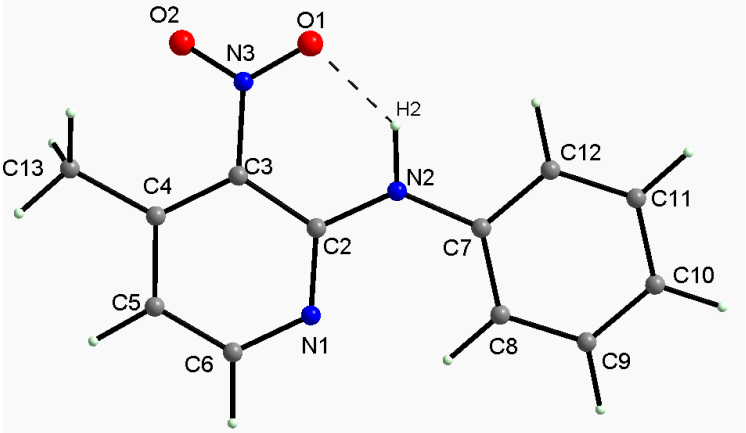
Supplementary Materials

Structure and optical properties of new 2-N-phenylamino-methyl-nitro-pyridine isomers

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Table S1. Optimized parameters (Å,°) for 2-*N*-phenylamino-3-nitro-4-methylpyridine (PA3N4MP- **1**).



N3–O1	1.242	N3–O2	1.226	N1–C2	1.343
C2–C3	1.443	C3–N3	1.454	C3–C4	1.410
C4–C13	1.508	C4–C5	1.394	C5–C6	1.390
C6–N1	1.325	C2–N2	1.360	N2–C7	1.411
C7–C8	1.401	C8–C9	1.394	C9–C10	1.392
C10–C11	1.395	C11–C12	1.388	C12–C7	1.406
C5–H5	1.082	C6–H6	1.087	C8–H8	1.077
C9–H9	1.084	C10–H10	1.084	C11–H11	1.084
C12–H12	1.085	C13–H13A	1.091	C13–H13B	1.091
C13–H13C	1.091				

O1–N3–O2	122.37	O1–N3–C3	118.78	N1–C2–C3	120.12
C2–C3–C4	120.07	C3–C4–C13	125.11	C3–C4–C5	116.76
C4–C5–C6	119.52	C5–C6–N1	124.30	C6–N1–C2	119.08
N1–C2–N2	118.28	C2–N2–H2	113.16	C7–N2–H2	115.16
C2–N2–C7	131.64	N2–C7–C8	125.50	C7–C8–C9	119.52
C8–C9–C10	121.39	C9–C10–C11	119.04	C10–C11–C12	120.27
C12–C7–N2	120.75				

N2–C2–C3–N3	5.17	C2–C3–N3–O1	-25.14	C2–C3–N3–O2	154.28
C2–C3–C4–C13	176.42	C3–C4–C5–C6	-1.43	C4–C5–C6–N1	2.70
C5–C6–N1–C2	-0.21	C6–N1–C2–N2	177.35	N1–C2–N2–C7	5.59
C2–N2–C7–C12	-171.16	C2–N2–C7–C8	10.44	N2–C7–C8–C9	178.41
C7–C8–C9–C10	0.01	C8–C9–C10–C11	-0.09	C9–C10–C11–C12	0.08
C10–C11–C12–C7	0.01				

Intramolecular hydrogen bond

N2–H2	1.014	H2···O1	1.814	N2···O1	2.632	N2–H2···O1	135.17

Angle between the plane of NO_2 (O1N3O2)and the plane of pyridine ring(N1,C2-C6) 25.50

Angle between the plane of pyridine ring (N1,C2-C6) and the plane of phenyl ring (C7-C12) 15.70

Optimization completed.

Optimized Parameters
(Angstroms and Degrees)

Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3431	-DE/DX = 0.0
R2	R(1,7)	1.3251	-DE/DX = 0.0
R3	R(2,3)	1.4433	-DE/DX = 0.0
R4	R(2,9)	1.3599	-DE/DX = 0.0
R5	R(3,4)	1.41	-DE/DX = 0.0
R6	R(3,22)	1.454	-DE/DX = 0.0
R7	R(4,5)	1.3939	-DE/DX = 0.0
R8	R(4,25)	1.5078	-DE/DX = 0.0
R9	R(5,6)	1.0824	-DE/DX = 0.0
R10	R(5,7)	1.3895	-DE/DX = 0.0
R11	R(7,8)	1.0872	-DE/DX = 0.0
R12	R(9,10)	1.0141	-DE/DX = 0.0
R13	R(9,11)	1.4115	-DE/DX = 0.0
R14	R(11,12)	1.4013	-DE/DX = 0.0
R15	R(11,20)	1.4056	-DE/DX = 0.0
R16	R(12,13)	1.0772	-DE/DX = 0.0
R17	R(12,14)	1.394	-DE/DX = 0.0
R18	R(14,15)	1.0845	-DE/DX = 0.0
R19	R(14,16)	1.3922	-DE/DX = 0.0
R20	R(16,17)	1.0836	-DE/DX = 0.0
R21	R(16,18)	1.3949	-DE/DX = 0.0
R22	R(18,19)	1.0841	-DE/DX = 0.0
R23	R(18,20)	1.3882	-DE/DX = 0.0
R24	R(20,21)	1.0854	-DE/DX = 0.0
R25	R(22,23)	1.2421	-DE/DX = 0.0
R26	R(22,24)	1.2256	-DE/DX = 0.0
R27	R(25,26)	1.0906	-DE/DX = 0.0
R28	R(25,27)	1.0909	-DE/DX = 0.0
R29	R(25,28)	1.0913	-DE/DX = 0.0
A1	A(2,1,7)	119.0782	-DE/DX = 0.0
A2	A(1,2,3)	120.1217	-DE/DX = 0.0
A3	A(1,2,9)	118.2802	-DE/DX = 0.0
A4	A(3,2,9)	121.5947	-DE/DX = 0.0
A5	A(2,3,4)	120.0706	-DE/DX = 0.0
A6	A(2,3,22)	120.7344	-DE/DX = 0.0
A7	A(4,3,22)	119.18	-DE/DX = 0.0
A8	A(3,4,5)	116.7545	-DE/DX = 0.0
A9	A(3,4,25)	125.1081	-DE/DX = 0.0
A10	A(5,4,25)	118.1178	-DE/DX = 0.0
A11	A(4,5,6)	120.1629	-DE/DX = 0.0
A12	A(4,5,7)	119.5174	-DE/DX = 0.0
A13	A(6,5,7)	120.3193	-DE/DX = 0.0
A14	A(1,7,5)	124.2995	-DE/DX = 0.0
A15	A(1,7,8)	115.645	-DE/DX = 0.0
A16	A(5,7,8)	120.0493	-DE/DX = 0.0
A17	A(2,9,10)	113.1558	-DE/DX = 0.0
A18	A(2,9,11)	131.6388	-DE/DX = 0.0
A19	A(10,9,11)	115.1574	-DE/DX = 0.0
A20	A(9,11,12)	125.4979	-DE/DX = 0.0
A21	A(9,11,20)	115.4508	-DE/DX = 0.0
A22	A(12,11,20)	119.0324	-DE/DX = 0.0
A23	A(11,12,13)	119.8023	-DE/DX = 0.0
A24	A(11,12,14)	119.5209	-DE/DX = 0.0

