Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Full article (*Cent. Eur. J. Energ. Mater.* 2019, *16*(4): 547-563; DOI 10.22211/cejem/113123) is available in PDF-format, in colour, at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963.pdf

Supporting Information

Please note:
1) The publisher is not responsible for the content of the section Supporting Information.
2) Any queries should be directed to the corresponding Author mentioned below.

Research paper

Crystal Structure and Thermal Behaviour of Imidazolium 2,4,5-Trinitroimidazolate

Chen Jian[1], Lian Pengbao[1], Chen Lizhen[1], Wang Jianlong[1,*], Chen Jun[2]
[1] *School of Chemical Engineering and Technology, North University of China, 030051 Taiyuan, Shanxi, China*
[2] *Oriental Chemical Co., Ltd., 441403 Xiangyang, Hubei, China*
**E-mail:* 619379961@qq.com

Content

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound 3 U(eq) defined as one third of the trace of the orthogonalized U^{ij} tensor

Atom	*x*	*y*	*z*	U(eq)
C1A	2357(3)	5572(2)	4948.1(16)	18.0(5)
C2A	4177(3)	6468(2)	3817.8(17)	19.7(5)
C3A	4304(3)	4990(2)	3901.5(17)	18.9(5)
C4A	2770(3)	672(2)	4606.1(19)	28.1(6)
C5A	1350(3)	913(3)	6071.3(19)	31.4(6)
C6A	1239(3)	–411(3)	6019.8(19)	30.8(6)
C1B	11238(3)	3577(2)	9085.7(16)	18.3(5)
C2B	9213(3)	3548(2)	8512.8(16)	19.1(5)
C3B	9261(3)	4982(2)	8450.8(16)	18.2(5)
C4B	986(3)	8805(2)	8757.8(17)	23.7(5)
C5B	3370(3)	8815(3)	9076(2)	33.9(6)
C6B	3373(3)	7475(3)	9016.1(19)	30.7(6)
N1A	3119(2)	4419.6(19)	4633.1(14)	19.9(4)
N2A	2922(2)	6835.2(19)	4497.6(13)	19.9(4)
N3A	998(2)	5442(2)	5772.4(14)	20.4(4)
N4A	5173(3)	7590(2)	3197.8(16)	29.3(5)
N5A	5411(2)	4040(2)	3364.0(15)	23.3(5)
N6A	2123(3)	–526(2)	5099.7(16)	25.3(5)
N7A	2315(3)	1558(2)	5186.2(16)	28.6(5)
N1B	10583(2)	4995.5(19)	8820.6(13)	19.0(4)
N2B	10498(2)	2639.9(19)	8918.7(13)	19.4(4)
N3B	12698(2)	3050(2)	9564.0(15)	24.1(5)
N4B	8047(3)	2906(2)	8256.5(14)	24.3(5)
N5B	8268(2)	6371(2)	8003.1(14)	22.7(5)
N6B	1878(3)	7492(2)	8814.6(15)	23.9(5)
N7B	1879(3)	9625(2)	8911.3(15)	27.1(5)
O1A	452(2)	4287.2(17)	6104.2(12)	27.2(4)
O2A	466(2)	6510.2(17)	6090.1(13)	31.3(4)
O3A	4582(3)	8853(2)	3117.4(16)	54.2(6)
O4A	6552(2)	7170(2)	2847.6(15)	44.2(5)
O5A	6306(2)	4594.6(19)	2583.9(14)	41.8(5)
O6A	5357(2)	2716.2(17)	3730.8(13)	29.7(4)
O1B	13264(2)	3945.8(18)	9765.4(13)	28.9(4)
O2B	13258(2)	1731.0(18)	9756.7(15)	39.5(5)
O3B	8558(2)	1772.7(19)	8023.1(15)	40.0(5)
O4B	6639(2)	3512.0(19)	8306.3(14)	35.5(5)
O5B	7173(2)	6378.6(18)	7564.6(13)	34.0(4)
O6B	8609(2)	7489.4(17)	8064.6(13)	32.2(4)

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S2. Bond lengths [Å] and angles [°] for compound 3

