

Electronic Supplementary Information (ESI)

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1. Experimental Section

1.1 Safety Precaution

In this work, compounds **MPT-1** and **MPT-2** are potential energetic materials that tend to explode under certain external stimuli. Therefore, the whole experimental process should be carried out by using proper safety equipment, such as safety shields, eye protection, and leather gloves.

1.2 General methods

All of the reactions were carried out in air. Ammonium 4-amino-3,5-dinitropyrazolate monohydrate, ^[1] 4-amino-5-nitro-1,2,3-triazole ^[2] were prepared following literature procedure, other commercial reagents and solvents were obtained from commercial providers and used without further purification. ¹H NMR and ¹³C NMR spectra were recorded at 25 °C on a Bruker 400 MHz and 125 MHz, respectively, and TMS as internal standard. Chemical shifts were reported in parts per million (ppm). The onset decomposition temperature was measured using a TA Instruments DSC25 differential scanning calorimeter at a heating rate of 10 °C min⁻¹ under dry nitrogen atmosphere. Infrared spectra (IR) were obtained on a PerkinElmer Spectrum BX FT-IR instrument equipped with an ATR unit at 25 °C. Elemental analyses of C/H/N were investigated on a Thermo Scientific Flash 2000 Elemental Analyzer. Impact and friction sensitivities were tested by a BAM fallhammer and friction tester. Densities were determined at room temperature by employing a Micromeritics AccuPyc 1340 gas pycnometer. The crystal structures were produced employing Mercury 2021.1.0 software.

1.3 X-ray crystallography

Single Crystal X-ray Diffraction (SCXRD). X-ray diffractions of all single crystals were carried out at 170(2) K or room temperature on a Bruker D8 VENTURE diffractometer using Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$). Integration and scaling of intensity data were performed using the SAINT program. Data were corrected for the effects of absorption using SADABS. The structures were solved by direct method and refined with full-matrix least-squares technique using SHELX-2014 software.

Non-hydrogen atoms were refined with anisotropic displacement parameters, and hydrogen atoms were placed in calculated positions and refined with a riding model.

Cell refinement: SAINT V8.40A (Bruker, 2016); data reduction: SAINT V8.40A (Bruker, 2016); program(s) used to solve structure: ShelXT (Sheldrick, 2015); program(s) used to refine structure: SHELXL (Sheldrick, 2015); ^[3] molecular graphics: Olex2 (Dolomanov et al., 2009); ^[4] software used to prepare material for publication: Olex2 (Dolomanov et al., 2009).^[4]

Data collection of MPT-1-170K

Bruker D8 VENTURE diffractometer	2018 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.072$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.0869 before and 0.0725 after correction. The Ratio of minimum to maximum transmission is 0.9399. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.701$, $T_{\text{max}} = 0.746$	$h = -8 \rightarrow 7$
14243 measured reflections	$k = -15 \rightarrow 14$
2626 independent reflections	$l = -20 \rightarrow 20$

Data collection of MPT-1-rt

Bruker D8 VENTURE diffractometer	2108 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.050$
Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(\text{int})$ was 0.1250 before and 0.0653 after correction. The Ratio of minimum to maximum transmission is 0.7952. The $\lambda/2$ correction factor is Not present.	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.593$, $T_{\text{max}} = 0.746$	$h = -8 \rightarrow 8$

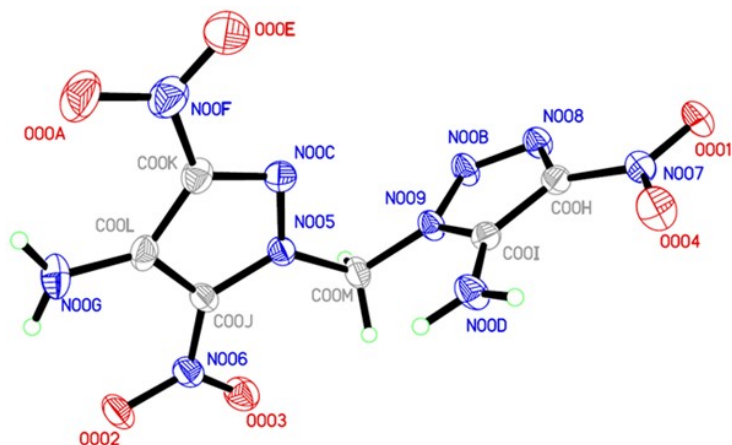
9578 measured reflections	$k = -15 \rightarrow 12$
2669 independent reflections	$l = -20 \rightarrow 20$

Data collection of MPT-2-170K

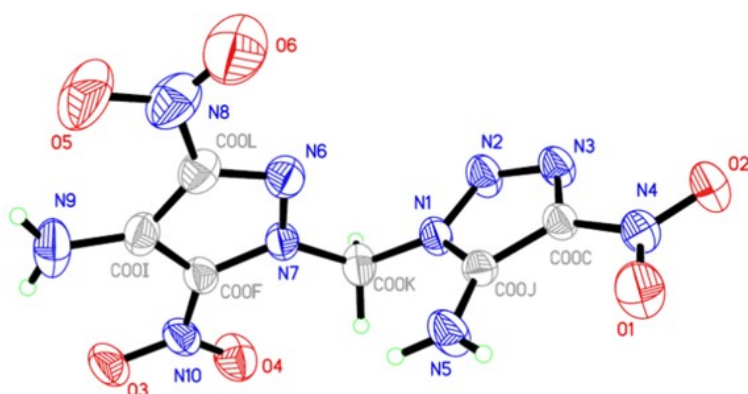
<p>Bruker D8 VENTURE diffractometer</p> <p>ϕ and ω scans</p> <p>Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.0663 before and 0.0543 after correction. The Ratio of minimum to maximum transmission is 0.8047. The $\lambda/2$ correction factor is Not present.</p> <p>$T_{min} = 0.600$, $T_{max} = 0.745$</p>	<p>1701 reflections with $I > 2\sigma(I)$</p> <p>$R_{int} = 0.043$</p> <p>$\theta_{max} = 26.5^\circ$, $\theta_{min} = 2.1^\circ$</p> <p>$h = -8 \rightarrow 8$</p> <p>8551 measured reflections</p> <p>2352 independent reflections</p>