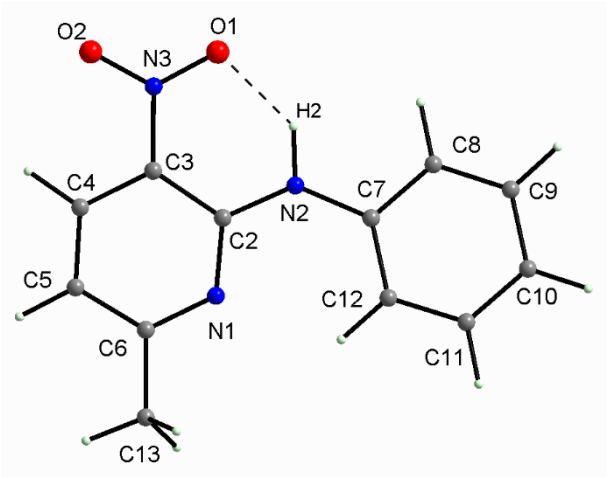
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! A25   A(13,12,14)          120.6735         -DE/DX =    0.0               !
! A26   A(12,14,15)          118.7241         -DE/DX =    0.0               !
! A27   A(12,14,16)          121.393          -DE/DX =    0.0               !
! A28   A(15,14,16)          119.8829         -DE/DX =    0.0               !
! A29   A(14,16,17)          120.5271         -DE/DX =    0.0               !
! A30   A(14,16,18)          119.0376         -DE/DX =    0.0               !
! A31   A(17,16,18)          120.4353         -DE/DX =    0.0               !
! A32   A(16,18,19)          120.3333         -DE/DX =    0.0               !
! A33   A(16,18,20)          120.2678         -DE/DX =    0.0               !
! A34   A(19,18,20)          119.3989         -DE/DX =    0.0               !
! A35   A(11,20,18)          120.7482         -DE/DX =    0.0               !
! A36   A(11,20,21)          119.4476         -DE/DX =    0.0               !
! A37   A(18,20,21)          119.8042         -DE/DX =    0.0               !
! A38   A(3,22,23)           118.7806         -DE/DX =    0.0               !
! A39   A(3,22,24)           118.8503         -DE/DX =    0.0               !
! A40   A(23,22,24)          122.3665         -DE/DX =    0.0               !
! A41   A(4,25,26)           112.2736         -DE/DX =    0.0               !
! A42   A(4,25,27)           109.1538         -DE/DX =    0.0               !
! A43   A(4,25,28)           111.0073         -DE/DX =    0.0               !
! A44   A(26,25,27)          108.9673         -DE/DX =    0.0               !
! A45   A(26,25,28)          106.4724         -DE/DX =    0.0               !
! A46   A(27,25,28)          108.8769         -DE/DX =    0.0               !
! D1    D(7,1,2,3)            -3.308          -DE/DX =    0.0               !
! D2    D(7,1,2,9)           177.3526         -DE/DX =    0.0               !
! D3    D(2,1,7,5)            -0.2091         -DE/DX =    0.0               !
! D4    D(2,1,7,8)          -179.2963         -DE/DX =    0.0               !
! D5    D(1,2,3,4)             4.4355         -DE/DX =    0.0               !
! D6    D(1,2,3,22)         -174.1435         -DE/DX =    0.0               !
! D7    D(9,2,3,4)          -176.2474         -DE/DX =    0.0               !
! D8    D(9,2,3,22)            5.1736         -DE/DX =    0.0               !
! D9    D(1,2,9,10)         -171.7174         -DE/DX =    0.0               !
! D10   D(1,2,9,11)            5.5916         -DE/DX =    0.0               !
! D11   D(3,2,9,10)            8.9534         -DE/DX =    0.0               !
! D12   D(3,2,9,11)         -173.7376         -DE/DX =    0.0               !
! D13   D(2,3,4,5)             -1.9342         -DE/DX =    0.0               !
! D14   D(2,3,4,25)           176.4201         -DE/DX =    0.0               !
! D15   D(22,3,4,5)           176.6669         -DE/DX =    0.0               !
! D16   D(22,3,4,25)           -4.9788         -DE/DX =    0.0               !
! D17   D(2,3,22,23)          -25.1423         -DE/DX =    0.0               !
! D18   D(2,3,22,24)          154.2841         -DE/DX =    0.0               !
! D19   D(4,3,22,23)          156.2662         -DE/DX =    0.0               !
! D20   D(4,3,22,24)          -24.3074         -DE/DX =    0.0               !
! D21   D(3,4,5,6)            178.8134         -DE/DX =    0.0               !
! D22   D(3,4,5,7)             -1.4303         -DE/DX =    0.0               !
! D23   D(25,4,5,6)             0.3398         -DE/DX =    0.0               !
! D24   D(25,4,5,7)          -179.9039         -DE/DX =    0.0               !
! D25   D(3,4,25,26)          -43.4482         -DE/DX =    0.0               !
! D26   D(3,4,25,27)         -164.3845         -DE/DX =    0.0               !
! D27   D(3,4,25,28)           75.5983         -DE/DX =    0.0               !
! D28   D(5,4,25,26)          134.8856         -DE/DX =    0.0               !
! D29   D(5,4,25,27)           13.9494         -DE/DX =    0.0               !
! D30   D(5,4,25,28)         -106.0678         -DE/DX =    0.0               !
! D31   D(4,5,7,1)              2.6968         -DE/DX =    0.0               !
! D32   D(4,5,7,8)           -178.2539         -DE/DX =    0.0               !
! D33   D(6,5,7,1)           -177.5473         -DE/DX =    0.0               !
! D34   D(6,5,7,8)              1.502          -DE/DX =    0.0               !
! D35   D(2,9,11,12)           10.4439         -DE/DX =    0.0               !
! D36   D(2,9,11,20)         -171.1634         -DE/DX =    0.0               !
! D37   D(10,9,11,12)        -172.2896         -DE/DX =    0.0               !
```

! D38	D(10,9,11,20)	6.1031	-DE/DX =	0.0 !
! D39	D(9,11,12,13)	-2.239	-DE/DX =	0.0 !
! D40	D(9,11,12,14)	178.4122	-DE/DX =	0.0 !
! D41	D(20,11,12,13)	179.4209	-DE/DX =	0.0 !
! D42	D(20,11,12,14)	0.0721	-DE/DX =	0.0 !
! D43	D(9,11,20,18)	-178.583	-DE/DX =	0.0 !
! D44	D(9,11,20,21)	1.3493	-DE/DX =	0.0 !
! D45	D(12,11,20,18)	-0.0796	-DE/DX =	0.0 !
! D46	D(12,11,20,21)	179.8527	-DE/DX =	0.0 !
! D47	D(11,12,14,15)	179.9762	-DE/DX =	0.0 !
! D48	D(11,12,14,16)	0.0134	-DE/DX =	0.0 !
! D49	D(13,12,14,15)	0.6332	-DE/DX =	0.0 !
! D50	D(13,12,14,16)	-179.3296	-DE/DX =	0.0 !
! D51	D(12,14,16,17)	179.9199	-DE/DX =	0.0 !
! D52	D(12,14,16,18)	-0.0921	-DE/DX =	0.0 !
! D53	D(15,14,16,17)	-0.0424	-DE/DX =	0.0 !
! D54	D(15,14,16,18)	179.9455	-DE/DX =	0.0 !
! D55	D(14,16,18,19)	-179.9205	-DE/DX =	0.0 !
! D56	D(14,16,18,20)	0.0845	-DE/DX =	0.0 !
! D57	D(17,16,18,19)	0.0674	-DE/DX =	0.0 !
! D58	D(17,16,18,20)	-179.9276	-DE/DX =	0.0 !
! D59	D(16,18,20,11)	0.0008	-DE/DX =	0.0 !
! D60	D(16,18,20,21)	-179.9313	-DE/DX =	0.0 !
! D61	D(19,18,20,11)	-179.9943	-DE/DX =	0.0 !
! D62	D(19,18,20,21)	0.0736	-DE/DX =	0.0 !

Optimized Parameters (xyz)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.030221	-0.020182	-0.040740
2	6	0	1.307905	-0.115503	0.025014
3	6	0	1.938112	-1.410661	0.117796
4	6	0	1.157832	-2.582822	0.045574
5	6	0	-0.220440	-2.412747	-0.074133
6	1	0	-0.869997	-3.274990	-0.153311
7	6	0	-0.753428	-1.129574	-0.085855
8	1	0	-1.829340	-0.987560	-0.150237
9	7	0	2.036882	1.032505	0.015347
10	1	0	3.034606	0.870658	-0.066742
11	6	0	1.649899	2.389463	0.048902
12	6	0	0.356052	2.860417	0.309279
13	1	0	-0.446477	2.159989	0.469585
14	6	0	0.119059	4.233711	0.344462
15	1	0	-0.887173	4.583940	0.546711
16	6	0	1.142268	5.152032	0.125718
17	1	0	0.942008	6.216588	0.155053
18	6	0	2.430136	4.682142	-0.131733
19	1	0	3.242859	5.378656	-0.303792
20	6	0	2.682471	3.317631	-0.169992
21	1	0	3.687706	2.960276	-0.369881
22	7	0	3.373801	-1.525903	0.316797
23	8	0	4.105586	-0.592906	-0.053031
24	8	0	3.817431	-2.534856	0.852755
25	6	0	1.702360	-3.988811	0.052611
26	1	0	2.577155	-4.096528	-0.589719
27	1	0	0.925781	-4.675112	-0.287900
28	1	0	2.017108	-4.281444	1.055771

Table S2. Optimized parameters (Å,°) for 2-N-phenylamino-3-nitro-6-methylpyridine, $C_{12}H_{11}N_3O_2$ (PA3N6MP - **2**)



N3–O1	1.243	N3–O2	1.226	N1–C2	1.344
C2–C3	1.438	C3–N3	1.450	C3–C4	1.393
C4–C5	1.380	C5–C6	1.404	C6–N1	1.331
C6–C13	1.505	C2–N2	1.358	N2–C7	1.410
C7–C8	1.406	C8–C9	1.388	C9–C10	1.395
C10–C11	1.392	C11–C12	1.394	C12–C7	1.401
C4–H4	1.081	C5–H5	1.082	C8–H8	1.085
C9–H9	1.084	C10–H10	1.084	C11–H11	1.084
C12–H12	1.077	C13–H13A	1.093	C13–H13B	1.091
C13–H13C	1.093				

O1–N3–O2	122.61	O1–N3–C3	118.69	N1–C2–C3	119.38
C2–C3–C4	118.92	C3–C4–C5	120.01	C4–C5–C6	118.13
C5–C6–C13	121.31	C5–C6–N1	122.47	C13–C6–N1	116.21
N1–C2–N2	119.23	C2–N2–C7	132.24	C2–N2–H2	112.41
N2–C7–C8	115.37	C7–C8–C9	120.74	C8–C9–C10	120.29
C9–C10–C11	119.03	C10–C11–C12	121.41	C11–C12–C7	119.52
C12–C7–C8	119.02	C12–C7–N2	125.59		

N2–C2–C3–N3	0.01	C2–C3–N3–O1	0.01	C2–C3–N3–O2	-179.99
C2–C3–C4–C5	0.00	C3–C4–C5–C6	-0.01	C4–C5–C6–N1	0.01
C5–C6–N1–C2	0.00	C6–N1–C2–N2	179.99	N1–C2–N2–C7	0.01
C2–N2–C7–C8	179.99	N2–C7–C8–C9	179.99	C7–C8–C9–C10	0.00
C8–C9–C10–C11	0.00	C9–C10–C11–C12	0.00	C10–C11–C12–C7	0.00

intramolecular hydrogen bond

N2–H2	1.016	H2···O1	1.818	N2···O1	2.649	N2–H2···O1	136.58

The conformation of the whole molecule is planar (without H atoms of CH_3).

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Optimization completed.

                          ----------------------------
                          !   Optimized Parameters   !
                          ! (Angstroms and Degrees)  !
 --------------------------                            --------------------------
 ! Name  Definition              Value          Derivative Info.                !
 --------------------------------------------------------------------------------
 ! R1    R(1,2)                  1.3439         -DE/DX =    0.0                 !
 ! R2    R(1,8)                  1.3314         -DE/DX =    0.0                 !
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! R3    R(2,3)                1.4376         -DE/DX =    0.0               !
! R4    R(2,9)                1.3578         -DE/DX =    0.0               !
! R5    R(3,4)                1.3931         -DE/DX =    0.0               !
