | 121.5(3) |
| C(19)-C(18)-H(18) | 119.2 |
| C(17)-C(18)-H(18) | 119.2 |
| C(18)-C(19)-C(20) | 119.1(2) |
| C(18)-C(19)-H(19) | 120.5 |
| C(20)-C(19)-H(19) | 120.5 |
| C(19)-C(20)-C(21) | 120.5(2) |
| C(19)-C(20)-H(20) | 119.8 |
| C(21)-C(20)-H(20) | 119.8 |
| C(16)-C(21)-C(20) | 119.9(2) |
| C(16)-C(21)-H(21) | 120.0 |
| C(20)-C(21)-H(21) | 120.0 |
| O(3)#1-O(3)-H(3C) | 115.1(19) |

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd28234.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| N(1) | 66(1) | 55(1) | 49(1) | 10(1) | 9(1) | 32(1) |
| N(2) | 51(1) | 71(1) | 53(1) | -9(1) | -14(1) | 17(1) |
| N(3) | 32(1) | 45(1) | 85(1) | -9(1) | -1(1) | 18(1) |
| N(4) | 66(1) | 57(1) | 53(1) | -7(1) | 1(1) | 39(1) |
| N(5) | 34(1) | 38(1) | 60(1) | 6(1) | -3(1) | 17(1) |
| O(1) | 40(1) | 63(1) | 76(1) | -1(1) | -23(1) | 17(1) |
| O(2) | 43(1) | 67(1) | 69(1) | 1(1) | 12(1) | 22(1) |
| C(1) | 32(1) | 35(1) | 36(1) | 3(1) | 2(1) | 16(1) |
| C(2) | 30(1) | 33(1) | 35(1) | -1(1) | -2(1) | 14(1) |
| C(3) | 31(1) | 37(1) | 38(1) | 4(1) | 1(1) | 18(1) |
| C(4) | 35(1) | 36(1) | 35(1) | 0(1) | 3(1) | 19(1) |
| C(5) | 35(1) | 37(1) | 36(1) | -6(1) | -5(1) | 16(1) |
| C(6) | 28(1) | 38(1) | 39(1) | 2(1) | -2(1) | 15(1) |
| C(7) | 36(1) | 36(1) | 40(1) | -2(1) | 1(1) | 17(1) |
| C(8) | 32(1) | 41(1) | 41(1) | 1(1) | 0(1) | 14(1) |
| C(9) | 41(1) | 41(1) | 38(1) | 0(1) | 2(1) | 20(1) |
| C(10) | 30(1) | 35(1) | 48(1) | -2(1) | 2(1) | 16(1) |
| C(11) | 59(1) | 53(1) | 49(1) | -4(1) | 1(1) | 33(1) |
| C(12) | 73(2) | 62(1) | 71(2) | -16(1) | 6(1) | 38(1) |
| C(13) | 60(1) | 51(1) | 94(2) | -2(1) | 16(1) | 35(1) |
| C(14) | 55(1) | 56(1) | 84(2) | 17(1) | 11(1) | 37(1) |
| C(15) | 45(1) | 49(1) | 55(1) | 3(1) | 3(1) | 28(1) |
| C(16) | 30(1) | 32(1) | 61(1) | -4(1) | 1(1) | 17(1) |
| C(17) | 59(1) | 42(1) | 61(1) | 8(1) | 2(1) | 21(1) |
| C(18) | 68(2) | 60(2) | 84(2) | 26(1) | 15(1) | 32(1) |
| C(19) | 51(2) | 55(2) | 133(3) | 36(2) | 27(2) | 29(1) |
| C(20) | 41(1) | 32(1) | 153(3) | -10(2) | 4(2) | 10(1) |
| C(21) | 41(1) | 45(1) | 88(2) | -16(1) | -1(1) | 18(1) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd28234.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 899 | 3796 | -499 | 41 |
| H(5) | 1283 | 4787 | 1215 | 44 |
| H(6) | 1134 | 3785 | 1060 | 43 |
| H(11) | 752 | 2918 | -1281 | 63 |
| H(12) | 878 | 2015 | -1538 | 80 |
| H(13) | 1149 | 1520 | -588 | 78 |
| H(14) | 1297 | 1930 | 612 | 73 |
| H(15) | 1145 | 2819 | 889 | 57 |
| H(17) | 1205 | 4805 | -815 | 67 |
| H(18) | 1816 | 5728 | -1535 | 85 |
| H(19) | 2513 | 6730 | -999 | 94 |
| H(20) | 2597 | 6816 | 292 | 95 |
| H(21) | 2012 | 5876 | 1041 | 71 |
| H(3A) | -999(9) | 3324(9) | 211(11) | 54(7) |
| H(3B) | -817(11) | 3946(10) | 589(13) | 73(8) |
| H(3C) | 9649(11) | 9530(11) | 9249(14) | 93(8) |