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
C1A–N1A	1.331(3)	N1A–C1A–N3A	121.09(19)
C1A–N2A	1.330(3)	N2A–C1A–N1A	117.8(2)
C1A–N3A	1.440(3)	N2A–C1A–N3A	121.06(19)
C2A–C3A	1.394(3)	C3A–C2A–N4A	132.6(2)
C2A–N2A	1.339(3)	N2A–C2A–C3A	109.55(1
C2A–N4A	1.462(3)	N2A–C2A–N4A	117.71(19)
C3A–N1A	1.340(3)	C2A–C3A–N5A	132.8(2)
C3A–N5A	1.446(3)	N1A–C3A–C2A	109.01(19)
C4A–N6A	1.317(3)	N1A–C3A–N5A	118.20(19)
C4A–N7A	1.319(3)	N6A–C4A–N7A	107.9(2)
C5A–C6A	1.349(3)	C6A–C5A–N7A	106.7(2)
C5A–N7A	1.361(3)	C5A–C6A–N6A	106.7(2)
C6A–N6A	1.360(3)	N1B–C1B–N2B	118.2(2)
C1B–N1B	1.327(3)	N1B–C1B–N3B	121.16(19)
C1B–N2B	1.333(3)	N2B–C1B–N3B	120.59(19)
C1B–N3B	1.448(3)	C3B–C2B–N4B	132.4(2)
C2B–C3B	1.387(3)	N2B–C2B–C3B	109.60(19)
C2B–N2B	1.339(3)	N2B–C2B–N4B	117.95(19)
C2B–N4B	1.455(3)	C2B–C3B–N5B	132.1(2)
C3B–N1B	1.345(3)	N1B–C3B–C2B	109.38(19)
C3B–N5B	1.441(3)	N1B–C3B–N5B	118.31(19)
C4B–N6B	1.324(3)	N7B–C4B–N6B	108.0(2)
C4B–N7B	1.323(3)	C6B–C5B–N7B	107.1(2)
C5B–C6B	1.344(3)	C5B–C6B–N6B	106.9(2)
C5B–N7B	1.362(3)	C1A–N1A–C3A	101.94(17)
C6B–N6B	1.365(3)	C1A–N2A–C2A	101.69(18)

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S2. continuation

Atom–Atom	Length [Å]	Atom–Atom–Atom	Angle [°]
N3A–O1A	1.226(2)	O1A–N3A–C1A	118.21(18)
N3A–O2A	1.229(2)	O1A–N3A–O2A	124.73(19)
N4A–O3A	1.202(3)	O2A–N3A–C1A	117.06(18)
N4A–O4A	1.215(3)	O3A–N4A–C2A	117.1(2)
N5A–O5A	1.216(2)	O3A–N4A–O4A	125.1(2)
N5A–O6A	1.227(2)	O4A–N4A–C2A	117.7(2)
N3B–O1B	1.228(2)	O5A–N5A–C3A	118.72(19)
N3B–O2B	1.227(2)	O5A–N5A–O6A	124.61(19)
N4B–O3B	1.222(2)	O6A–N5A–C3A	116.66(19)
N4B–O4B	1.218(3)	C4A–N6A–C6A	109.3(2)
N5B–O5B	1.220(2)	C4A–N7A–C5A	109.3(2)
N5B–O6B	1.231(2)	C1B–N1B–C3B	101.40(18)
		C1B–N2B–C2B	101.38(18)
		O1B–N3B–C1B	117.75(18)
		O2B–N3B–C1B	117.34(19)
		O2B–N3B–O1B	124.9(2)
		O3B–N4B–C2B	117.0(2)
		O4B–N4B–C2B	118.25(19)
		O4B–N4B–O3B	124.7(2)
		O5B–N5B–C3B	118.51(19)
		O5B–N5B–O6B	123.9(2)
		O6B–N5B–C3B	117.5(2)
		C4B–N6B–C6B	109.0(2)
		C4B–N7B–C5B	109.0(2)