! R6    R(3,22)               1.4502         -DE/DX =    0.0               !
! R7    R(4,5)                1.0814         -DE/DX =    0.0               !
! R8    R(4,6)                1.3804         -DE/DX =    0.0               !
! R9    R(6,7)                1.0819         -DE/DX =    0.0               !
! R10   R(6,8)                1.4035         -DE/DX =    0.0               !
! R11   R(8,25)               1.5043         -DE/DX =    0.0               !
! R12   R(9,10)               1.0159         -DE/DX =    0.0               !
! R13   R(9,11)               1.4105         -DE/DX =    0.0               !
! R14   R(11,12)              1.406          -DE/DX =    0.0               !
! R15   R(11,20)              1.4014         -DE/DX =    0.0               !
! R16   R(12,13)              1.0854         -DE/DX =    0.0               !
! R17   R(12,14)              1.3879         -DE/DX =    0.0               !
! R18   R(14,15)              1.0841         -DE/DX =    0.0               !
! R19   R(14,16)              1.3951         -DE/DX =    0.0               !
! R20   R(16,17)              1.0836         -DE/DX =    0.0               !
! R21   R(16,18)              1.3919         -DE/DX =    0.0               !
! R22   R(18,19)              1.0845         -DE/DX =    0.0               !
! R23   R(18,20)              1.3943         -DE/DX =    0.0               !
! R24   R(20,21)              1.077          -DE/DX =    0.0               !
! R25   R(22,23)              1.2261         -DE/DX =    0.0               !
! R26   R(22,24)              1.2433         -DE/DX =    0.0               !
! R27   R(25,26)              1.0933         -DE/DX =    0.0               !
! R28   R(25,27)              1.0906         -DE/DX =    0.0               !
! R29   R(25,28)              1.0933         -DE/DX =    0.0               !
! A1    A(2,1,8)            121.0978         -DE/DX =    0.0               !
! A2    A(1,2,3)            119.3757         -DE/DX =    0.0               !
! A3    A(1,2,9)            119.2257         -DE/DX =    0.0               !
! A4    A(3,2,9)            121.3987         -DE/DX =    0.0               !
! A5    A(2,3,4)            118.9156         -DE/DX =    0.0               !
! A6    A(2,3,22)           124.0585         -DE/DX =    0.0               !
! A7    A(4,3,22)           117.0259         -DE/DX =    0.0               !
! A8    A(3,4,5)            118.242          -DE/DX =    0.0               !
! A9    A(3,4,6)            120.0067         -DE/DX =    0.0               !
! A10   A(5,4,6)            121.7513         -DE/DX =    0.0               !
! A11   A(4,6,7)            120.997          -DE/DX =    0.0               !
! A12   A(4,6,8)            118.1288         -DE/DX =    0.0               !
! A13   A(7,6,8)            120.8741         -DE/DX =    0.0               !
! A14   A(1,8,6)            122.4755         -DE/DX =    0.0               !
! A15   A(1,8,25)           116.2121         -DE/DX =    0.0               !
! A16   A(6,8,25)           121.3124         -DE/DX =    0.0               !
! A17   A(2,9,10)           112.4105         -DE/DX =    0.0               !
! A18   A(2,9,11)           132.2435         -DE/DX =    0.0               !
! A19   A(10,9,11)          115.346          -DE/DX =    0.0               !
! A20   A(9,11,12)          115.3899         -DE/DX =    0.0               !
! A21   A(9,11,20)          125.5889         -DE/DX =    0.0               !
! A22   A(12,11,20)         119.0212         -DE/DX =    0.0               !
! A23   A(11,12,13)         119.4661         -DE/DX =    0.0               !
! A24   A(11,12,14)         120.7377         -DE/DX =    0.0               !
! A25   A(13,12,14)         119.7963         -DE/DX =    0.0               !
! A26   A(12,14,15)         119.3801         -DE/DX =    0.0               !
! A27   A(12,14,16)         120.2935         -DE/DX =    0.0               !
! A28   A(15,14,16)         120.3264         -DE/DX =    0.0               !
! A29   A(14,16,17)         120.4241         -DE/DX =    0.0               !
! A30   A(14,16,18)         119.0261         -DE/DX =    0.0               !
! A31   A(17,16,18)         120.5498         -DE/DX =    0.0               !
! A32   A(16,18,19)         119.8762         -DE/DX =    0.0               !
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! A33   A(16,18,20)          121.4012         -DE/DX =    0.0                 !
! A34   A(19,18,20)          118.7227         -DE/DX =    0.0                 !
! A35   A(11,20,18)          119.5204         -DE/DX =    0.0                 !
! A36   A(11,20,21)          119.6292         -DE/DX =    0.0                 !
! A37   A(18,20,21)          120.8504         -DE/DX =    0.0                 !
! A38   A(3,22,23)           118.7011         -DE/DX =    0.0                 !
! A39   A(3,22,24)           118.6853         -DE/DX =    0.0                 !
! A40   A(23,22,24)          122.6136         -DE/DX =    0.0                 !
! A41   A(8,25,26)           110.0258         -DE/DX =    0.0                 !
! A42   A(8,25,27)           111.7814         -DE/DX =    0.0                 !
! A43   A(8,25,28)           110.0281         -DE/DX =    0.0                 !
! A44   A(26,25,27)          108.858          -DE/DX =    0.0                 !
! A45   A(26,25,28)          107.1655         -DE/DX =    0.0                 !
! A46   A(27,25,28)          108.8587         -DE/DX =    0.0                 !
! D1    D(8,1,2,3)            -0.0027         -DE/DX =    0.0                 !
! D2    D(8,1,2,9)           179.9952         -DE/DX =    0.0                 !
! D3    D(2,1,8,6)            -0.0017         -DE/DX =    0.0                 !
! D4    D(2,1,8,25)          179.9972         -DE/DX =    0.0                 !
! D5    D(1,2,3,4)             0.0046         -DE/DX =    0.0                 !
! D6    D(1,2,3,22)         -179.9941         -DE/DX =    0.0                 !
! D7    D(9,2,3,4)          -179.9933         -DE/DX =    0.0                 !
! D8    D(9,2,3,22)            0.008          -DE/DX =    0.0                 !
! D9    D(1,2,9,10)          179.9926         -DE/DX =    0.0                 !
! D10   D(1,2,9,11)            0.0024         -DE/DX =    0.0                 !
! D11   D(3,2,9,10)           -0.0095         -DE/DX =    0.0                 !
! D12   D(3,2,9,11)          180.0003         -DE/DX =    0.0                 !
! D13   D(2,3,4,5)           179.9982         -DE/DX =    0.0                 !
! D14   D(2,3,4,6)            -0.0021         -DE/DX =    0.0                 !
! D15   D(22,3,4,5)           -0.003          -DE/DX =    0.0                 !
! D16   D(22,3,4,6)          179.9967         -DE/DX =    0.0                 !
! D17   D(2,3,22,23)         180.0035         -DE/DX =    0.0                 !
! D18   D(2,3,22,24)           0.0038         -DE/DX =    0.0                 !
! D19   D(4,3,22,23)           0.0047         -DE/DX =    0.0                 !
! D20   D(4,3,22,24)        -179.9949         -DE/DX =    0.0                 !
! D21   D(3,4,6,7)           179.999          -DE/DX =    0.0                 !
! D22   D(3,4,6,8)            -0.0021         -DE/DX =    0.0                 !
! D23   D(5,4,6,7)            -0.0013         -DE/DX =    0.0                 !
! D24   D(5,4,6,8)           179.9975         -DE/DX =    0.0                 !
! D25   D(4,6,8,1)             0.0042         -DE/DX =    0.0                 !
! D26   D(4,6,8,25)         -179.9946         -DE/DX =    0.0                 !
! D27   D(7,6,8,1)          -179.9969         -DE/DX =    0.0                 !
! D28   D(7,6,8,25)            0.0042         -DE/DX =    0.0                 !
! D29   D(1,8,25,26)         -58.9406         -DE/DX =    0.0                 !
! D30   D(1,8,25,27)        -180.0128         -DE/DX =    0.0                 !
! D31   D(1,8,25,28)          58.9125         -DE/DX =    0.0                 !
! D32   D(6,8,25,26)         121.0583         -DE/DX =    0.0                 !
! D33   D(6,8,25,27)           -0.0139         -DE/DX =    0.0                 !
! D34   D(6,8,25,28)        -121.0885         -DE/DX =    0.0                 !
! D35   D(2,9,11,12)         179.9994         -DE/DX =    0.0                 !
! D36   D(2,9,11,20)           -0.0012         -DE/DX =    0.0                 !
! D37   D(10,9,11,12)           0.0093         -DE/DX =    0.0                 !
! D38   D(10,9,11,20)        -179.9913         -DE/DX =    0.0                 !
! D39   D(9,11,12,13)          -0.001          -DE/DX =    0.0                 !
! D40   D(9,11,12,14)         179.9992         -DE/DX =    0.0                 !
! D41   D(20,11,12,13)        179.9996         -DE/DX =    0.0                 !
! D42   D(20,11,12,14)         -0.0002         -DE/DX =    0.0                 !
! D43   D(9,11,20,18)        -179.999          -DE/DX =    0.0                 !
! D44   D(9,11,20,21)           0.0015         -DE/DX =    0.0                 !
! D45   D(12,11,20,18)          0.0004         -DE/DX =    0.0                 !
```