Table 6. Torsion angles [deg] for cd28234.

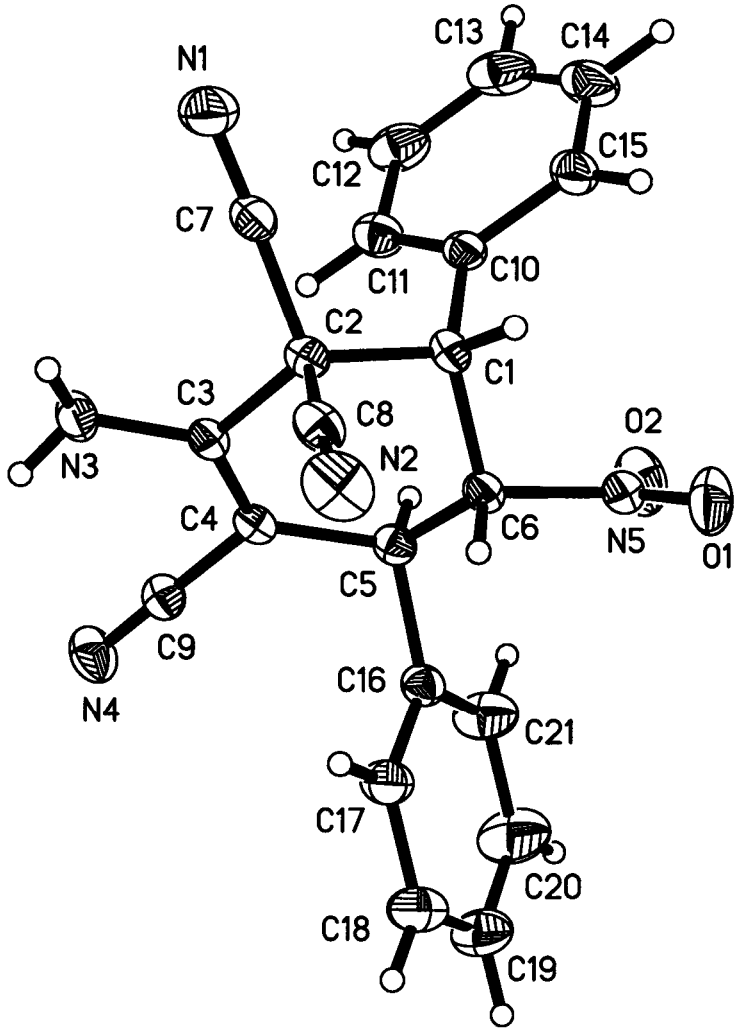
| | |
|---|---|
| C(6)-C(1)-C(2)-C(7) | -71.35(17) |
| C(10)-C(1)-C(2)-C(7) | 54.95(18) |
| C(6)-C(1)-C(2)-C(8) | 168.77(14) |
| C(10)-C(1)-C(2)-C(8) | -64.93(17) |
| C(6)-C(1)-C(2)-C(3) | 47.99(18) |
| C(10)-C(1)-C(2)-C(3) | 174.29(13) |
| C(7)-C(2)-C(3)-C(4) | 100.52(18) |
| C(8)-C(2)-C(3)-C(4) | -140.68(16) |
| C(1)-C(2)-C(3)-C(4) | -20.5(2) |
| C(7)-C(2)-C(3)-N(3) | -73.70(19) |
| C(8)-C(2)-C(3)-N(3) | 45.1(2) |
| C(1)-C(2)-C(3)-N(3) | 165.30(16) |
| N(3)-C(3)-C(4)-C(9) | -4.7(3) |
| C(2)-C(3)-C(4)-C(9) | -178.37(15) |
| N(3)-C(3)-C(4)-C(5) | 173.75(18) |
| C(2)-C(3)-C(4)-C(5) | 0.1(3) |
| C(3)-C(4)-C(5)-C(16) | 120.80(19) |
| C(9)-C(4)-C(5)-C(16) | -60.68(19) |
| C(3)-C(4)-C(5)-C(6) | -9.3(2) |
| C(9)-C(4)-C(5)-C(6) | 169.18(15) |
| O(2)-N(5)-C(6)-C(1) | 16.6(2) |
| O(1)-N(5)-C(6)-C(1) | -165.06(14) |
| O(2)-N(5)-C(6)-C(5) | -110.09(17) |
| O(1)-N(5)-C(6)-C(5) | 68.26(18) |
| C(10)-C(1)-C(6)-N(5) | 54.97(19) |
| C(2)-C(1)-C(6)-N(5) | 177.77(13) |
| C(10)-C(1)-C(6)-C(5) | 177.25(14) |
| C(2)-C(1)-C(6)-C(5) | -59.95(18) |
| C(4)-C(5)-C(6)-N(5) | 165.20(14) |
| C(16)-C(5)-C(6)-N(5) | 38.51(19) |
| C(4)-C(5)-C(6)-C(1) | 40.9(2) |
| C(16)-C(5)-C(6)-C(1) | -85.76(18) |
| C(8)-C(2)-C(7)-N(1) | -173.7(19) |
| C(3)-C(2)-C(7)-N(1) | -56(2) |
| C(1)-C(2)-C(7)-N(1) | 68(2) |
| C(7)-C(2)-C(8)-N(2) | 150(4) |
| C(3)-C(2)-C(8)-N(2) | 33(4) |
| C(1)-C(2)-C(8)-N(2) | -91(4) |
| C(3)-C(4)-C(9)-N(4) | -134(100) |
| C(5)-C(4)-C(9)-N(4) | 47(98) |
| C(6)-C(1)-C(10)-C(11) | -146.71(17) |
| C(2)-C(1)-C(10)-C(11) | 92.12(19) |
| C(6)-C(1)-C(10)-C(15) | 34.4(2) |