Data collection of MPT-2-rt

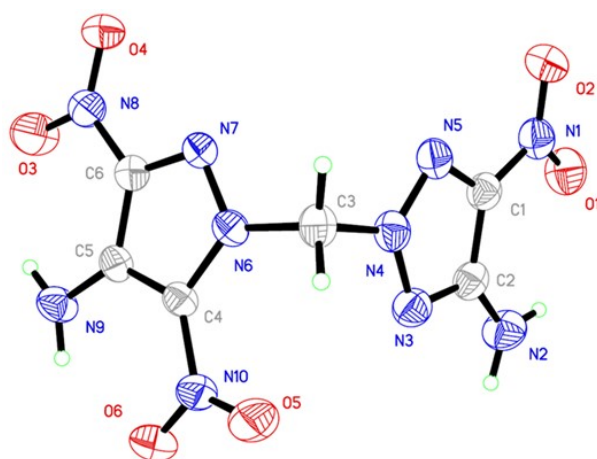
<p>Bruker APEX-II CCD diffractometer</p> <p>ϕ and ω scans</p> <p>Absorption correction: multi-scan <i>SADABS2016/2</i> (Bruker,2016/2) was used for absorption correction. $wR2(int)$ was 0.1055 before and 0.0582 after correction. The Ratio of minimum to maximum transmission is 0.8450. The $\lambda/2$ correction factor is Not present.</p> <p>$T_{min} = 0.630$, $T_{max} = 0.746$</p>	<p>1323 reflections with $I > 2\sigma(I)$</p> <p>$R_{int} = 0.064$</p> <p>$\theta_{max} = 27.5^\circ$, $\theta_{min} = 2.1^\circ$</p> <p>$h = -9 \rightarrow 9$</p> <p>8693 measured reflections</p> <p>2689 independent reflections</p>



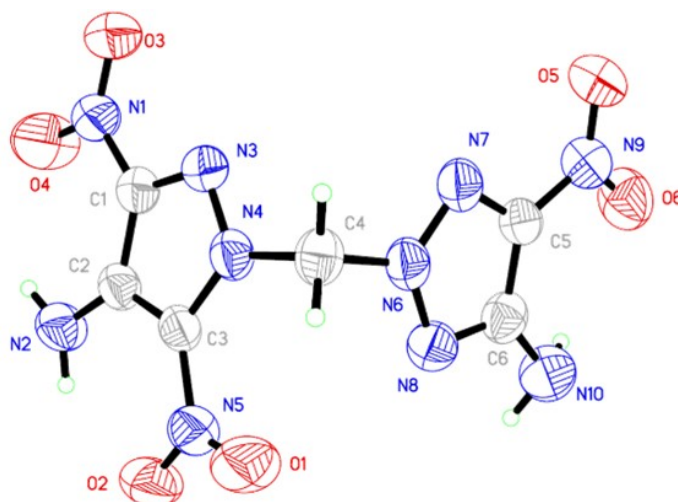
Thermal ellipsoid plot (50%) and labeling scheme for MPT-1-170K.



Thermal ellipsoid plot (50%) and labeling scheme for MPT-1-rt.



Thermal ellipsoid plot (50%) and labeling scheme for MPT-2-170K.



Thermal ellipsoid plot (50%) and labeling scheme for MPT-2-rt.

1.4 Synthetic Procedures

1-(Chloromethyl)-3,5-dinitro-1H-pyrazol-4-amine (CDPA): ClCH_2I (2 mL) was added to 100 mL round-bottom flask equipped with condenser, ammonium 4-amino-3,5-dinitropyrazolate monohydrate (1 mmol) in DMF (2 mL) was dropped into ClCH_2I . Then the reaction was stirred at 50 °C for 30 min. The reaction was monitored by TLC. After reaction completion, the reaction mixture was allowed to cool down to rt, and H_2O (10 mL) and ether (10 mL) were added to the vessel. The resulting suspension was extracted with ether (3×30 mL). The organic phases were combined and dried over Na_2SO_4 . After filtration, the solvent was removed from the filtrate under reduced pressure. The acquired residue was subjected to silica gel column chromatography to give 1-(chloromethyl)-3,5-dinitro-1H-pyrazol-4-amine (50 mg, 25%). $^1\text{H NMR}$ (d_6 -DMSO): δ 7.25 (s, 2 H), 6.46 (s, 2 H) ppm. $^{13}\text{C NMR}$ (d_6 -DMSO): δ 142.0, 130.9, 129.9, 59.8 ppm.

((4-Amino-3,5-dinitro-1H-pyrazol-1-yl)methyl)-4-nitro-1H-1,2,3-triazol-5-amine: 1-(Chloromethyl)-3,5-dinitro-1H-pyrazol-4-amine CDPA (1mmol), 5-nitro-2H-1,2,3-triazol-4-amine (2 mmol), KOH (2 mmol), KI (1 mmol) and DMF (5 mL) were added to 100 mL round-bottom flask equipped with condenser. Then the reaction was stirred at 80 °C for 12 h. The reaction mixture was allowed to cool down

to rt, and H₂O (15 mL) was added to the vessel. The resulting suspension was extracted with ethyl acetate (3 × 30 mL). The organic phases were combined and dried over Na₂SO₄. After filtration, the solvent was removed from the solution under reduced pressure. The acquired residue was subjected to silica gel column chromatography to give 1-((4-amino-3,5-dinitro-1H-pyrazol-1-yl)methyl)-4-nitro-1H-1,2,3-triazol-5-amine (**MPT-1**, 94 mg) and 2-((4-amino-3,5-dinitro-1H-pyrazol-1-yl)methyl)-5-nitro-2H-1,2,3-triazol-4-amine (**MPT-2**, 126 mg).

Compound **MPT-1** (1-((4-amino-3,5-dinitro-1H-pyrazol-1-yl)methyl)-4-nitro-1H-1,2,3-triazol-5-amine)

Yellow solid, 30% yield. $T_m = 175\text{ }^\circ\text{C}$, T_d (onset) = 190 °C. ¹H NMR (400 MHz, *d*₆-DMSO) δ 8.13 (s, 2 H), 7.40 (s, 2 H), 7.00 (s, 2 H) ppm. ¹³C NMR (101 MHz, *d*₆-DMSO) δ 142.6, 141.1, 135.7, 131.4, 130.6, 61.7 ppm. IR (KBr): $\tilde{\nu}$ 3595, 3365, 2838, 1759, 1734, 1662, 1605, 1548, 1479, 1422, 1333, 1288, 1241, 1201, 1183, 1075, 1007, 966, 849, 793, 770, 725, 698, 633, 561, 530, 425 cm⁻¹. Elemental analysis of C₆H₆N₁₀O₆ (314.05): calcd C 22.94, H 1.93, N 44.58%; found: C 22.56, H 1.67, N 44.12%.