! D46	D(12,11,20,21)	-179.9991	-DE/DX =	0.0 !
! D47	D(11,12,14,15)	180.0	-DE/DX =	0.0 !
! D48	D(11,12,14,16)	-0.0003	-DE/DX =	0.0 !
! D49	D(13,12,14,15)	0.0002	-DE/DX =	0.0 !
! D50	D(13,12,14,16)	-180.0001	-DE/DX =	0.0 !
! D51	D(12,14,16,17)	-179.9994	-DE/DX =	0.0 !
! D52	D(12,14,16,18)	0.0005	-DE/DX =	0.0 !
! D53	D(15,14,16,17)	0.0004	-DE/DX =	0.0 !
! D54	D(15,14,16,18)	-179.9997	-DE/DX =	0.0 !
! D55	D(14,16,18,19)	179.9995	-DE/DX =	0.0 !
! D56	D(14,16,18,20)	-0.0004	-DE/DX =	0.0 !
! D57	D(17,16,18,19)	-0.0006	-DE/DX =	0.0 !
! D58	D(17,16,18,20)	179.9996	-DE/DX =	0.0 !
! D59	D(16,18,20,11)	-0.0001	-DE/DX =	0.0 !
! D60	D(16,18,20,21)	179.9994	-DE/DX =	0.0 !
! D61	D(19,18,20,11)	-180.0	-DE/DX =	0.0 !
! D62	D(19,18,20,21)	-0.0004	-DE/DX =	0.0 !