| C(2)-C(1)-C(10)-C(15) | -86.8(2) |
| C(15)-C(10)-C(11)-C(12) | 0.9(3) |
| C(1)-C(10)-C(11)-C(12) | -178.06(18) |
| C(10)-C(11)-C(12)-C(13) | -0.8(3) |
| C(11)-C(12)-C(13)-C(14) | -0.1(3) |
| C(12)-C(13)-C(14)-C(15) | 1.0(3) |
| C(11)-C(10)-C(15)-C(14) | 0.0(3) |
| C(1)-C(10)-C(15)-C(14) | 178.89(16) |
| C(13)-C(14)-C(15)-C(10) | -0.9(3) |
| C(4)-C(5)-C(16)-C(17) | -65.3(2) |
| C(6)-C(5)-C(16)-C(17) | 61.2(2) |
| C(4)-C(5)-C(16)-C(21) | 110.64(18) |
| C(6)-C(5)-C(16)-C(21) | -122.80(18) |
| C(21)-C(16)-C(17)-C(18) | 2.2(3) |
| C(5)-C(16)-C(17)-C(18) | 178.19(18) |
| C(16)-C(17)-C(18)-C(19) | -1.6(3) |
| C(17)-C(18)-C(19)-C(20) | -0.3(4) |
| C(18)-C(19)-C(20)-C(21) | 1.7(4) |
| C(17)-C(16)-C(21)-C(20) | -0.9(3) |
| C(5)-C(16)-C(21)-C(20) | -177.02(17) |
| C(19)-C(20)-C(21)-C(16) | -1.1(3) |

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+2

Table 7. Hydrogen bonds for cd28234 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(3)-H(3A)...O(2)#2 | 0.814(15) | 2.632(17) | 3.346(2) | 147.3(19) |

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+2 #2 x-y,x,-z




The crystal data of compound **4a-2** have been deposited in CCDC with number 688759. Empirical Formula: $C_{21}H_{15}N_5O_2$; Formula Weight: 369.38; Crystal size: 0.321 x 0.236 x 0.051; Crystal Color, Habit: colorless, prismatic; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters: a = 13.2254(13)Å, b = 11.3377(12)Å, c = 14.1441(15)Å, $\alpha = 90^o$, $\beta = 117.874(2)^o$, $\gamma = 90^o$, V = 1874.8(3)Å$^3$; Space group: P2(1)/c; Z = 4; $D_{calc} = 1.309$ g/cm$^3$; $F_{000} = 768$; R1 = 0.0561, wR2 = 0.1011. Diffractometer: Rigaku AFC7R.