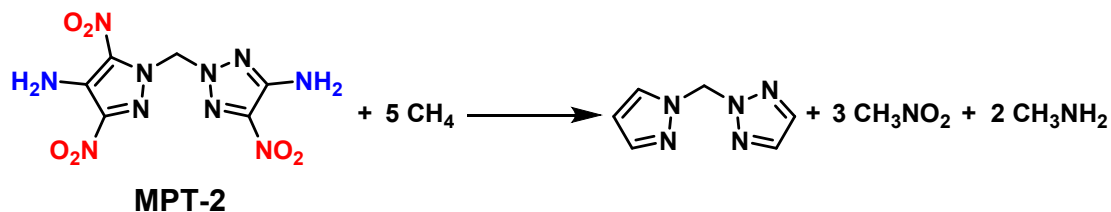
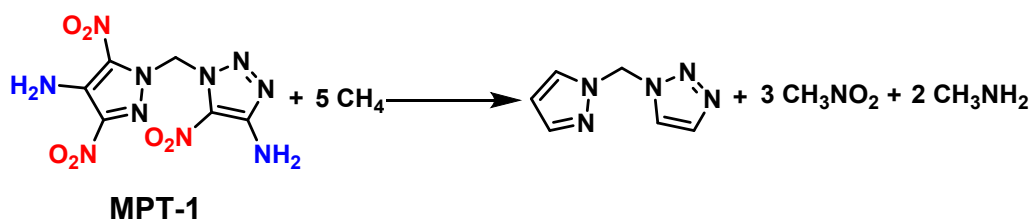
Compound **MPT-2** (2-((4-amino-3,5-dinitro-1H-pyrazol-1-yl)methyl)-4-nitro-1H-1,2,3-triazol-5-amine)

Yellow solid, 40% yield. $T_m = 194\text{ }^\circ\text{C}$, T_d (onset) = 269 °C. ¹H NMR (400 MHz, *d*₆-DMSO) δ 7.45 (s, 2 H), 6.99 (s, 2 H), 6.86 (s, 2 H) ppm. ¹³C NMR (101 MHz, *d*₆-DMSO) δ 149.3, 142.1, 138.9, 130.7, 130.6, 68.7 ppm. IR (KBr): $\tilde{\nu}$ 3595, 3365, 2838, 1759, 1734, 1662, 1605, 1548, 1479, 1422, 1333, 1288, 1241, 1201, 1183, 1074, 1007, 966, 849, 793, 770, 725, 698, 633, 561, 530, 425 cm⁻¹. Elemental analysis of C₆H₆N₁₀O₆ (314.05): calcd C 22.94, H 1.93, N 44.58%; found: C 23.12, H 2.04, N 44.09%.

2. Computational Details

The heats of formation of compounds **MPT-1** and **MPT-2** were performed by using the Gaussian 09 suite of programs.^[5] Gas phase heats of formation of the title compounds were computed based on an isodesmic reaction (Fig. S1). The enthalpy of reaction was carried out by combining the M062X/6-311++G** energy difference for the reactions, the scaled zero-point energies (ZPE), values of thermal correction (HT), and other thermal factors. The solid state heats of formation were further obtained by employing Trouton's rule according to equation 1 (T represents either melting point or decomposition temperature when no melting occurs prior to decomposition).^[6]

$$\Delta H_{sub} = 188/J\ mol^{-1}\ K^{-1} \times T\ (1)$$



3. Crystallographic data for MPT-1 and MPT-2

	MPT-1-170K	MPT-2-170K
CCDC No.	2182866	2178121
Empirical Formula	C ₆ H ₆ N ₁₀ O ₆	C ₆ H ₆ N ₁₀ O ₆
Formula Weight	314.21	314.21
Temperature (K)	170	170
Crystal System	orthorhombic	Monoclinic
Space group	<i>P2₁/2₁/2₁</i>	<i>P2₁/n</i>
Unit cell dimensions		
a (Å)	6.2740(4)	7.1538(55)
b (Å)	11.6263(7)	8.2580(14)
c (Å)	15.6940 (9)	19.830(3)
α (°)	90	90
β (°)	90	95.353(5)
γ (°)	90	90
Volume (Å ³)	1144.77(12)	1166.4(3)
Z	4	4
Density (g cm ⁻³) (calculated)	1.823	1.789
F(000)	640.0	640
Crystal size (mm ³)	0.130 x 0.050 x 0.040	0.08 x 0.05 x 0.04
Goodness-of-fit on F ²	1.075	1.107
Final R indexes [I>=2σ (I)]	R ₁ = 0.0435 wR ₂ = 0.0845	R ₁ = 0.0715, wR ₂ = 0.1668
Final R indexes [all data]	R ₁ = 0.0711, wR ₂ = = 0.0975	R ₁ = 0.1026, wR ₂ = 0.1830

	MPT-1rt	MPT-2rt
CCDC No.	2194551	2182865
Empirical Formula	C ₆ H ₆ N ₁₀ O ₆	C ₆ H ₆ N ₁₀ O ₆
Formula Weight	314.21	314.21
Temperature (K)	298	298
Crystal System	orthorhombic	Monoclinic
Space group	<i>P2₁/2₁/2₁</i>	<i>P2₁/n</i>
Unit cell dimensions		
a (Å)	6.2935(3)	7.1738(8)
b (Å)	11.7191(5)	8.3136(10)

c (Å)	15.8519(7)	19.948 (3)
α (°)	90	90
β (°)	90	95.253(4)
γ (°)	90	90
Volume (Å ³)	1169.14(9)	1184.7(2)
Z	4	4
Density (g cm ⁻³) (calculated)	1.785	1.762
F(000)	640.0	640
Crystal size (mm ³)	0.12 x 0.08 x 0.05	0.12 x 0.08 x 0.05
Goodness-of-fit on F ²	1.045	1.059
Final R indexes [$I \geq 2\sigma$ (I)]	R ₁ = 0.0392 wR ₂ = 0.0835	R ₁ = 0.0717, wR ₂ = 0.1699
Final R indexes [all data]	R ₁ = 0.0583, wR ₂ = = 0.0945	R ₁ = 0.1650, wR ₂ = 0.2161