Optimized Parameters (xyz)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000392	-0.020716	-0.016252
2	6	0	-1.322494	0.220072	-0.014598
3	6	0	-2.240726	-0.886028	-0.018637
4	6	0	-1.732702	-2.183223	-0.024082
5	1	0	-2.433194	-3.007131	-0.027053
6	6	0	-0.367874	-2.390114	-0.025568
7	1	0	0.044000	-3.390522	-0.029760
8	6	0	0.471867	-1.265520	-0.021509
9	7	0	-1.762392	1.504630	-0.009099
10	1	0	-2.776372	1.566766	-0.008455
11	6	0	-1.081752	2.740000	-0.004408
12	6	0	-1.903357	3.880965	0.000695
13	1	0	-2.982191	3.762028	0.000766
14	6	0	-1.349819	5.153695	0.005623
15	1	0	-2.003969	6.018164	0.009506
16	6	0	0.035497	5.318601	0.005583
17	1	0	0.469934	6.311296	0.009435
18	6	0	0.849979	4.189906	0.000527
19	1	0	1.928655	4.302107	0.000421
20	6	0	0.310004	2.904383	-0.004464
21	1	0	0.948566	2.037165	-0.008364
22	7	0	-3.683945	-0.743527	-0.017446
23	8	0	-4.375623	-1.755955	-0.021141
24	8	0	-4.170646	0.400495	-0.012725
25	6	0	1.969388	-1.408031	-0.022924
26	1	0	2.391817	-0.912393	-0.901129
27	1	0	2.276294	-2.454503	-0.027066
28	1	0	2.392887	-0.919032	0.858476