Table 1. Crystal data and structure refinement for cd28232.

| | |
|---|---|
| Identification code | cd28232 |
| Empirical formula | C21 H15 N5 O2 |
| Formula weight | 369.38 |
| Temperature | 293(2) K |
| Wavelength | 0.71073 A |
| Crystal system, space group | Monoclinic, P2(1)/n |
| Unit cell dimensions | a = 13.2254(13) A alpha = 90 deg.<br>b = 11.3377(12) A beta = 117.874(2) deg.<br>c = 14.1441(15) A gamma = 90 deg. |
| Volume | 1874.8(3) A^3 |
| Z, Calculated density | 4, 1.309 Mg/m^3 |
| Absorption coefficient | 0.088 mm^-1 |
| F(000) | 768 |
| Crystal size | 0.321 x 0.236 x 0.051 mm |
| Theta range for data collection | 1.74 to 26.99 deg. |
| Limiting indices | -16<=h<=13, -10<=k<=14, -18<=l<=18 |
| Reflections collected / unique | 10802 / 4078 [R(int) = 0.0527] |
| Completeness to theta = 26.99 | 99.8 % |
| Absorption correction | Empirical |
| Max. and min. transmission | 1.00000 and 0.86356 |
| Refinement method | Full-matrix least-squares on F^2 |
| Data / restraints / parameters | 4078 / 0 / 261 |
| Goodness-of-fit on F^2 | 0.993 |
| Final R indices [I>2sigma(I)] | R1 = 0.0561, wR2 = 0.1011 |
| R indices (all data) | R1 = 0.0884, wR2 = 0.1131 |
| Largest diff. peak and hole | 0.169 and -0.162 e.A^-3 |

Table 2. Atomic coordinates ( x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd28232.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| N(1) | 2283(2) | 4290(2) | 3016(2) | 56(1) |
| N(2) | 4589(2) | 1524(2) | 3299(2) | 64(1) |
| N(3) | 1286(2) | 1756(2) | 1555(2) | 42(1) |
| N(4) | 316(2) | 408(2) | -962(1) | 53(1) |
| N(5) | 4464(2) | 3434(2) | 237(2) | 44(1) |
| O(1) | 5484(1) | 3456(2) | 830(1) | 70(1) |
| O(2) | 3994(2) | 3896(2) | -635(1) | 69(1) |
| C(1) | 3562(2) | 3655(2) | 1403(1) | 32(1) |
| C(2) | 2982(2) | 2918(2) | 1952(1) | 32(1) |
| C(3) | 1999(1) | 2131(2) | 1176(1) | 30(1) |
| C(4) | 1910(2) | 1844(2) | 215(1) | 31(1) |
| C(5) | 2662(2) | 2304(2) | -254(1) | 32(1) |
| C(6) | 3749(2) | 2804(2) | 652(1) | 33(1) |
| C(7) | 2587(2) | 3709(2) | 2546(2) | 37(1) |
| C(8) | 3871(2) | 2120(2) | 2737(2) | 39(1) |
| C(9) | 1023(2) | 1049(2) | -441(2) | 36(1) |
| C(10) | 2965(2) | 4800(2) | 903(2) | 35(1) |
| C(11) | 1797(2) | 4896(2) | 246(2) | 45(1) |
| C(12) | 1316(2) | 5976(2) | -181(2) | 58(1) |
| C(13) | 1989(3) | 6968(2) | 47(2) | 67(1) |
| C(14) | 3143(3) | 6879(2) | 693(2) | 62(1) |
| C(15) | 3635(2) | 5807(2) | 1115(2) | 47(1) |
| C(16) | 2948(2) | 1340(2) | -844(2) | 36(1) |
| C(17) | 3322(2) | 251(2) | -390(2) | 48(1) |
| C(18) | 3615(2) | -603(2) | -915(2) | 62(1) |
| C(19) | 3536(2) | -376(2) | -1893(2) | 67(1) |
| C(20) | 3159(2) | 696(3) | -2355(2) | 78(1) |
| C(21) | 2859(2) | 1553(2) | -1841(2) | 60(1) |