4. Crystallographic bond lengths [Å] and angles [°] for MPT-1

MPT-1-170K

O(001)-N(007)	1.239(3)	N(009)-C(00I)	1.354(4)
O(002)-N(006)	1.241(4)	N(009)-C(00M)	1.433(4)
O(003)-N(006)	1.238(4)	O(00A)-N(00F)	1.238(4)
O(004)-N(007)	1.243(3)	N(00C)-C(00K)	1.332(4)
N(005)-N(00C)	1.329(4)	N(00D)-C(00I)	1.318(4)
N(005)-C(00J)	1.378(4)	O(00E)-N(00F)	1.225(4)
N(005)-C(00M)	1.474(4)	N(00F)-C(00K)	1.427(5)
N(006)-C(00J)	1.391(4)	N(00G)-C(00L)	1.339(4)
N(007)-C(00H)	1.396(4)	C(00H)-C(00I)	1.392(5)
N(008)-N(00B)	1.291(4)	C(00J)-C(00L)	1.393(5)
N(008)-C(00H)	1.354(4)	C(00K)-C(00L)	1.405(5)
N(009)-N(00B)	1.387(4)		
N(00C)-N(005)-C(00J)	111.3(3)	O(00E)-N(00F)-C(00K)	120.1(3)
N(00C)-N(005)-C(00M)	120.5(3)	N(008)-C(00H)-N(007)	122.5(3)
C(00J)-N(005)-C(00M)	128.2(3)	N(008)-C(00H)-C(00I)	110.9(3)
O(002)-N(006)-C(00J)	117.1(3)	C(00I)-C(00H)-N(007)	126.6(3)
O(003)-N(006)-O(002)	123.1(3)	N(009)-C(00I)-C(00H)	102.0(3)
O(003)-N(006)-C(00J)	119.8(3)	N(00D)-C(00I)-N(009)	125.9(3)
O(001)-N(007)-O(004)	123.3(3)	N(00D)-C(00I)-C(00H)	132.1(3)
O(001)-N(007)-C(00H)	119.1(3)	N(005)-C(00J)-N(006)	123.8(3)
O(004)-N(007)-C(00H)	117.6(3)	N(005)-C(00J)-C(00L)	108.3(3)
N(00B)-N(008)-C(00H)	108.6(3)	N(006)-C(00J)-C(00L)	127.8(3)
N(00B)-N(009)-C(00M)	119.3(3)	N(00C)-C(00K)-N(00F)	119.6(3)
C(00I)-N(009)-N(00B)	111.3(3)	N(00C)-C(00K)-C(00L)	114.3(3)
C(00I)-N(009)-C(00M)	128.8(3)	C(00L)-C(00K)-N(00F)	126.1(3)
N(005)-N(00B)-N(009)	107.2(3)	N(00G)-C(00L)-C(00J)	128.3(3)
N(005)-N(00C)-C(00K)	104.6(3)	N(00G)-C(00L)-C(00K)	130.2(3)
O(00A)-N(00F)-C(00K)	115.3(3)	C(00J)-C(00L)-C(00K)	101.5(3)
O(00E)-N(00F)-O(00A)	124.7(3)	N(009)-C(00M)-C(005)	110.1 (3)

MPT-1-rt

O2—N4	1.230 (3)	N3—C00C	1.351 (3)
N7—N6	1.326 (3)	N10—C00F	1.402 (4)
N7—C00F	1.370 (3)	N6—C00L	1.331 (4)
N7—C00K	1.464 (4)	C00C—C00J	1.385 (4)
O3—N10	1.236 (3)	O5—N8	1.237 (4)
O4—N10	1.220 (3)	N8—C00L	1.434 (4)
O1—N4	1.234 (3)	N8—O6	1.209 (4)
N4—C00C	1.395 (4)	C00F—C00I	1.394 (4)
N1—N2	1.386 (3)	N5—C00J	1.319 (3)
N1—C00J	1.354 (4)	N9—C00I	1.333 (4)
N1—C00K	1.431 (3)	C00I—C00L	1.401 (4)
N3—N2	1.287 (3)		
N6—N7—C00F	111.2 (2)	C00J—C00C—N4	126.7 (2)
N6—N7—C00K	120.2 (2)	O5—N8—C00L	114.7 (3)
C00F—N7—C00K	128.5 (2)	O6—N8—O5	125.3 (3)
O2—N4—O1	123.1 (2)	O6—N8—C00L	120.1 (3)
O2—N4—C00C	119.4 (2)	N7—C00F—N10	123.8 (3)
O1—N4—C00C	117.5 (2)	N7—C00F—C00I	108.7 (2)
N2—N1—C00K	119.5 (2)	C00I—C00F—N10	127.5 (3)
C00J—N1—N2	110.9 (2)	C00F—C00I—C00L	100.9 (2)
C00J—N1—C00K	129.1 (2)	N9—C00I—C00F	128.7 (3)
N2—N3—C00C	108.6 (2)	N9—C00I—C00L	130.4 (3)
O3—N10—C00F	116.9 (3)	N1—C00J—C00C	102.3 (2)
O4—N10—O3	123.5 (3)	N5—C00J—N1	125.4 (3)
O4—N10—C00F	119.6 (2)	N5—C00J—C00C	132.3 (3)
N3—N2—N1	107.4 (2)	N1—C00K—N7	110.8 (2)
N7—N6—C00L	104.5 (2)	N6—C00L—N8	119.1 (3)
N3—C00C—N4	122.4 (2)	N6—C00L—C00I	114.6 (3)
N3—C00C—C00J	110.8 (2)	C00I—C00L—N8	126.3 (3)