Table S3. Experimental and calculated wavenumbers with assignment of the observed bands to respective normal modes for monomer.

PA3N4MP				PA3N6MP				
Exp.		Calc.		Exp.		Exp.		
IR	RS	IR	RS	IR	RS	IR	RS	Assignment
3367	3367	3433m		3344	3344	3311w		νN-H····O
		3304m						
3132	3132	3135m		3135	3135	3146vw		$\nu(C-H)_{\phi}$
				3100	3100		3082w	
3074	3074			3077	3077			$\nu(C-H)_{\theta}$
3069	3069			3069	3069		3067w	$\nu(C-H)_{\phi}$
3056	3056	3053w	3056w	3056	3056			
3046	3046			3046	3046	3047vw		
3038	3038	3036w		3038	3038			
3025	3025							$\nu(C_{\tau}-H)_{\theta}$
3002	3002			3003	3003			$\nu_{as}(CH_3)$
2994	2994	2988w	2989w					
		2981w		2974	2974			
2937	2937	2932w	2935w	2924	2924	2914vw	2915w	$\nu_{s}(CH_3)$
						1619s		
		1607s	1607m			1613s	1606m	
			1596m			1596vs	1591w	
1585	1585	1579s	1579w	1589	1589	1580vs	1585w	$\delta(CNH)_{\phi}+\nu(\phi)$
1574	1574	1566s	1567w	1578	1578		1578w	$\delta(CNH)_{\theta}+\nu(\phi)+\nu_{as}(NO_2)$
				1562	1562			
1549	1549	1548s	1547m	1548	1548	1548vw	1545w	$\nu_{as}(NO_2)+\nu(\phi)+\nu(\theta)+\delta(C_{\phi}NC_{\theta})$
1543	1543							
1521	1521	1511vs	1500w	1519	1519	1502s	1500w	
1481	1481	1485w				1491m	1486w	$\nu_{as}(NO_2)+\nu(\phi)+\nu(\theta)$
1471	1471			1472	1472			$\nu_{as}(NO_2)+\nu(\theta)$
		1448m	1450w	1466	1466	1465m	1458w	
				1433	1433	1432w	1434w	$\nu_{as}(NO_2)+\delta_{as}(CH_3)$
1436	1436	1437m						
1429	1429	1429sh		1430	1430			$\delta_{as}(CH_3)+\delta(\theta)$
1423	1423			1423	1423			
1416	1416							$\nu_{as}(NO_2)$
				1403	1403	1396w	1394v	$\nu_{as}(NO_2)+\delta_{as}(CH_3)+\delta(\phi)+\delta($

							w	θ)
1366	1366	1378	1378m	1378	1378	1373w	1371w	$\nu_s(NO_2)$ $\delta_s(CH_3)$
1350	1350	1361		1357	1357	1357w		$\nu(CN)_\phi+\nu_s(NO_2)+\delta(\phi)+\delta_s(CH_3)$
		1341	1348w				1339w	
1324	1324	1326	1326vw	1309		1329vw	1315w	$\nu_s(NO_2)+\delta(\phi)+\delta(\theta)+\delta_s(CH_3)$
1304	1304	1307vw	1308w	1304	1309	1314w		
		1301vw			1304	1302w	1302w	
1279	1279	1286vw	1272vw	1280	1280	1271w	1271w	$\nu_s(NO_2)+\delta(CH)+\nu(\phi+\theta)+\delta_s(CH_3)$
1256	1256	1248sh	1238vs	1240	1240	1239vs	1236vs	$\nu_s(NO_2)+\delta(CH)+\nu(\phi+\theta)+\delta_s(CH_3)$
1226	1226	1237m	1212s	1227	1227	1219vs	1216s	$\nu(\phi)+\nu_s(NO)+\nu(CN)_{\phi\alpha}+\nu(CNH)_\phi$
1197	1197	1220s	1192sh	1195	1195	1186s	1188s	$\nu_s(NO_2)+(CNH)_\theta$
1184	1184	1203sh						$\nu_s(NO_2)+\nu(NCN)_\phi$
		1177m				1177s		
1159	1159	1166sh	1162w	1159	1159	1159m	1156m	$\nu_s(NO_2)+\delta(CH)_\phi$
				1157	1157			
1137	1137	1143w	1150vw	1138	1138			
				1136	1136			
1122	1122	1081vw				1110vw	1084vw	$\delta(CH)_\theta$
1069	1069	1063m	1062m	1070	1070	1073w	1073w	$\delta(CH)_\phi$
1044	1044	1048w		1051	1051			$\delta(\phi)_\phi+\nu(NO_2)$
1027	1027	1035w	1031vw			1031w	1034vw	
1017	1017	1027w		1016	1016			$\rho(CH_3)$
				1015	1015			
1008	1008		1001m	1009	1009			$\delta(\phi)_\theta+\rho(CH_3)$
977	977	998vw		977	977	997w	998m	
		981w	984w					
964	964	964vw		963	963	963w	964w	$\rho(CH)$
960	960			962	962			$\rho(CH_3)$
957	957							
946	946			945	945			$\delta(CH)_\theta$
				944	944			
883	883	903w		883	883	903w		

		865m	868m			854w	856w	
840	840	838vw	833vw	831	831	844w	845w	$\delta_s(NO)_\phi+\tau(\phi)$
				823	823			
810	810		810vw	811	811	813vw		$\delta(CH)_\phi$
807	807	807m						$\nu(CNHC)$
794	794			798	798			$\rho(CH_3)$
790	790							$\nu(CNHC)_{\phi+\theta}+\delta_s(NO)_\phi$
775	775	777m	761vw					$\rho(CH_3)$
		757s		749	749	751s	759vw	
735	735			735	735		745vw	$\delta(CH)_\theta$
				728	728			
719	719	720w	724w	724	724			$\delta_{as}(NO)_\phi$
707	707			710	710			$\delta(NH)$
699	699	691m				694m		$\delta(CNHC)_{\phi+\theta}$
672	672	682m		674	674	679w	681m	$\delta(CH)_\theta$
				665	665			
610	610	618vw	620w	614	614		628w	$\tau(\phi_\theta)$
590	590	600w	600w	606	606		592m	$\tau(\phi)+\tau(\theta)$
580	580	585w		578	578			$\rho(CH_3)$
531	531	536w	541m	522	522	534w	536vw	$\gamma(\phi)+\nu_{as}(NO)_\phi$
522	522	510m	510w			512s	511vw	$\delta(\phi)$
492	492	470w		493	493	458w		$\delta(CH)_\theta$
463	463			430	430	436w	436vw	$\rho(CH_3)$
401	401		403w	401	401	419w		$\delta(CH)_\theta$
395	395		386w	386	386	394w	395vw	$\delta(CCH_3)+\delta(CNO)_\phi$
373	373			367	367	375w	383w	$\delta(\phi)+\nu(C\text{-}NO_2)$
						353w		
						342w		
						335w		
			331w			328w		
						324w	323w	
				311	311	315vw		
308	308		301w			303m		
290	290		289w			295m	295vw	$\delta(CNHC)_{\phi+\theta}$
				280	280	282m		
				250	250	278m		$\tau(CH_3)$
266	266			248	248	266s	264vw	
			242w			254w		
						248w		
231	231		210w			245w		
224	224					227w		