Table 3. Bond lengths [A] and angles [deg] for cd28232.

| | |
|---|---|
| N(1)-C(7) | 1.135(2) |
| N(2)-C(8) | 1.133(2) |
| N(3)-C(3) | 1.353(2) |
| N(3)-H(3A) | 0.88(2) |
| N(3)-H(3B) | 0.88(2) |
| N(4)-C(9) | 1.141(2) |
| N(5)-O(2) | 1.210(2) |
| N(5)-O(1) | 1.211(2) |
| N(5)-C(6) | 1.505(2) |
| C(1)-C(10) | 1.512(2) |
| C(1)-C(6) | 1.538(2) |
| C(1)-C(2) | 1.565(2) |
| C(1)-H(1) | 0.9800 |
| C(2)-C(7) | 1.481(3) |
| C(2)-C(8) | 1.487(3) |
| C(2)-C(3) | 1.535(2) |
| C(3)-C(4) | 1.349(2) |
| C(4)-C(9) | 1.425(3) |
| C(4)-C(5) | 1.522(2) |
| C(5)-C(6) | 1.518(2) |
| C(5)-C(16) | 1.526(2) |
| C(5)-H(5) | 0.9800 |
| C(6)-H(6) | 0.9800 |
| C(10)-C(11) | 1.385(3) |
| C(10)-C(15) | 1.389(2) |
| C(11)-C(12) | 1.382(3) |
| C(11)-H(11) | 0.9300 |
| C(12)-C(13) | 1.375(3) |
| C(12)-H(12) | 0.9300 |
| C(13)-C(14) | 1.368(3) |
| C(13)-H(13) | 0.9300 |
| C(14)-C(15) | 1.376(3) |
| C(14)-H(14) | 0.9300 |
| C(15)-H(15) | 0.9300 |
| C(16)-C(17) | 1.372(3) |
| C(16)-C(21) | 1.381(3) |
| C(17)-C(18) | 1.382(3) |
| C(17)-H(17) | 0.9300 |
| C(18)-C(19) | 1.362(3) |
| C(18)-H(18) | 0.9300 |
| C(19)-C(20) | 1.359(3) |
| C(19)-H(19) | 0.9300 |
| C(20)-C(21) | 1.378(3) |
| C(20)-H(20) | 0.9300 |
| C(21)-H(21) | 0.9300 |

| | |
|---|---|
| C(3)-N(3)-H(3A) | 117.6(12) |
| C(3)-N(3)-H(3B) | 121.4(14) |
| H(3A)-N(3)-H(3B) | 115.2(19) |
| O(2)-N(5)-O(1) | 124.88(18) |
| O(2)-N(5)-C(6) | 119.02(17) |
| O(1)-N(5)-C(6) | 116.08(18) |
| C(10)-C(1)-C(6) | 115.65(15) |
| C(10)-C(1)-C(2) | 114.87(14) |
| C(6)-C(1)-C(2) | 106.37(14) |
| C(10)-C(1)-H(1) | 106.4 |
| C(6)-C(1)-H(1) | 106.4 |
| C(2)-C(1)-H(1) | 106.4 |
| C(7)-C(2)-C(8) | 108.09(15) |
| C(7)-C(2)-C(3) | 110.62(14) |
| C(8)-C(2)-C(3) | 106.84(15) |
| C(7)-C(2)-C(1) | 110.03(15) |
| C(8)-C(2)-C(1) | 107.18(14) |
| C(3)-C(2)-C(1) | 113.80(14) |
| C(4)-C(3)-N(3) | 125.13(17) |
| C(4)-C(3)-C(2) | 120.42(15) |
| N(3)-C(3)-C(2) | 114.44(16) |
| C(3)-C(4)-C(9) | 117.76(16) |

