Supplementary Material (ESI) for Chemical Communications

Sorting of polymorphs based on mechanical properties.

Trimorphs of 6-chloro-2,4-dinitroaniline

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Supplementary Material (ESI)
(7 pages)

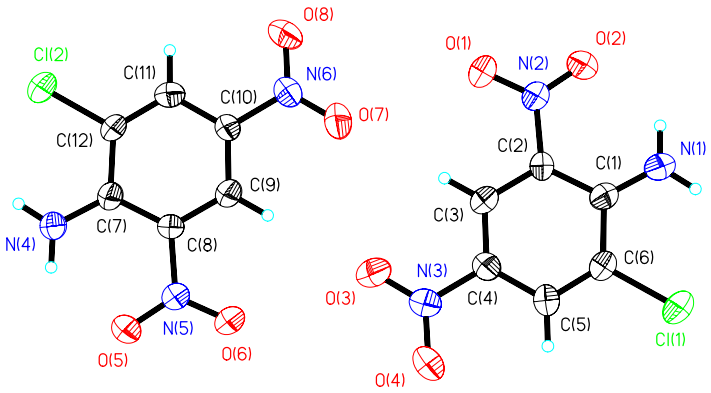

Fig. 1 ORTEP diagram for Form **I**.

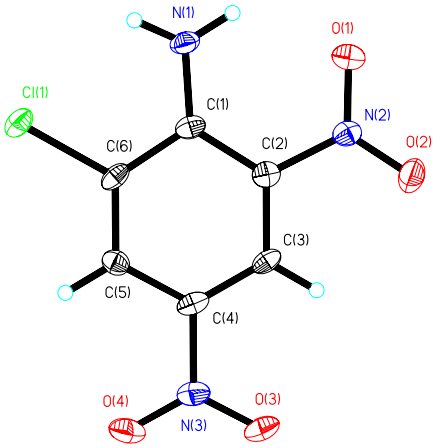

Fig. 2 ORTEP diagram for Form **II**.

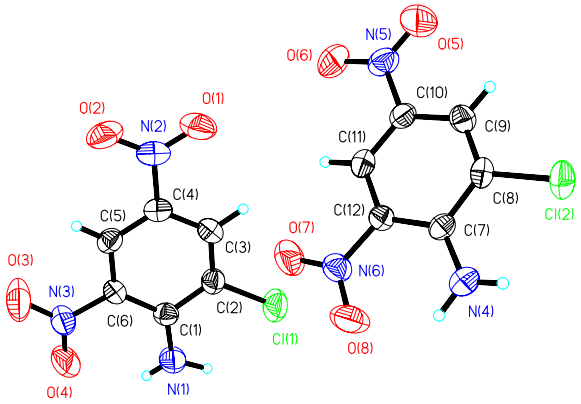

Fig. 3 ORTEP diagram for Form **III**.

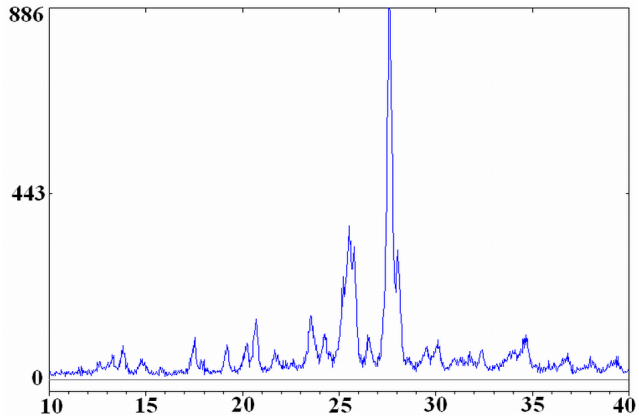

Fig. **4** PXRD pattern of mixture of Forms I and III obtained by grinding the chunky crystals from CH_2Cl_2. Note that lines corresponding to both the forms are observed.