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound 3

Note: The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

Atom	*U*11	*U*22	*U*33	*U*23	*U*13	*U*12
C1A	16.1(13)	21.7(12)	16.8(11)	–7.1(10)	–0.5(10)	–4.2(10)
C2A	20.9(14)	22.7(12)	16.6(11)	–6(1)	–0.9(10)	–7.9(10)
C3A	18.6(13)	23.3(12)	16.4(11)	–8.4(10)	–1.2(10)	–4.4(10)
C4A	31.3(16)	21.9(13)	29.0(14)	–7.4(11)	–2.2(12)	–3.0(12)
C5A	39.1(17)	26.2(14)	26.5(14)	–7.9(11)	1.9(13)	–7.7(12)
C6A	38.2(17)	25.5(14)	27.9(14)	–5.9(11)	–2.2(12)	–9.9(12)
C1B	17.0(13)	21.2(13)	16.5(11)	–6.2(9)	–1.1(10)	–3.7(10)
C2B	21.7(14)	23.1(12)	13.8(11)	–6.8(9)	–0.7(10)	–6.7(11)
C3B	16.8(13)	20.5(12)	16.0(11)	–5.7(9)	–1.1(10)	–1.8(10)
C4B	28.5(15)	22.3(13)	20.4(12)	–5.5(10)	–3.8(11)	–6.3(11)
C5B	32.7(17)	30.9(15)	41.6(16)	–10.2(12)	–10.5(13)	–9.5(13)
C6B	29.2(16)	26.5(14)	36.0(15)	–9.0(12)	–6.0(12)	–4.2(12)
N1A	20.4(11)	21.6(10)	19.6(10)	–9.2(8)	–2.7(9)	–3.1(9)
N2A	21.0(11)	22(1)	18.1(10)	–7.7(8)	–0.9(9)	–5.9(9)
N3A	20.7(11)	21.6(11)	18.7(10)	–6.7(8)	–1.9(9)	–3.5(9)
N4A	28.1(14)	35.8(13)	27.5(11)	–17(1)	4.8(10)	–9.4(10)
N5A	18.4(11)	29.6(12)	24.2(11)	–13.1(9)	–3.4(9)	–0.6(9)
N6A	32.5(13)	18.9(11)	27.7(11)	–10.3(9)	–6.4(10)	–4.3(10)
N7A	36.2(14)	17.2(11)	32.3(12)	–7.3(10)	–3.4(11)	–6.4(10)
N1B	19.9(11)	19.9(11)	17(1)	–7.7(8)	0.9(8)	–3.2(9)
N2B	20.6(11)	20.8(10)	16.9(10)	–5.9(8)	–1.2(9)	–5.1(9)
N3B	24.6(12)	24.9(12)	23.3(11)	–8.1(9)	–3.6(9)	–4(1)
N4B	26.8(13)	26.9(12)	18.3(10)	–3.9(9)	–4.4(9)	–6.6(10)
N5B	22.9(12)	22.6(11)	19.4(10)	–6.0(9)	1.9(9)	–2.8(9)
N6B	30.7(13)	19.4(11)	25.0(11)	–10.1(9)	–2.8(10)	–7.1(10)
N7B	34.6(14)	18.5(11)	29.5(12)	–7.3(9)	–7(1)	–5.3(10)
O1A	29.8(11)	24.8(9)	27.0(9)	–5.4(7)	1.5(8)	–14.2(8)
O2A	33.1(11)	27.7(10)	32.1(10)	–16.7(8)	8.0(8)	–3.5(8)
O3A	61.6(15)	23.9(11)	66.8(14)	–12.1(10)	20.4(12)	–18(1)
O4A	36.4(13)	48.0(12)	48.1(12)	–20.1(10)	15.9(10)	–19.7(10)
O5A	38.0(12)	43.0(11)	39.7(11)	–19.5(9)	19.5(10)	–10.8(9)
O6A	32.0(11)	22.3(10)	35.8(10)	–13.0(8)	–4.9(8)	–0.1(8)
O1B	27.3(10)	33.4(10)	32.1(10)	–13.3(8)	–7.2(8)	–9.5(8)
O2B	40.2(12)	24.7(10)	56.3(12)	–12.4(9)	–25.8(10)	6.4(9)
O3B	43.8(12)	34.5(11)	54.9(12)	–26.2(9)	–10.8(10)	–9.7(9)
O4B	26.2(11)	39.7(11)	41.8(11)	–10.1(9)	–9.8(9)	–8.1(9)
O5B	27.5(11)	34.3(10)	40.2(11)	–6.8(8)	–16.2(9)	–2.3(8)
O6B	36.6(12)	19.0(9)	41.8(11)	–10.6(8)	–6.9(9)	–3.4(8)

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S4. Hydrogen coordinates ($Å^2 \times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for compound 3

Atom	*x*	*y*	*z*	U(eq)
H4A	3445	865	3948	34
H5A	851	1316	6619	38
H6A	656	–1124	6528	37
H4B	–104	9104	8629	28
H5B	4244	9137	9209	41
H6B	4248	6670	9098	37
H6AA	2340(30)	–1290(30)	4878(19)	30
H7AA	2600(30)	2410(30)	5019(19)	34
H6BA	1550(30)	6750(30)	8758(18)	29
H7BA	1500(30)	10530(30)	8918(19)	32