				212m	210w	
205	205		205	205	208m	
					203m	
					194w	
187	187		184	184	188w		$\delta(CNHC)_{\phi+\theta}$
107	107		94	94	177w		$\delta(CNHC)_{\phi+\theta}$
83	83		84	84	150m		$\delta_s(NO)_{\phi}+\delta(CNHC)_{\phi+\theta}$
			79	79	122m	107m	
62	62		55	55			$\nu(NO)_{\phi}$
38	38		42	42		77m	
19	19		20	20		54s	

Figure S1. The deconvolution of 2DFP plot for individual interactions in the crystal of PA3N4MP.

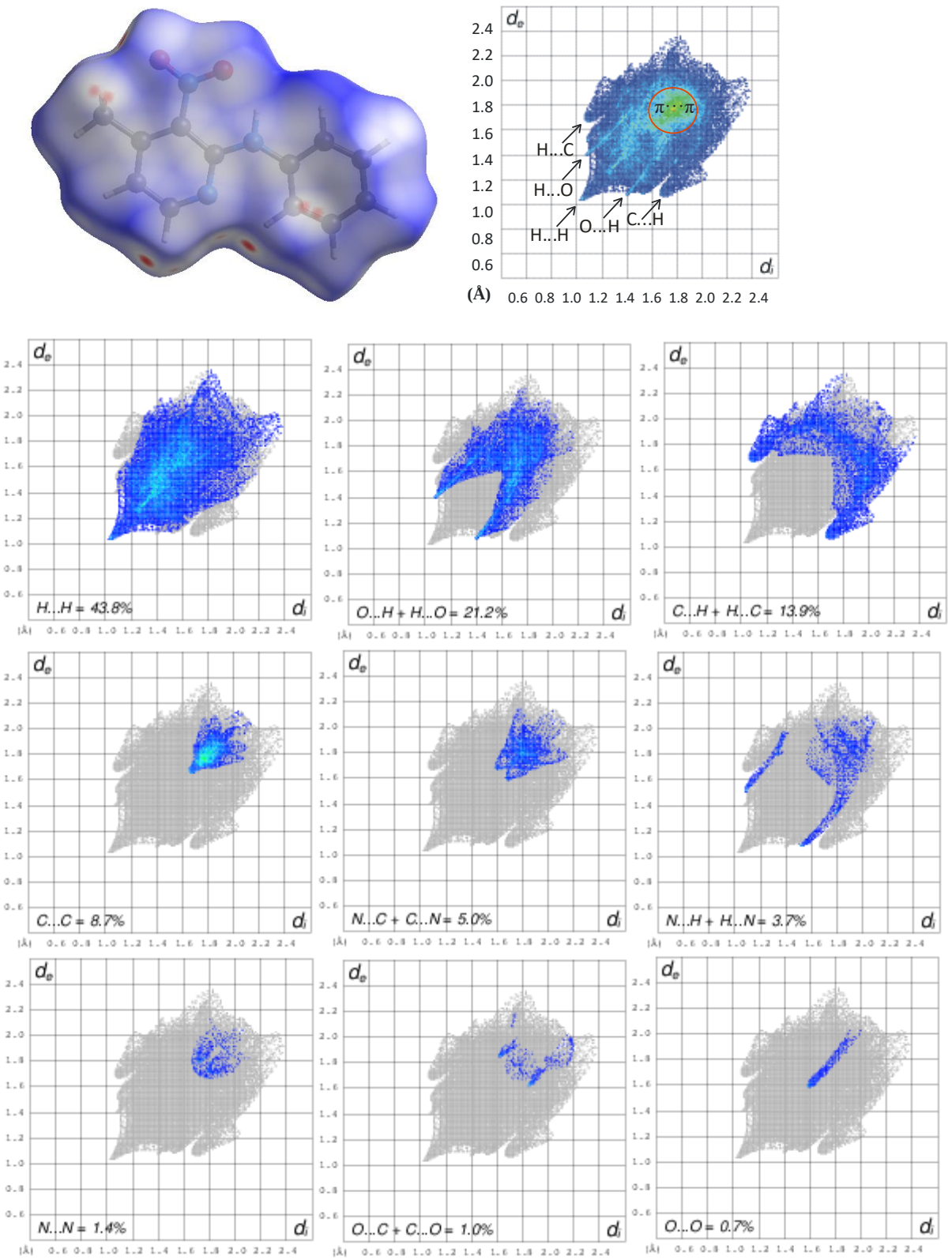


Figure S2. The deconvolution of 2DFP plot for individual interactions in the crystal of PA3N6MP.