5. Crystallographic bond Lengths [Å] and angles [°] for MPT-2

MPT-2-170K

N6—N7	1.329 (4)	O4—N8	1.230 (4)
N6—C4	1.382 (5)	N4—N3	1.356 (4)
N6—C3	1.458 (5)	N4—C3	1.438 (5)
N7—C6	1.327 (5)	N4—N5	1.312 (5)
C5—C6	1.412 (5)	N3—C2	1.337 (5)
C5—C4	1.392 (5)	N2—C2	1.339 (5)
C5—N9	1.345 (5)	N5—C1	1.334 (5)
C6—N8	1.418 (5)	C1—C2	1.418 (5)
C4—N10	1.408 (5)	C1—N1	1.415 (5)
O6—N10	1.251 (4)	O1—N1	1.235 (5)
N10—O5	1.227 (4)	O2—N1	1.223 (4)
O3—N8	1.228 (4)		
N7—N6—C4	111.2 (3)	O3—N8—O4	123.9 (4)
N7—N6—C3	117.3 (3)	O4—N8—C6	119.9 (3)
C4—N6—C3	131.2 (3)	N3—N4—C3	122.3 (3)
C6—N7—N6	105.1 (3)	N5—N4—N3	117.4 (3)
C4—C5—C6	101.7 (3)	N5—N4—C3	120.1 (3)
N9—C5—C6	129.4 (4)	C2—N3—N4	103.3 (3)
N9—C5—C4	128.9 (4)	N4—C3—N6	110.2 (3)
N7—C6—C5	113.9 (3)	N4—N5—C1	101.7 (3)
N7—C6—N8	119.2 (3)	N5—C1—C2	111.2 (4)
C5—C6—N8	126.9 (3)	N5—C1—N1	120.9 (4)
N6—C4—C5	108.1 (3)	N1—C1—C2	127.9 (4)
N6—C4—N10	124.6 (3)	N3—C2—C1	106.4 (3)
C5—C4—N10	127.3 (3)	N2—C2—N3	124.0 (4)
O6—N10—C4	115.6 (3)	N2—C2—C1	129.5 (4)
O5—N10—C4	120.6 (3)	O1—N1—C1	116.1 (3)
O5—N10—O6	123.8 (3)	O2—N1—C1	118.7 (4)
O3—N8—C6	116.3 (3)	O2—N1—O1	125.2 (4)

MPT-2-rt

N4—N3	1.321 (4)	N2—C2	1.338 (5)
N4—C3	1.380 (5)	N2—H2A	0.854 (19)
N4—C4	1.447 (5)	N2—H2B	0.860 (19)
N6—N7	1.310 (4)	N9—C5	1.419 (6)
N6—N8	1.345 (5)	N1—C1	1.419 (5)
N6—C4	1.432 (5)	N1—O4	1.219 (5)
O3—N1	1.218 (4)	C3—C2	1.374 (5)
N3—C1	1.324 (5)	N10—H10A	0.8600
O2—N5	1.249 (4)	N10—H10B	0.8600
N7—C5	1.325 (5)	N10—C6	1.331 (5)
N5—O1	1.225 (5)	C1—C2	1.403 (5)
N5—C3	1.418 (5)	C5—C6	1.398 (5)
O5—N9	1.214 (5)	C4—H4A	0.9700
O6—N9	1.236 (5)	C4—H4B	0.9700
N8—C6	1.341 (6)		
N3—N4—C3	110.9 (3)	C2—C3—N5	127.7 (4)
N3—N4—C4	117.1 (3)	H10A—N10—H10B	120.0
C3—N4—C4	131.6 (3)	C6—N10—H10A	120.0
N7—N6—N8	117.0 (3)	C6—N10—H10B	120.0
N7—N6—C4	120.2 (3)	N3—C1—N1	118.8 (4)
N8—N6—C4	122.6 (3)	N3—C1—C2	114.2 (4)
N4—N3—C1	104.8 (3)	C2—C1—N1	127.0 (4)
N6—N7—C5	101.5 (3)	N7—C5—N9	120.4 (4)
O2—N5—C3	115.4 (4)	N7—C5—C6	112.0 (4)
O1—N5—O2	123.7 (4)	C6—C5—N9	127.6 (4)
O1—N5—C3	121.0 (4)	N2—C2—C3	129.0 (4)
C6—N8—N6	103.5 (3)	N2—C2—C1	129.4 (4)
C2—N2—H2A	115 (3)	C3—C2—C1	101.5 (3)
C2—N2—H2B	117 (3)	N4—C4—H4A	109.4
H2A—N2—H2B	128 (4)	N4—C4—H4B	109.4

O5—N9—O6	124.8 (4)	N6—C4—N4	111.0 (3)
O5—N9—C5	119.2 (4)	N6—C4—H4A	109.4
O6—N9—C5	115.9 (4)	N6—C4—H4B	109.4
O3—N1—C1	120.3 (4)	H4A—C4—H4B	108.0
O3—N1—O4	123.0 (4)	N8—C6—C5	105.9 (4)
O4—N1—C1	116.6 (4)	N10—C6—N8	123.8 (4)
N4—C3—N5	123.7 (4)	N10—C6—C5	130.2 (4)
C2—C3—N4	108.6 (3)		

6. ^1H and ^{13}C NMR spectra for all new compounds.