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

Table S5. Thirty-nine forms of the kinetic model function

Function no.	Integral form, $G(\alpha)$	Differential form, $f(\alpha)$
1	α^2	$(1/2)\alpha^{-1}$
2	$\alpha + (1-\alpha)\ln(1-\alpha)$	$[-\ln(1-\alpha)]^{-1}$
3	$[1-(1-\alpha)^{1/2}]^{1/2}$	$4(1-\alpha)^{1/2}[1-(1-\alpha)^{1/2}]^{1/2}$
4	$[1-(1-\alpha)^{1/2}]^2$	$(1-\alpha)^{1/2}\,[1-(1-\alpha)^{1/2}]^{-1}$
5	$[1-(1-\alpha)^{1/3}]^{1/2}$	$6(1-\alpha)^{2/3}[1-(1-\alpha)^{1/3}]^{1/2}$
6	$[1-(1-\alpha)^{1/3}]^2$	$(3/2)(1-\alpha)^{2/3}[1-(1-\alpha)^{1/3}]^{-1}$
7	$1-(2/3)\alpha-(1-\alpha)^{2/3}$	$(3/2)[(1-\alpha)^{-1/3}-1]^{-1}$
8	$[(1+\alpha)^{1/3}-1]^2$	$(3/2)(1+\alpha)^{2/3}[(1+\alpha)^{1/3}-1]^{-1}$
9	$[(1-\alpha)^{-1/3}-1]^2$	$(3/2)(1-\alpha)^{4/3}[(1+\alpha)^{-1/3}-1]^{-1}$
10	$[-\ln(1-\alpha)]^{1/4}$	$4(1-\alpha)[-\ln(1-\alpha)]^{3/4}$
11	$[-\ln(1-\alpha)]^{1/3}$	$3(1-\alpha)[-\ln(1-\alpha)]^{2/3}$
12	$[-\ln(1-\alpha)]^{2/5}$	$(5/2)(1-\alpha)[-\ln(1-\alpha)]^{3/5}$
13	$[-\ln(1-\alpha)]^{1/2}$	$2(1-\alpha)[-\ln(1-\alpha)]^{1/2}$
14	$[-\ln(1-\alpha)]^{2/3}$	$(3/2)(1-\alpha)[-\ln(1-\alpha)]^{1/3}$
15	$[-\ln(1-\alpha)]^{3/4}$	$(4/3)(1-\alpha)[-\ln(1-\alpha)]^{1/4}$
16	$-\ln(1-\alpha)$	$1-\alpha$
17	$[-\ln(1-\alpha)]^{3/2}$	$(2/3)(1-\alpha)[-\ln(1-\alpha)]^{-1/2}$
18	$[-\ln(1-\alpha)]^2$	$(1/2)(1-\alpha)[-\ln(1-\alpha)]^{-1}$
19	$[-\ln(1-\alpha)]^3$	$(1/3)(1-\alpha)[-\ln(1-\alpha)]^{-2}$
20	$[-\ln(1-\alpha)]^4$	$(1/4)(1-\alpha)[-\ln(1-\alpha)]^{-3}$
21	$\mathrm{Ln}[\alpha/(1-\alpha)]$	$\alpha(1-\alpha)$
22	$\alpha^{1/4}$	$4\alpha^{3/4}$
23	$\alpha^{1/3}$	$3\alpha^{2/3}$
24	$\alpha^{1/2}$	$2\alpha^{1/2}$
25	α	1
26	$\alpha^{3/2}$	$(2/3)\alpha^{-1/2}$
27	$1-(1-\alpha)^{1/4}$	$4(1-\alpha)^{3/4}$
28	$1-(1-\alpha)^{1/3}$	$3(1-\alpha)^{2/3}$
29	$3[1-(1-\alpha)^{1/3}]$	$(1-\alpha)^{2/3}$
30	$1-(1-\alpha)^{1/2}$	$2(1-\alpha)^{1/2}$
31	$2[1-(1-\alpha)^{1/2}]$	$(1-\alpha)^{1/2}$
32	$1-(1-\alpha)^2$	$(1/2)(1-\alpha)^{-1}$
33	$1-(1-\alpha)^3$	$(1/3)(1-\alpha)^{-2}$
34	$1-(1-\alpha)^4$	$(1/4)(1-\alpha)^{-3}$
35	$(1-\alpha)^{-1}$	$(1-\alpha)^2$
36	$(1-\alpha)^{-1}-1$	
37	$(1-\alpha)^{-1/2}$	$2(1-\alpha)^{3/2}$
38	$\ln\alpha$	α
39	$\ln\alpha^2$	$(1/2)\alpha$