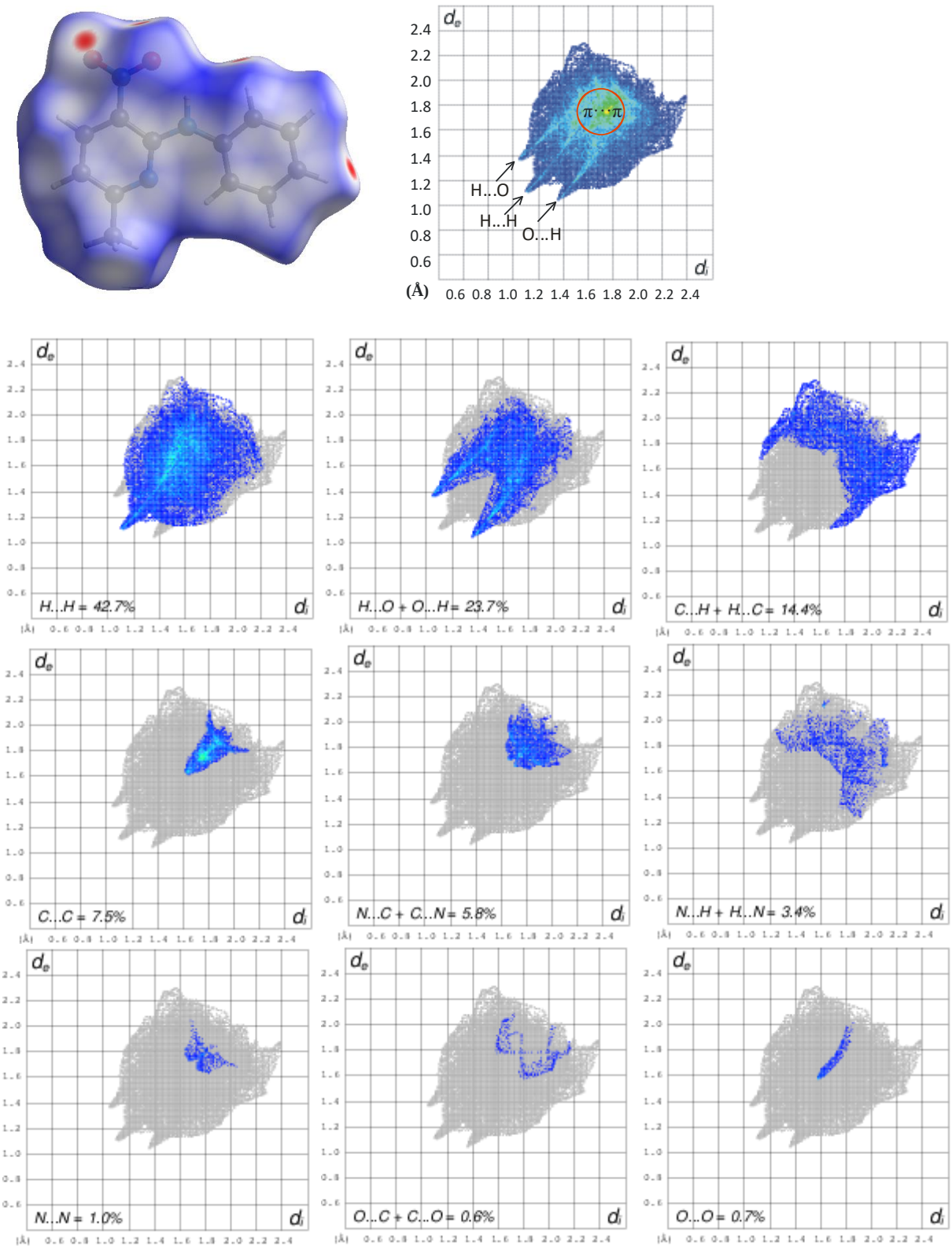


Figure S3. [1]H NMR spectra of the studied isomers: A) 2-*N*-phenylamino-4-methyl-3-nitro- and B) 2-*N*-phenylamino-6-methyl-3-nitro- pyridines.

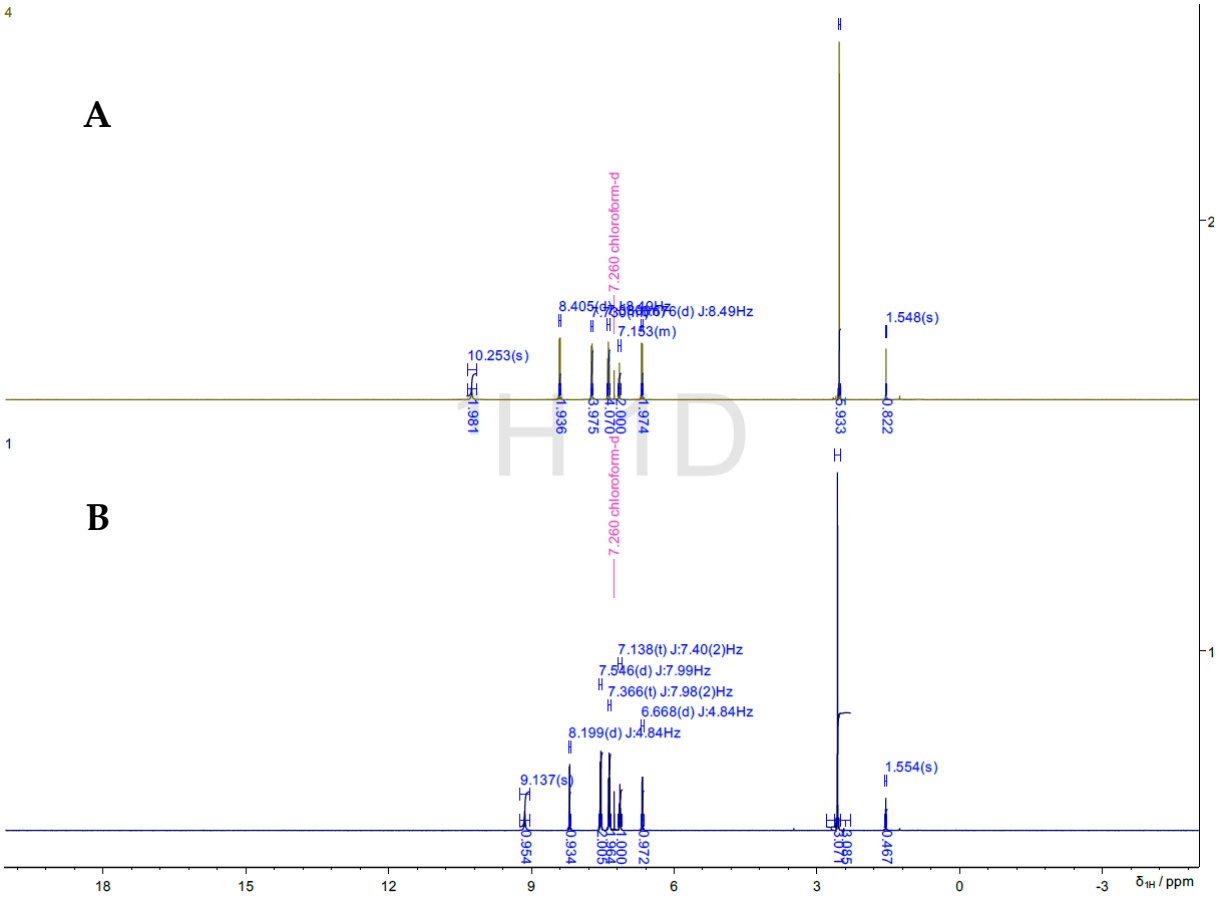


Figure S4. ^{13}C NMR spectra of the studied isomers: A) 2-*N*-phenylamino-4-methyl-3-nitro- and B) 2-*N*-pheny lamino-6-methyl-3-nitro- pyridines.