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Form-I. PXRD overlay coordinates.

```
CELL   11.3606   18.3200    7.9469    90.000    90.492    90.000
Cl1     17   -0.2085    0.8745    0.0022    1.0000    4.9733
O1       8    0.2100    0.9536    0.4268    1.0000    5.3890
O2       8    0.0797    1.0296    0.3591    1.0000    5.6635
O3       8    0.1687    0.7010    0.3748    1.0000    5.2273
O4       8    0.0335    0.6569    0.2098    1.0000    5.3475
N1       7   -0.0841    0.9889    0.1556    1.0000    4.1473
H1A      1   -0.0532    1.0261    0.2007    1.0000    7.1724
H1B      1   -0.1470    0.9913    0.0939    1.0000    5.2980
N2       7    0.1168    0.9682    0.3586    1.0000    3.8240
N3       7    0.0825    0.7076    0.2781    1.0000    3.6597
C1       6   -0.0345    0.9222    0.1812    1.0000    3.0716
C2       6    0.0543    0.9085    0.2794    1.0000    2.9887
C3       6    0.0968    0.8387    0.3154    1.0000    3.1582
H3       1    0.1617    0.8316    0.3742    1.0000    3.1338
C4       6    0.0378    0.7800    0.2414    1.0000    3.1206
C5       6   -0.0435    0.7897    0.1378    1.0000    3.2950
H5       1   -0.0807    0.7494    0.0837    1.0000    4.1650
C6       6   -0.0853    0.8582    0.1147    1.0000    3.2195
Cl2     17    0.7253    0.6450    0.9852    1.0000    4.5119
O5       8    0.4060    0.4822    0.6352    1.0000    6.8336
O6       8    0.2839    0.5593    0.5313    1.0000    5.0344
O7       8    0.3401    0.8172    0.5834    1.0000    4.9994
O8       8    0.4725    0.8616    0.7531    1.0000    5.2951
N4       7    0.5900    0.5286    0.8349    1.0000    3.9854
H4A      1    0.5557    0.4896    0.7973    1.0000    5.6786
H4B      1    0.6520    0.5252    0.8987    1.0000    4.1594
N5       7    0.3788    0.5483    0.6218    1.0000    3.9717
N6       7    0.4221    0.8105    0.6848    1.0000    3.5602
C7       6    0.5471    0.5949    0.7969    1.0000    2.9530
C8       6    0.4466    0.6083    0.6947    1.0000    3.0353
C9       6    0.4052    0.6779    0.6581    1.0000    2.9830
H9       1    0.3382    0.6843    0.5902    1.0000    3.2672
C10      6    0.4644    0.7372    0.7229    1.0000    2.8896
C11      6    0.5641    0.7279    0.8248    1.0000    3.2869
H11      1    0.6039    0.7686    0.8680    1.0000    4.4784
C12      6    0.6033    0.6593    0.8611    1.0000    3.1114
RGNR   14
TITL grd57a                          P21/c
CELL  0.71073   11.2850   18.2200    7.8860    90.000    90.440
90.000
ZERR 1           0.0030    0.0030    0.0080     0.000     0.040
0.000
LATT 1
SYMM - X ,    0.50000 + Y ,    0.50000 - Z
SFAC C  H  Cl N  O
UNIT 6 4 1 3 4
L.S. 4
ACTA
```

```
BOND $H
FMAP 2
PLAN 6
WGHT  0.042400  0.311800
FVAR  0.135660
Cl1    3  -0.217382  0.876156 -0.010426 11.000000  0.052150  0.058430 =
           0.077830 -0.000960 -0.035590 -0.000880
O1     5   0.218820  0.959075  0.439434 11.000000  0.058590  0.050500 =
           0.094980  0.010060 -0.044270 -0.003730
O2     5   0.083261  1.035132  0.367352 11.000000  0.067960  0.033900 =
           0.112690  0.004490 -0.040680 -0.003860
O3     5   0.175344  0.704775  0.378122 11.000000  0.066000  0.050640 =
           0.081450  0.002910 -0.033550 -0.014470
O4     5   0.041187  0.660593  0.212256 11.000000  0.082850  0.032800 =
           0.087110  0.006940 -0.026690  0.004140
N1     4  -0.092923  0.993060  0.168288 11.000000  0.049980  0.039620 =
           0.067620 -0.003990 -0.022920 -0.004500
AFIX 3
H1A    2  -0.062023  1.031619  0.213389 11.000000  0.090840
H1B    2  -0.155823  0.996820  0.106588 11.000000  0.067100
AFIX 0
N2     4   0.124543  0.973438  0.371263 11.000000  0.042440  0.038850 =
           0.063690  0.002170 -0.020180 -0.000200
N3     4   0.091268  0.712117  0.282177 11.000000  0.050190  0.034900 =
           0.053840 -0.000900 -0.007460 -0.004520
C1     1  -0.043389  0.927726  0.193889 11.000000  0.039490  0.037210 =
           0.039870 -0.004360 -0.008680 -0.000870
C2     1   0.059378  0.913468  0.291891 11.000000  0.037690  0.031770 =
           0.043920  0.003480 -0.011230  0.004220
C3     1   0.103231  0.843959  0.320089 11.000000  0.034950  0.040430 =
           0.044440  0.000370 -0.011220 -0.003330
AFIX 3
H3     2   0.170531  0.837099  0.386890 11.000000  0.039690
AFIX 0
C4     1   0.046651  0.785537  0.249012 11.000000  0.046570  0.031700 =
           0.040200  0.000870 -0.006000 -0.000250
C5     1  -0.052340  0.795137  0.145960 11.000000  0.044750  0.036370 =
           0.043930  0.005740 -0.008980  0.003980
AFIX 3
H5     2  -0.089540  0.754878  0.096360 11.000000  0.052750
AFIX 0
```