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

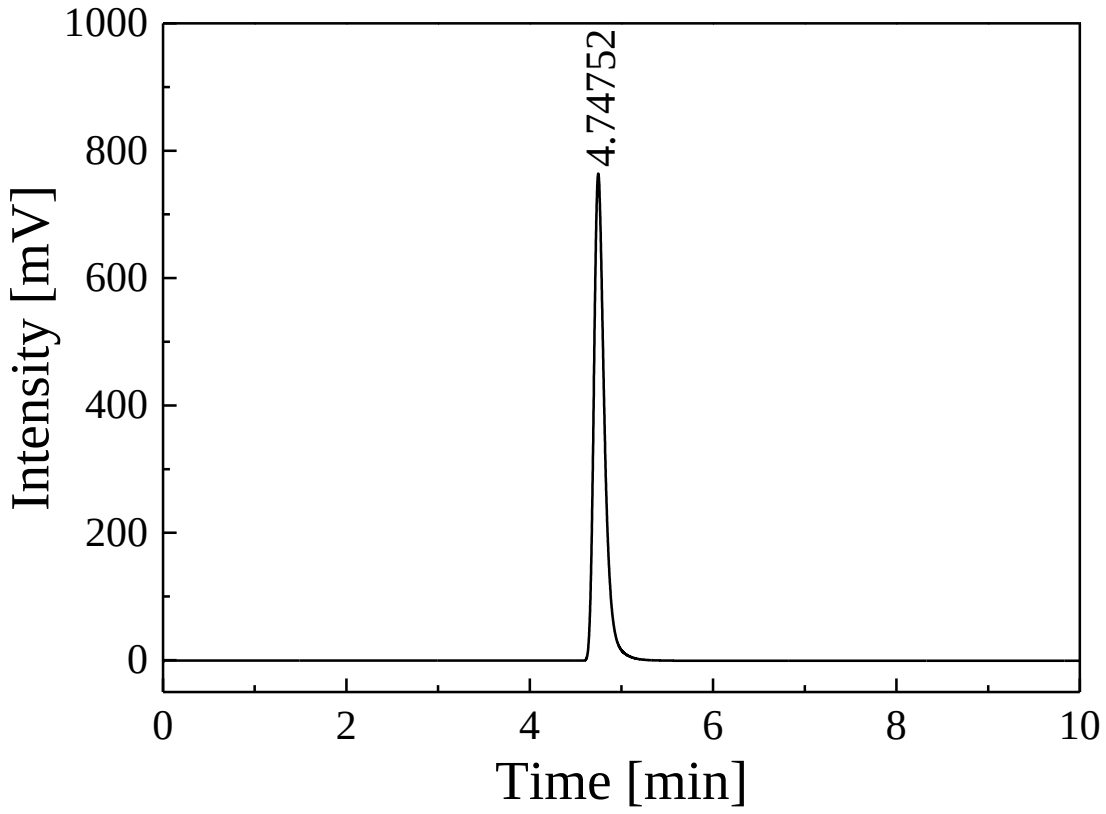


Figure S1. HPLC of compound 3

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