| | |
|---|---|
| C(3)-C(4)-C(5) | 126.14(16) |
| C(9)-C(4)-C(5) | 116.09(15) |
| C(6)-C(5)-C(4) | 108.30(14) |
| C(6)-C(5)-C(16) | 110.51(14) |
| C(4)-C(5)-C(16) | 111.84(15) |
| C(6)-C(5)-H(5) | 108.7 |
| C(4)-C(5)-H(5) | 108.7 |
| C(16)-C(5)-H(5) | 108.7 |
| N(5)-C(6)-C(5) | 111.59(15) |
| N(5)-C(6)-C(1) | 107.71(14) |
| C(5)-C(6)-C(1) | 115.01(14) |
| N(5)-C(6)-H(6) | 107.4 |
| C(5)-C(6)-H(6) | 107.4 |
| C(1)-C(6)-H(6) | 107.4 |
| N(1)-C(7)-C(2) | 178.2(2) |
| N(2)-C(8)-C(2) | 175.4(2) |
| N(4)-C(9)-C(4) | 179.7(3) |
| C(11)-C(10)-C(15) | 118.58(19) |
| C(11)-C(10)-C(1) | 123.79(17) |
| C(15)-C(10)-C(1) | 117.63(18) |
| C(12)-C(11)-C(10) | 120.3(2) |
| C(12)-C(11)-H(11) | 119.9 |
| C(10)-C(11)-H(11) | 119.9 |
| C(13)-C(12)-C(11) | 120.5(2) |
| C(13)-C(12)-H(12) | 119.8 |
| C(11)-C(12)-H(12) | 119.8 |
| C(14)-C(13)-C(12) | 119.6(2) |
| C(14)-C(13)-H(13) | 120.2 |
| C(12)-C(13)-H(13) | 120.2 |
| C(13)-C(14)-C(15) | 120.5(2) |
| C(13)-C(14)-H(14) | 119.7 |
| C(15)-C(14)-H(14) | 119.7 |
| C(14)-C(15)-C(10) | 120.6(2) |
| C(14)-C(15)-H(15) | 119.7 |
| C(10)-C(15)-H(15) | 119.7 |
| C(17)-C(16)-C(21) | 118.38(19) |
| C(17)-C(16)-C(5) | 121.01(17) |
| C(21)-C(16)-C(5) | 120.59(18) |
| C(16)-C(17)-C(18) | 120.6(2) |
| C(16)-C(17)-H(17) | 119.7 |
| C(18)-C(17)-H(17) | 119.7 |
| C(19)-C(18)-C(17) | 120.3(2) |
| C(19)-C(18)-H(18) | 119.8 |
| C(17)-C(18)-H(18) | 119.8 |
| C(20)-C(19)-C(18) | 119.7(2) |
| C(20)-C(19)-H(19) | 120.2 |
| C(18)-C(19)-H(19) | 120.2 |
| C(19)-C(20)-C(21) | 120.5(2) |
| C(19)-C(20)-H(20) | 119.7 |
| C(21)-C(20)-H(20) | 119.7 |
| C(20)-C(21)-C(16) | 120.5(2) |
| C(20)-C(21)-H(21) | 119.8 |
| C(16)-C(21)-H(21) | 119.8 |

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd28232.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [ h^2 a*^2 U11 + ... + 2 h k a* b* U12 ]