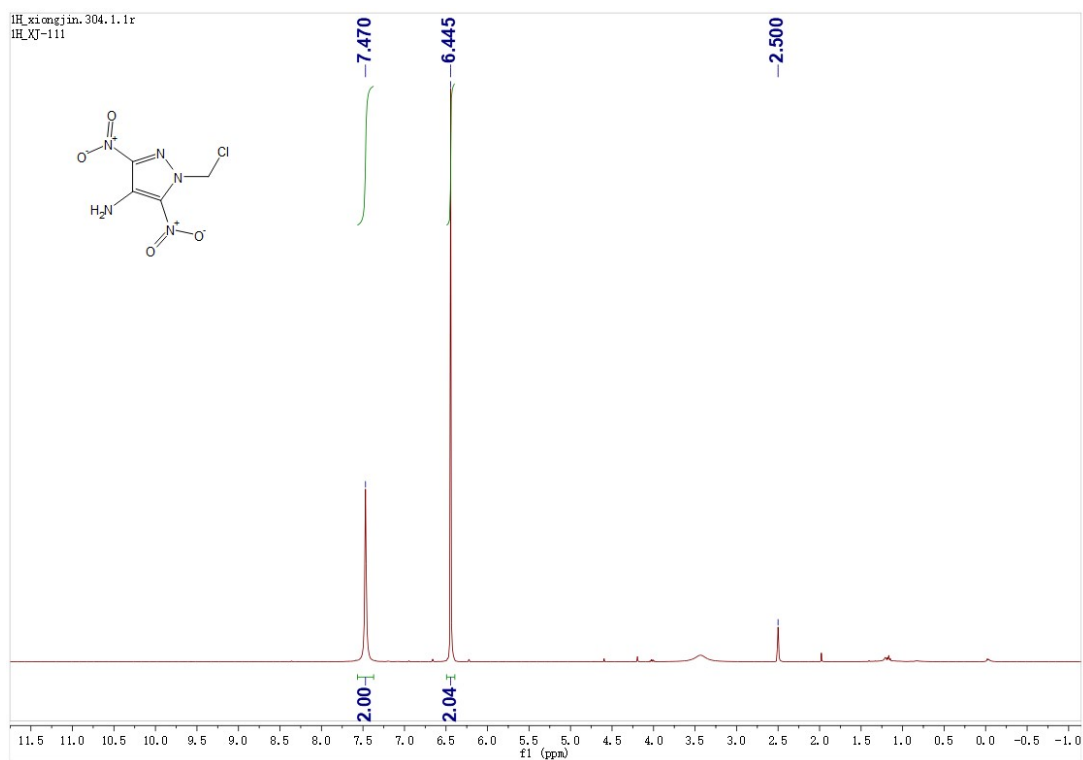


Figure 1. ^1H NMR spectrum of CDPA in d_6 -DMSO.

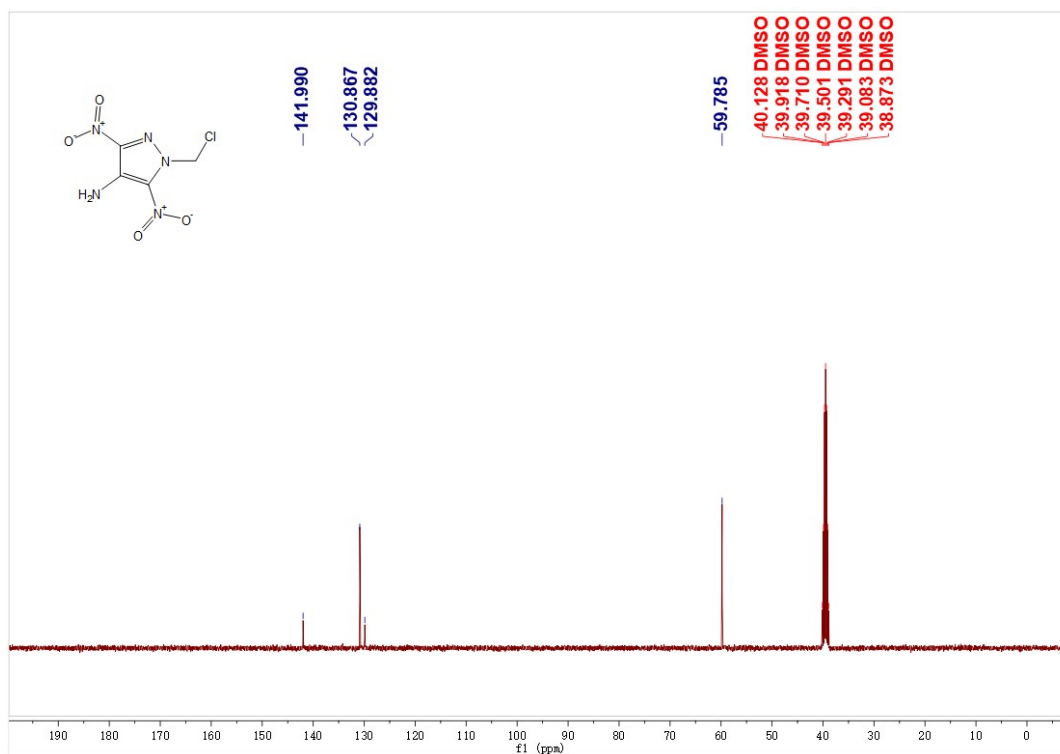


Figure 2. ^{13}C NMR spectrum of CDPA in d_6 -DMSO.

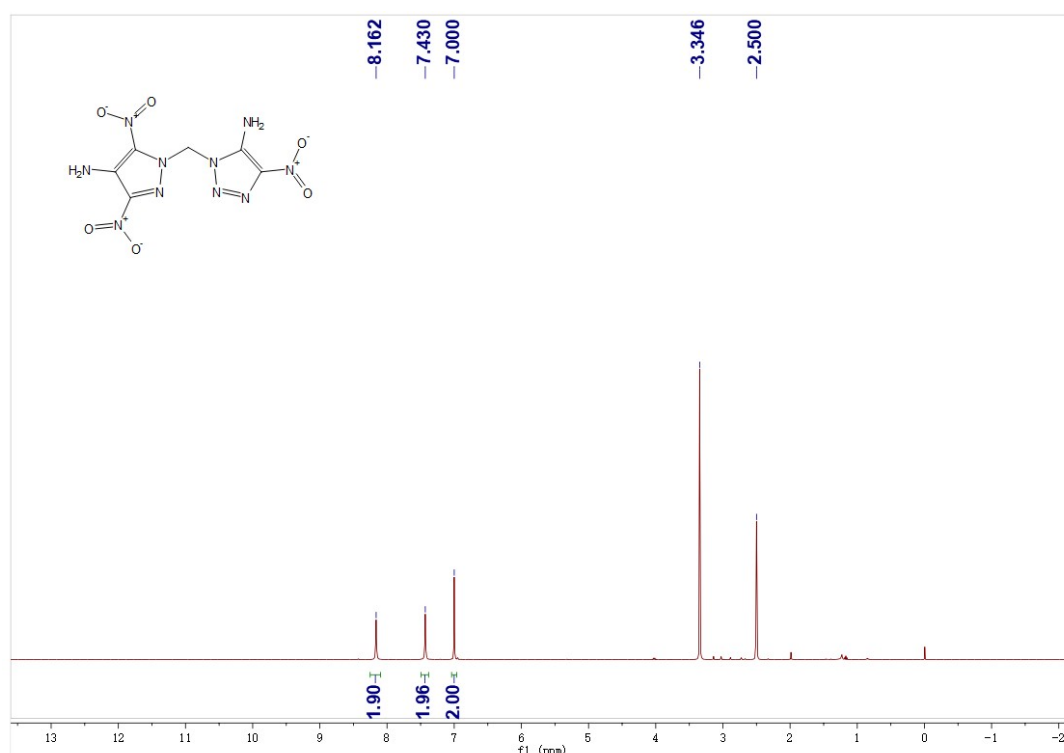


Figure 3. ^1H NMR spectrum of MPT-1 in d_6 -DMSO.