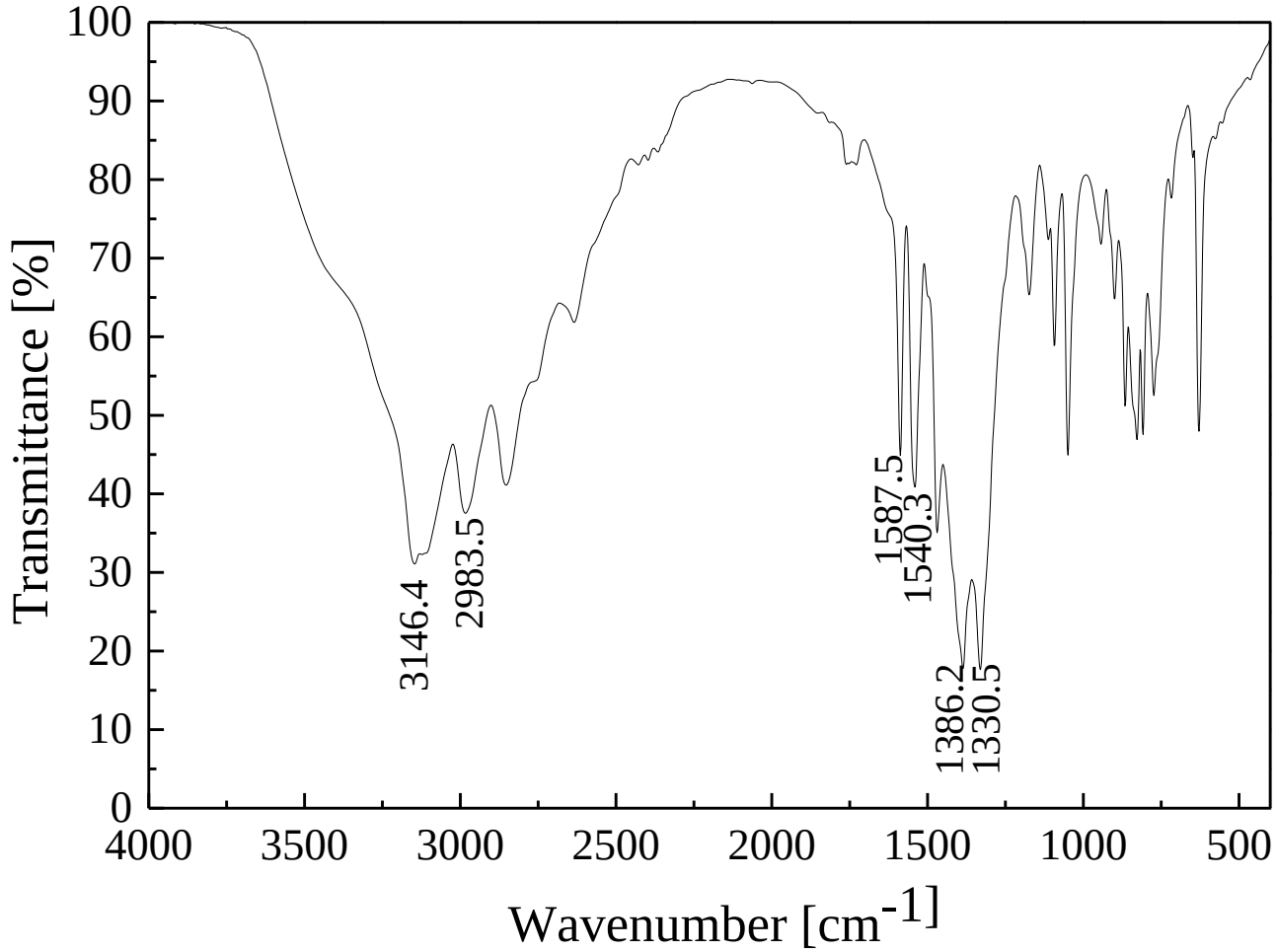


Figure S2. FTIR spectrum of compound 3

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

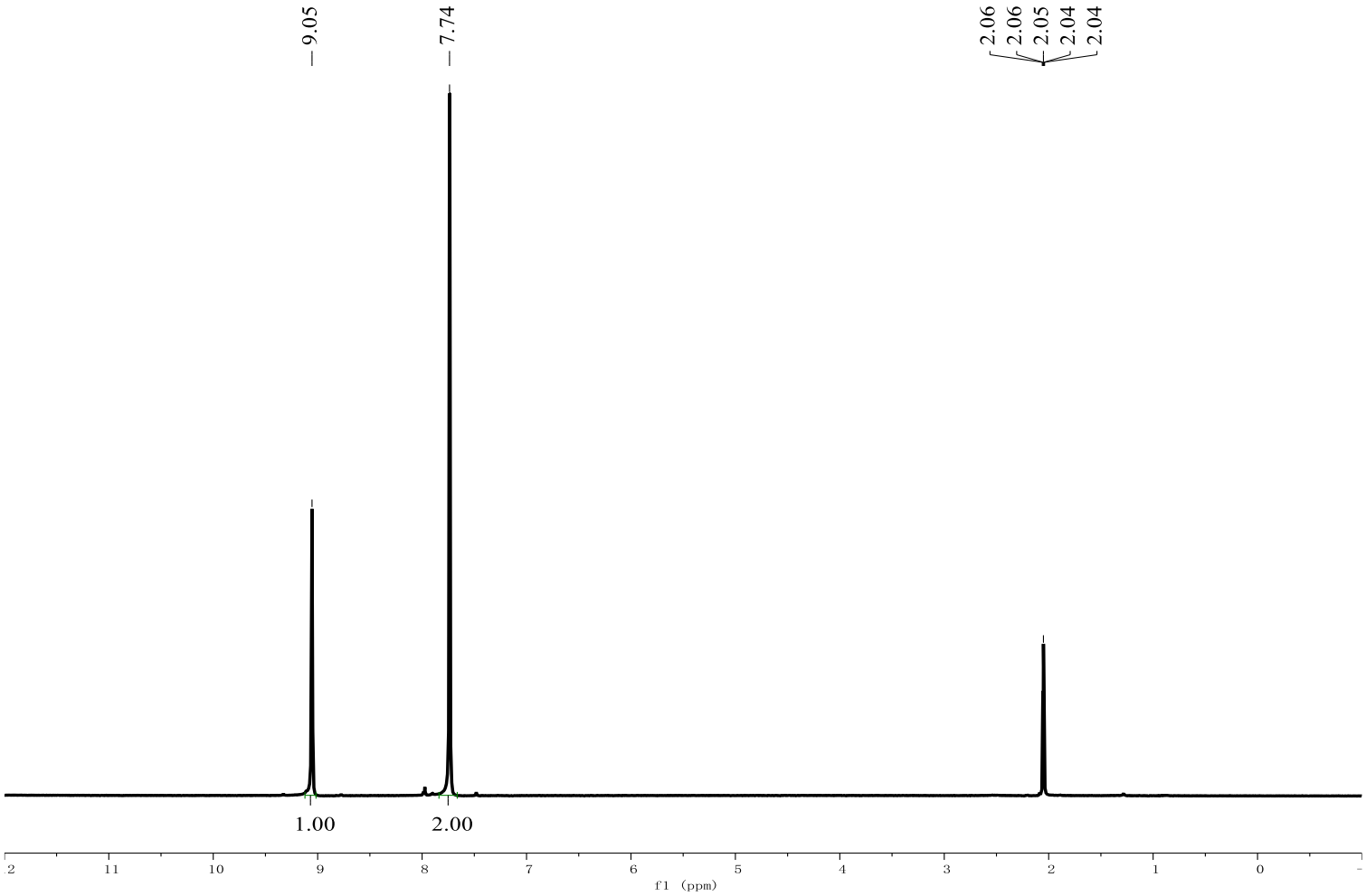


Figure S3. ^{1}H NMR spectrum of compound 3