Form-III. PXRD overlay coordinates.

```
CELL   7.9551    8.9268   12.9862    89.482    85.667    63.936
C1       6    0.9986    0.7358    0.0031    1.0000    3.1131
C2       6    0.9397    0.7453    0.1012    1.0000    3.5852
C3       6    0.7748    0.8805    0.1363    1.0000    3.4929
C4       6    0.6759    1.0068    0.0749    1.0000    3.2046
C5       6    0.7528    0.9996   -0.0150    1.0000    3.3757
C6       6    0.9108    0.8687   -0.0498    1.0000    3.1695
```

```
Cl1     17    1.0262    0.5962    0.1905    1.0000    5.7932
N1       7    1.1581    0.5964   -0.0143    1.0000    4.3013
N2       7    0.5191    1.1499    0.1152    1.0000    3.8692
N3       7    0.9798    0.8748   -0.1562    1.0000    4.4368
O1       8    0.4530    1.1521    0.2038    1.0000    5.4693
O2       8    0.4319    1.2596    0.0475    1.0000    5.2560
O3       8    0.8921    0.9916   -0.2080    1.0000    8.0503
O4       8    1.1177    0.7634   -0.1887    1.0000    6.2668
C7       6    0.3127    0.5800    0.4136    1.0000    2.8758
C8       6    0.2266    0.6515    0.5125    1.0000    3.4850
C9       6    0.2071    0.8025    0.5468    1.0000    3.3871
C10      6    0.2730    0.8921    0.4820    1.0000    3.2177
C11      6    0.3590    0.8325    0.3858    1.0000    3.5370
C12      6    0.3787    0.6788    0.3532    1.0000    2.9748
Cl2     17    0.1478    0.5367    0.5931    1.0000    5.4516
N4       7    0.3293    0.4320    0.3861    1.0000    4.0921
N5       7    0.2536    1.0423    0.5166    1.0000    4.2933
N6       7    0.4751    0.6207    0.2515    1.0000    3.7359
O5       8    0.1821    1.0931    0.6029    1.0000    6.5641
O6       8    0.3095    1.1200    0.4570    1.0000    6.7571
O7       8    0.5346    0.7072    0.2032    1.0000    6.4185
O8       8    0.4954    0.4869    0.2174    1.0000    5.4848
H1A      1    1.2319    0.5180    0.0199    1.0000    6.4642
H1B      1    1.2032    0.5927   -0.0705    1.0000    5.4038
H3       1    0.7309    0.9097    0.2058    1.0000    4.0781
H5       1    0.6998    1.0827   -0.0550    1.0000    3.3801
H4A      1    0.2773    0.3720    0.4197    1.0000    4.2905
H4B      1    0.3772    0.3767    0.3180    1.0000    5.2814
H9       1    0.1395    0.8298    0.6029    1.0000    3.2064
H11      1    0.3954    0.8790    0.3348    1.0000    3.8791
RGNR   2