| | U11 | U22 | U33 | U23 | U13 | U12 |
|---|---|---|---|---|---|---|
| N(1) | 79(1) | 45(1) | 59(1) | -7(1) | 43(1) | -4(1) |
| N(2) | 59(1) | 60(1) | 52(1) | 12(1) | 9(1) | 5(1) |
| N(3) | 49(1) | 42(1) | 41(1) | -8(1) | 26(1) | -17(1) |
| N(4) | 52(1) | 55(1) | 47(1) | -10(1) | 19(1) | -20(1) |
| N(5) | 50(1) | 34(1) | 59(1) | -8(1) | 36(1) | -8(1) |
| O(1) | 41(1) | 74(1) | 101(1) | -1(1) | 37(1) | -12(1) |
| O(2) | 82(1) | 73(1) | 60(1) | 13(1) | 41(1) | -18(1) |
| C(1) | 31(1) | 30(1) | 33(1) | -3(1) | 13(1) | -7(1) |
| C(2) | 36(1) | 28(1) | 30(1) | -1(1) | 15(1) | -2(1) |
| C(3) | 31(1) | 25(1) | 32(1) | 2(1) | 14(1) | -2(1) |
| C(4) | 32(1) | 26(1) | 31(1) | -1(1) | 11(1) | -2(1) |
| C(5) | 37(1) | 29(1) | 30(1) | 2(1) | 15(1) | 0(1) |
| C(6) | 36(1) | 27(1) | 36(1) | 1(1) | 18(1) | -2(1) |
| C(7) | 45(1) | 31(1) | 35(1) | -3(1) | 20(1) | -8(1) |
| C(8) | 43(1) | 36(1) | 32(1) | 0(1) | 12(1) | -6(1) |
| C(9) | 38(1) | 37(1) | 31(1) | 1(1) | 15(1) | -3(1) |
| C(10) | 50(1) | 28(1) | 34(1) | -3(1) | 27(1) | -4(1) |
| C(11) | 52(1) | 36(1) | 46(1) | 1(1) | 23(1) | 3(1) |
| C(12) | 73(2) | 53(2) | 54(2) | 11(1) | 34(1) | 23(1) |
| C(13) | 116(2) | 37(1) | 68(2) | 15(1) | 60(2) | 22(2) |
| C(14) | 106(2) | 32(1) | 72(2) | -2(1) | 61(2) | -9(1) |
| C(15) | 67(2) | 37(1) | 51(1) | -6(1) | 40(1) | -11(1) |
| C(16) | 41(1) | 34(1) | 34(1) | -5(1) | 18(1) | -4(1) |
| C(17) | 64(1) | 37(1) | 51(1) | -1(1) | 34(1) | 2(1) |
| C(18) | 76(2) | 43(1) | 76(2) | -7(1) | 43(2) | 6(1) |
| C(19) | 78(2) | 61(2) | 73(2) | -24(2) | 44(2) | 0(2) |
| C(20) | 110(2) | 86(2) | 49(2) | -10(2) | 47(2) | 13(2) |
| C(21) | 88(2) | 56(2) | 41(1) | 5(1) | 35(1) | 15(1) |

Table 5. Hydrogen coordinates ( x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd28232.

| | x | y | z | U(eq) |
|---|---|---|---|---|
| H(1) | 4324 | 3869 | 1968 | 38 |
| H(5) | 2255 | 2940 | -758 | 39 |
| H(6) | 4200 | 2138 | 1085 | 39 |
| H(11) | 1335 | 4231 | 91 | 54 |
| H(12) | 532 | 6033 | -625 | 70 |
| H(13) | 1661 | 7694 | -236 | 80 |
| H(14) | 3599 | 7549 | 848 | 75 |
| H(15) | 4422 | 5756 | 1545 | 56 |
| H(17) | 3378 | 87 | 277 | 57 |
| H(18) | 3868 | -1338 | -599 | 74 |
| H(19) | 3740 | -950 | -2242 | 81 |
| H(20) | 3102 | 851 | -3024 | 93 |
| H(21) | 2596 | 2281 | -2168 | 72 |
| H(3A) | 835(16) | 1160(18) | 1231(16) | 44(6) |
| H(3B) | 1458(17) | 1846(19) | 2230(18) | 59(7) |

Table 6. Torsion angles [deg] for cd28232.