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

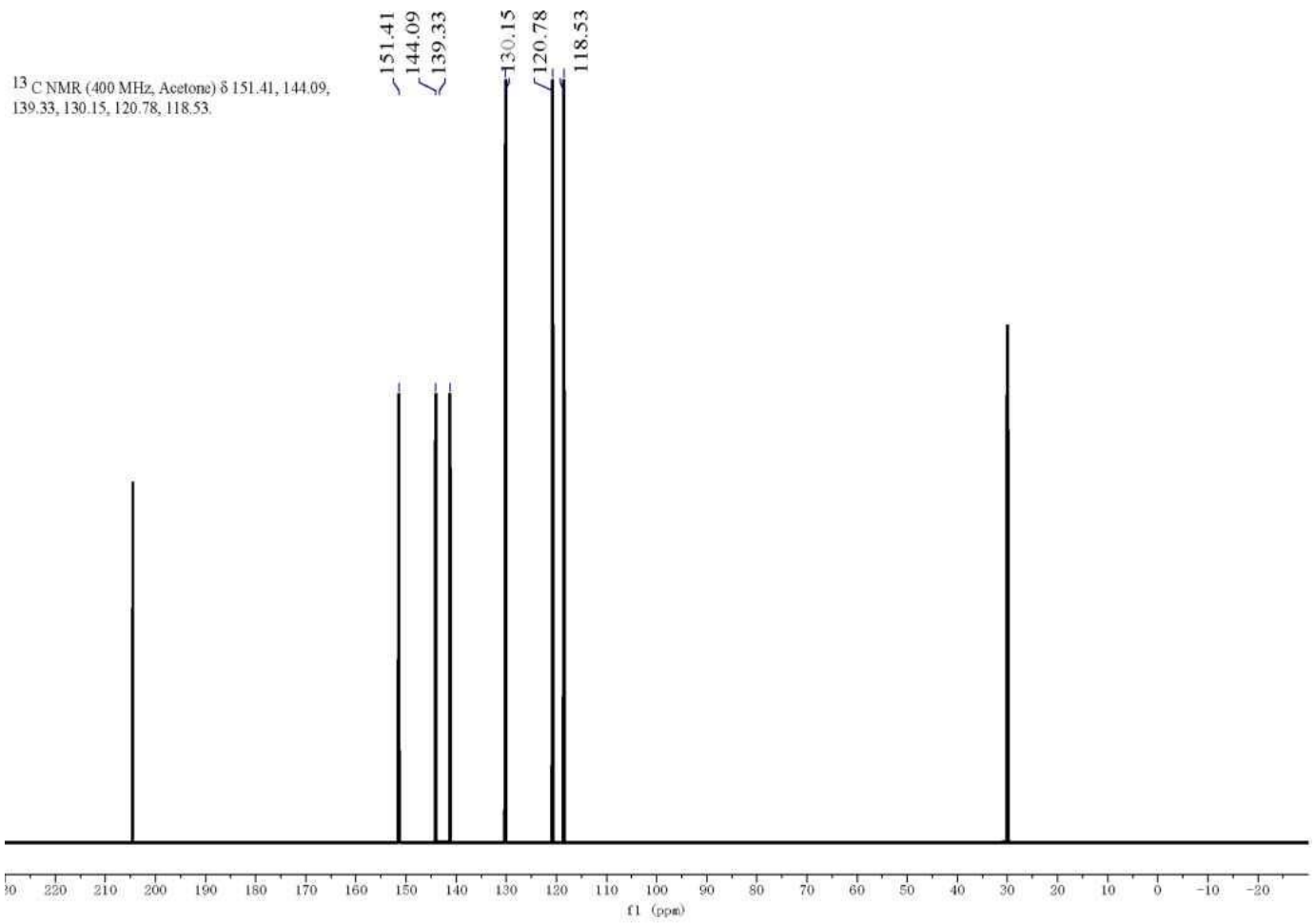
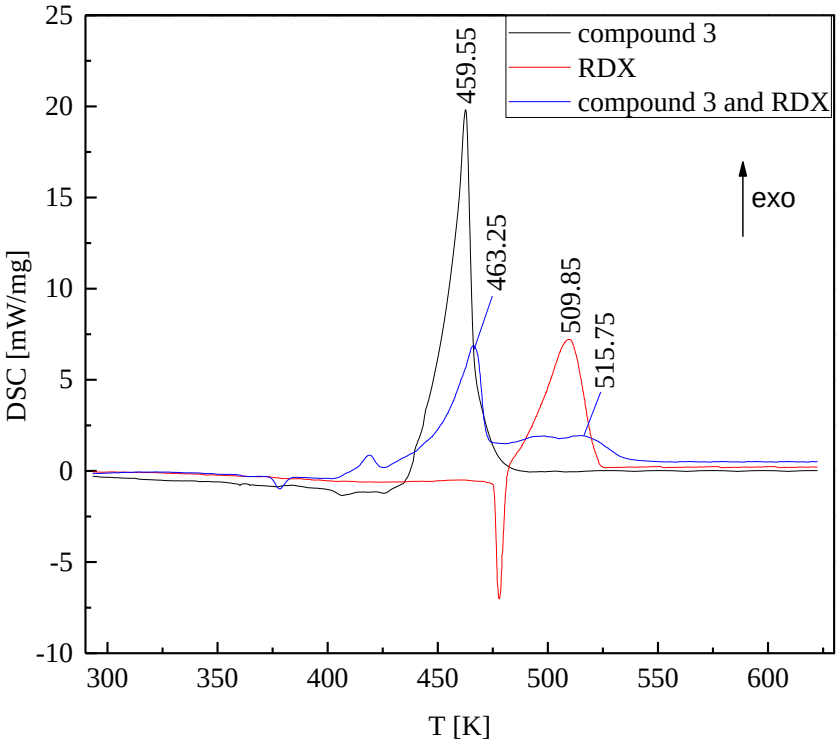
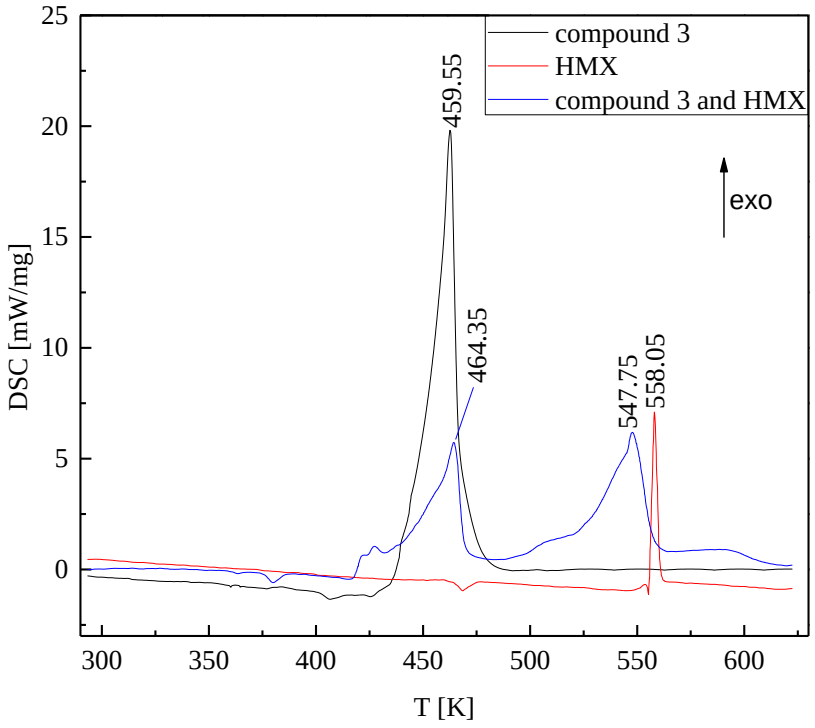