TITL grd56 in P -1
CELL  0.71073   7.9465   8.9166  12.9801   89.352   85.575   63.978
ZERR     2.00   0.0012   0.0028   0.0042    0.026    0.019    0.015
LATT 1
SFAC C  H  Cl N  O
UNIT 12 8 2 6 8
MERG 2
L.S. 4
ACTA
BOND $H
FMAP 2
PLAN 5
FREE C8   H9
FREE C12  H11
FREE C2   H3
WGHT  0.044900  0.346500
FVAR  1.372370
MOLE 1
C1     1   1.011185  0.740537  0.005769 11.000000  0.033380  0.034780 =
           0.036630 -0.002290 -0.002820 -0.012080
```

```
C2      1   0.927152  0.756509  0.108868 11.000000  0.039340  0.038620 =
            0.035310  0.004700 -0.005460 -0.015570
C3      1   0.767478  0.891082  0.144011 11.000000  0.040620  0.043800 =
            0.032500 -0.004270  0.001370 -0.019090
C4      1   0.678149  1.018010  0.077216 11.000000  0.034280  0.034150 =
            0.042800 -0.005250 -0.001840 -0.012790
C5      1   0.748200  1.010814 -0.022758 11.000000  0.037110  0.031990 =
            0.040890  0.002930 -0.009480 -0.013850
C6      1   0.911303  0.874735 -0.057517 11.000000  0.036570  0.038480 =
            0.028220 -0.000520 -0.001430 -0.017030
Cl1     3   1.038809  0.597523  0.191364 11.000000  0.060550  0.059160 =
            0.049700  0.020640 -0.005720 -0.008270
N1      4   1.170685  0.607604 -0.022048 11.000000  0.046160  0.046190 =
            0.045390  0.001840  0.005940 -0.002470
N2      4   0.506496  1.161156  0.113741 11.000000  0.043310  0.038690 =
            0.057850 -0.012120  0.002390 -0.013510
N3      4   0.980053  0.878193 -0.163930 11.000000  0.046340  0.055780 =
            0.036630  0.005260 -0.002290 -0.020180
O1      5   0.445309  1.163356  0.202984 11.000000  0.068650  0.056880 =
            0.065570 -0.016570  0.024550 -0.016460
O2      5   0.429995  1.270810  0.053103 11.000000  0.060870  0.040930 =
            0.076770 -0.002130 -0.011450  0.005610
O3      5   0.890139  0.995158 -0.215704 11.000000  0.071670  0.101100 =
            0.052840  0.035990 -0.004510 -0.015270
O4      5   1.130260  0.766897 -0.196395 11.000000  0.079480  0.074940 =
            0.043720 -0.000870  0.019090 -0.006850
C7      1   0.313461  0.580631  0.414060 11.000000  0.028360  0.027340 =
            0.036850  0.004090 -0.007290 -0.009950
C8      1   0.227257  0.652134  0.513017 11.000000  0.034460  0.036880 =
            0.033530  0.010620 -0.006440 -0.018040
```