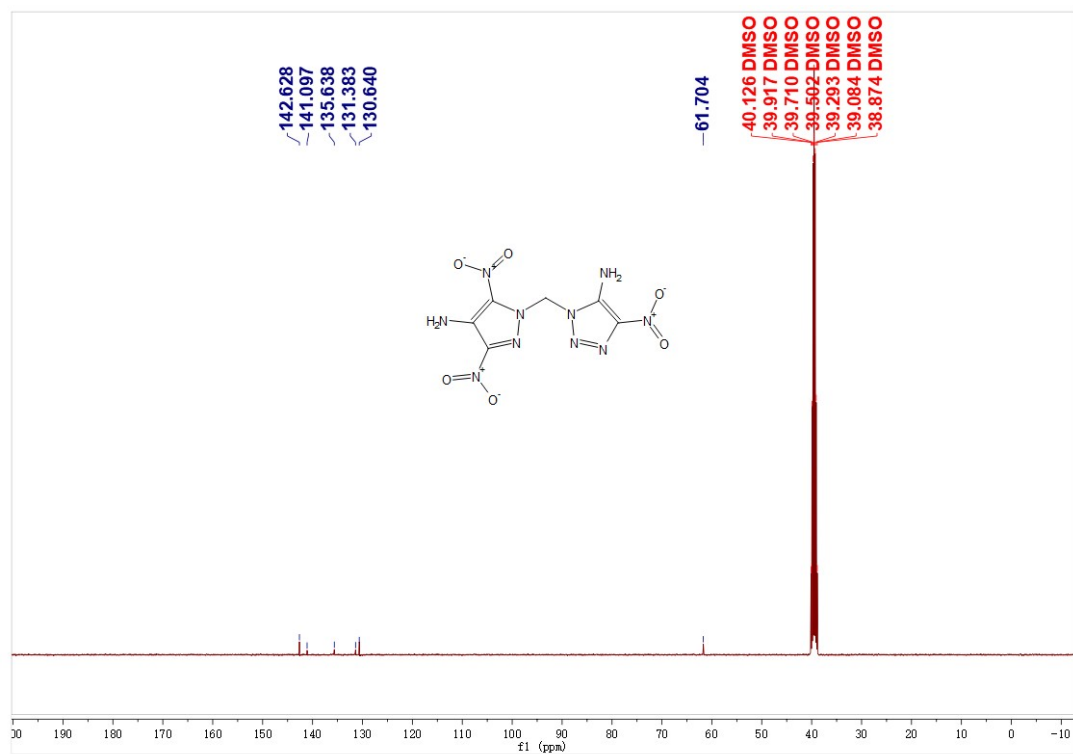


Figure 4. ^{13}C NMR spectrum of MPT-1 in d_6 -DMSO.

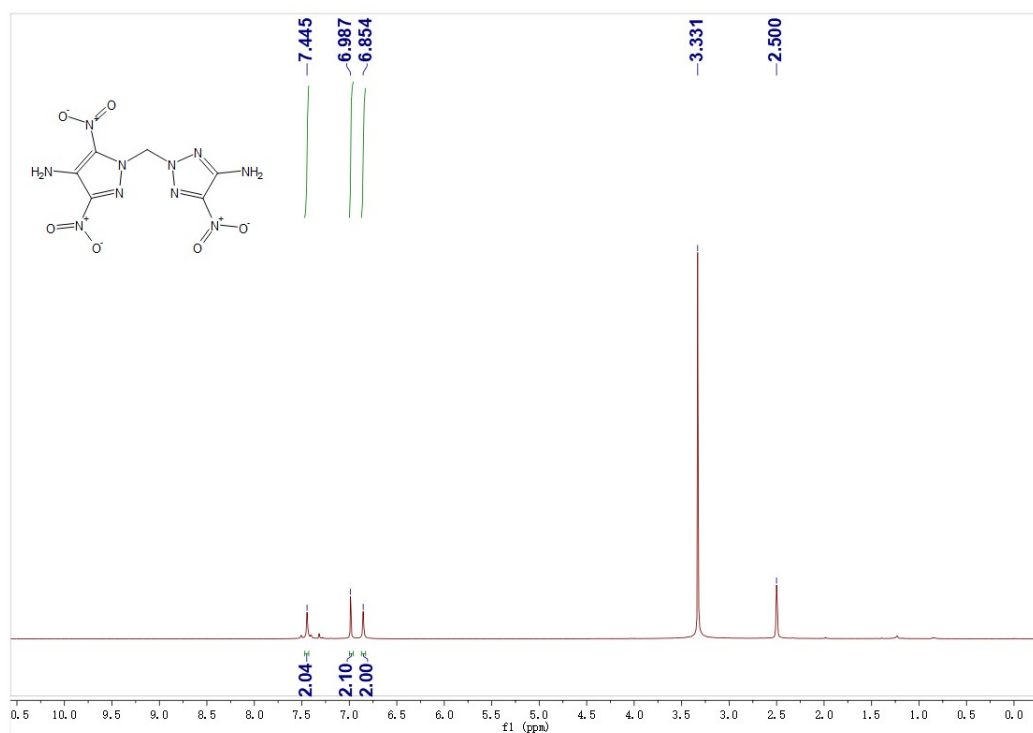


Figure 5. ^1H NMR spectrum of MPT-2 in d_6 -DMSO.