Figure S4. ^{13}C NMR spectrum of compound 3

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf

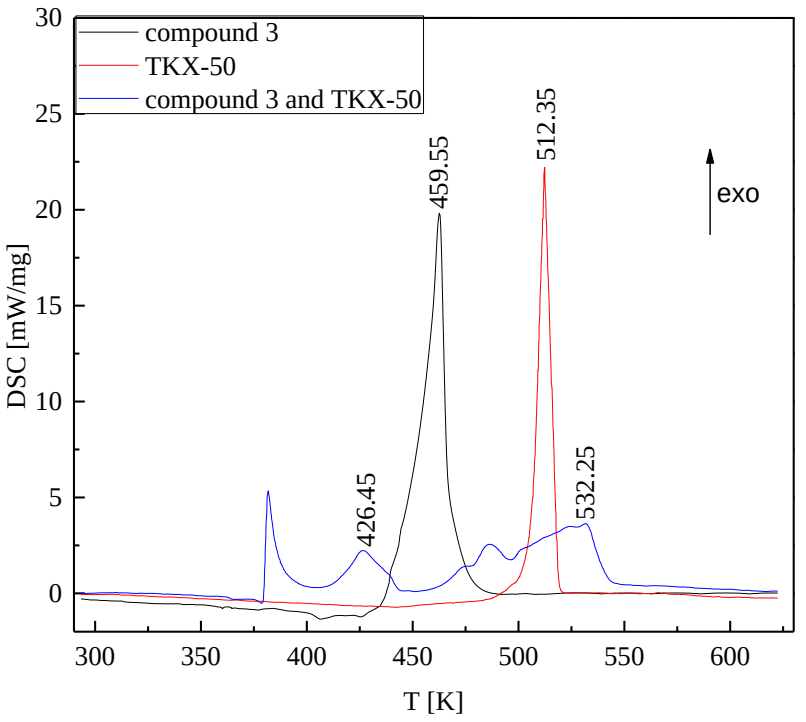


(a)

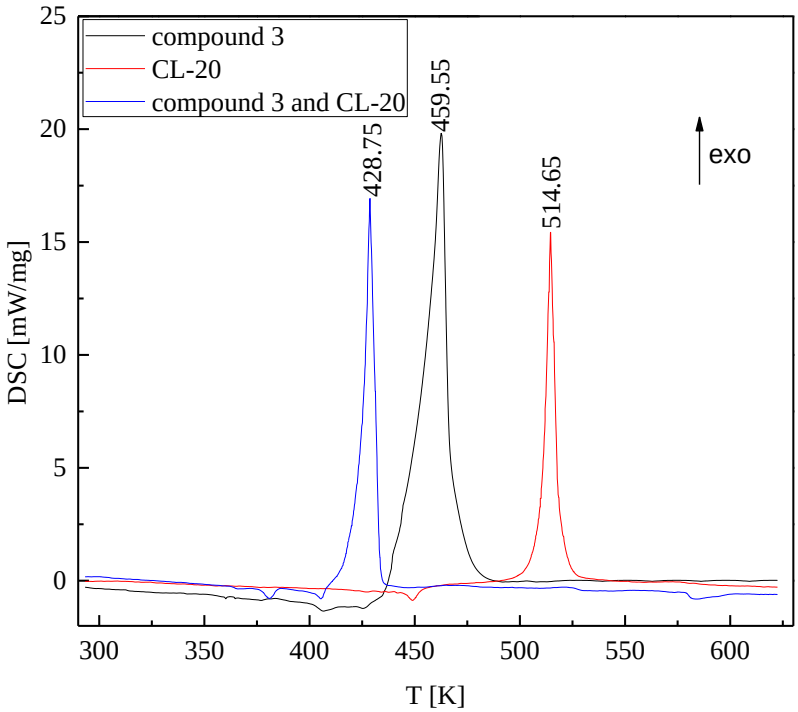


(b)

Cent. Eur. J. Energ. Mater. 2019, *16*(4)
ISSN 1733-7178; e-ISSN 2353-1843
Supporting Information is available at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-16-Number-4-2019/CEJEM_00963_SI.pdf



(c)



(d)

Figure S5. DSC curves of single and mixture systems

Received: July 21, 2018
First published online: December 20, 2019