| | |
|---|---|
| C(10)-C(1)-C(2)-C(7) | -40.9(2) |
| C(6)-C(1)-C(2)-C(7) | -170.18(14) |
| C(10)-C(1)-C(2)-C(8) | -158.18(15) |
| C(6)-C(1)-C(2)-C(8) | 72.51(17) |
| C(10)-C(1)-C(2)-C(3) | 83.92(19) |
| C(6)-C(1)-C(2)-C(3) | -45.39(19) |
| C(7)-C(2)-C(3)-C(4) | 143.89(17) |
| C(8)-C(2)-C(3)-C(4) | -98.68(19) |
| C(1)-C(2)-C(3)-C(4) | 19.4(2) |
| C(7)-C(2)-C(3)-N(3) | -37.5(2) |
| C(8)-C(2)-C(3)-N(3) | 79.96(19) |
| C(1)-C(2)-C(3)-N(3) | -161.95(16) |
| N(3)-C(3)-C(4)-C(9) | -2.5(3) |
| C(2)-C(3)-C(4)-C(9) | 175.99(16) |
| N(3)-C(3)-C(4)-C(5) | 176.55(17) |
| C(2)-C(3)-C(4)-C(5) | -5.0(3) |
| C(3)-C(4)-C(5)-C(6) | 18.4(2) |
| C(9)-C(4)-C(5)-C(6) | -162.53(16) |
| C(3)-C(4)-C(5)-C(16) | 140.43(18) |
| C(9)-C(4)-C(5)-C(16) | -40.5(2) |
| O(2)-N(5)-C(6)-C(5) | 29.3(2) |
| O(1)-N(5)-C(6)-C(5) | -152.22(17) |
| O(2)-N(5)-C(6)-C(1) | -97.8(2) |
| O(1)-N(5)-C(6)-C(1) | 80.6(2) |
| C(4)-C(5)-C(6)-N(5) | -171.84(14) |
| C(16)-C(5)-C(6)-N(5) | 65.33(19) |
| C(4)-C(5)-C(6)-C(1) | -48.8(2) |
| C(16)-C(5)-C(6)-C(1) | -171.61(15) |
| C(10)-C(1)-C(6)-N(5) | 59.6(2) |
| C(2)-C(1)-C(6)-N(5) | -171.57(15) |
| C(10)-C(1)-C(6)-C(5) | -65.5(2) |
| C(2)-C(1)-C(6)-C(5) | 63.32(19) |
| C(8)-C(2)-C(7)-N(1) | -46(7) |
| C(3)-C(2)-C(7)-N(1) | 70(7) |
| C(1)-C(2)-C(7)-N(1) | -163(7) |
| C(7)-C(2)-C(8)-N(2) | -137(3) |
| C(3)-C(2)-C(8)-N(2) | 104(3) |
| C(1)-C(2)-C(8)-N(2) | -18(3) |
| C(3)-C(4)-C(9)-N(4) | -70(40) |
| C(5)-C(4)-C(9)-N(4) | 111(40) |
| C(6)-C(1)-C(10)-C(11) | 77.2(2) |
| C(2)-C(1)-C(10)-C(11) | -47.4(2) |
| C(6)-C(1)-C(10)-C(15) | -102.46(19) |
| C(2)-C(1)-C(10)-C(15) | 132.98(17) |
| C(15)-C(10)-C(11)-C(12) | -0.4(3) |
| C(1)-C(10)-C(11)-C(12) | -179.99(18) |
| C(10)-C(11)-C(12)-C(13) | -0.4(3) |
| C(11)-C(12)-C(13)-C(14) | 0.6(4) |
| C(12)-C(13)-C(14)-C(15) | 0.0(3) |
| C(13)-C(14)-C(15)-C(10) | -0.8(3) |
| C(11)-C(10)-C(15)-C(14) | 1.0(3) |
| C(1)-C(10)-C(15)-C(14) | -179.37(18) |
| C(6)-C(5)-C(16)-C(17) | 73.3(2) |
| C(4)-C(5)-C(16)-C(17) | -47.5(2) |
| C(6)-C(5)-C(16)-C(21) | -105.3(2) |
| C(4)-C(5)-C(16)-C(21) | 133.99(19) |
| C(21)-C(16)-C(17)-C(18) | 0.8(3) |
| C(5)-C(16)-C(17)-C(18) | -177.79(18) |
| C(16)-C(17)-C(18)-C(19) | 0.0(3) |
| C(17)-C(18)-C(19)-C(20) | -0.5(4) |
| C(18)-C(19)-C(20)-C(21) | 0.2(4) |
| C(19)-C(20)-C(21)-C(16) | 0.5(4) |
| C(17)-C(16)-C(21)-C(20) | -1.0(3) |
| C(5)-C(16)-C(21)-C(20) | 177.5(2) |

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd28232 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| N(3)-H(3A)...N(4)#1 | 0.88(2) | 2.26(2) | 3.091(3) | 159.6(17) |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z