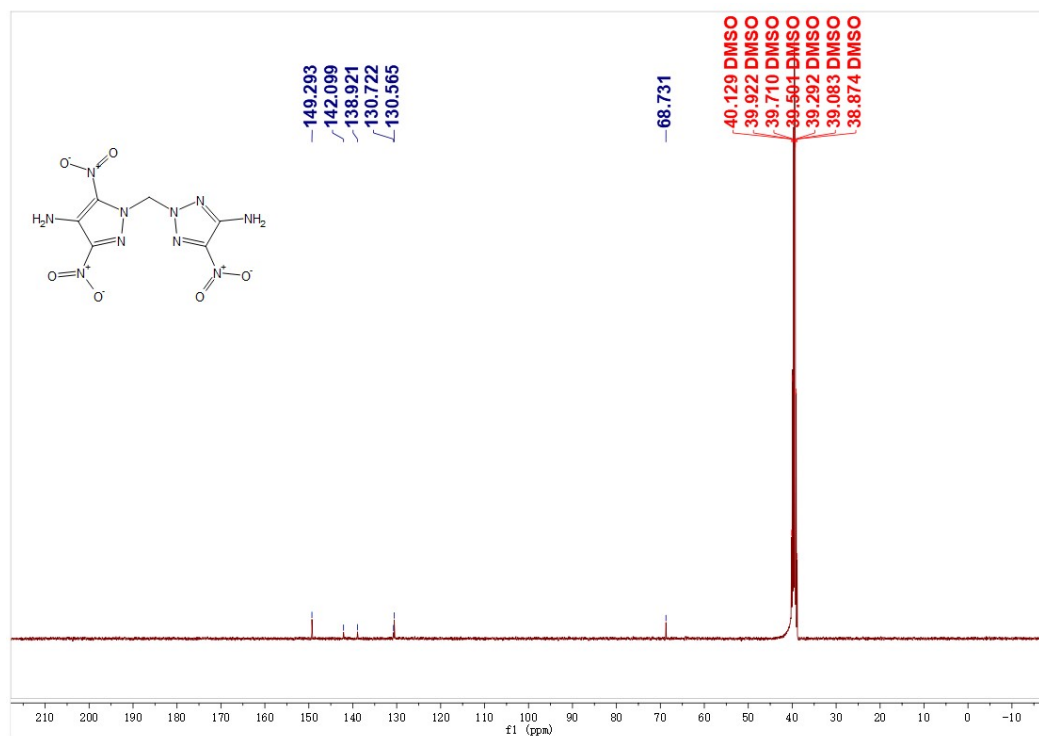


Figure 6. ¹³C NMR spectrum of MPT-2 in d₆-DMSO.

7. DSC curves of the title compounds

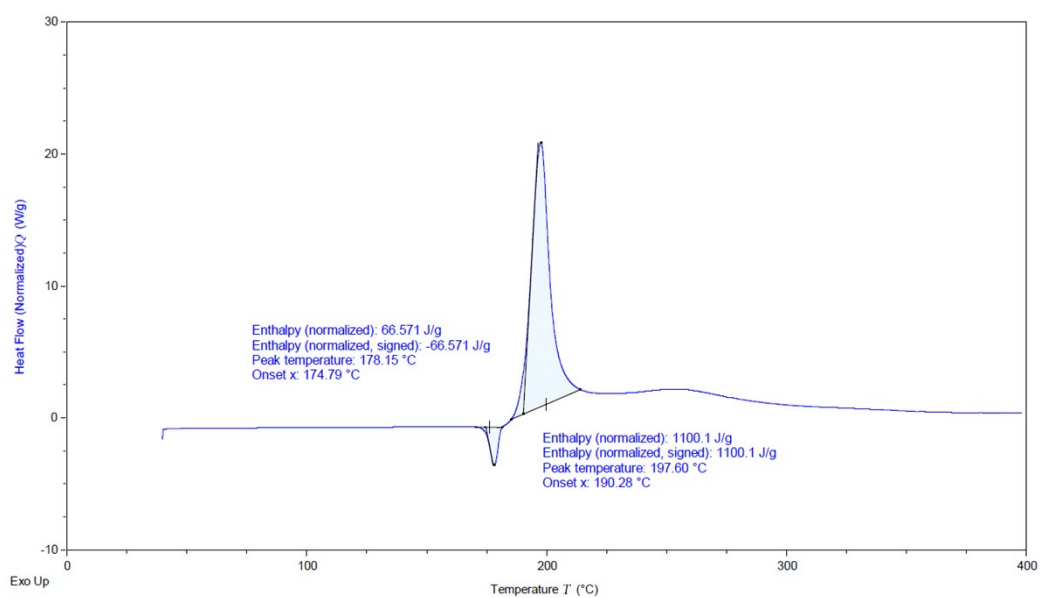


Figure 7. DSC curve of compound MPT-1 at 10 °C min⁻¹

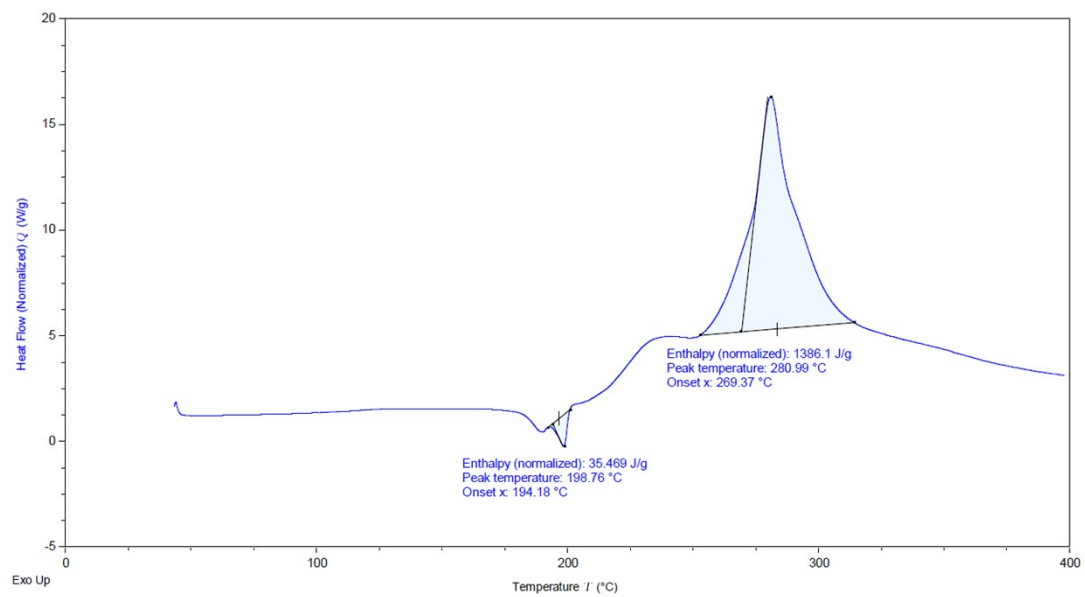


Figure 8. DSC curve of compound **MPT-2** at 10 °C min^{-1}

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