

# **Supporting Information**

## **Studies on the Synthesis and Properties of 1,1,1-Trinitroprop-2-yl Urea, Carbamate and Nitrocarbamate**

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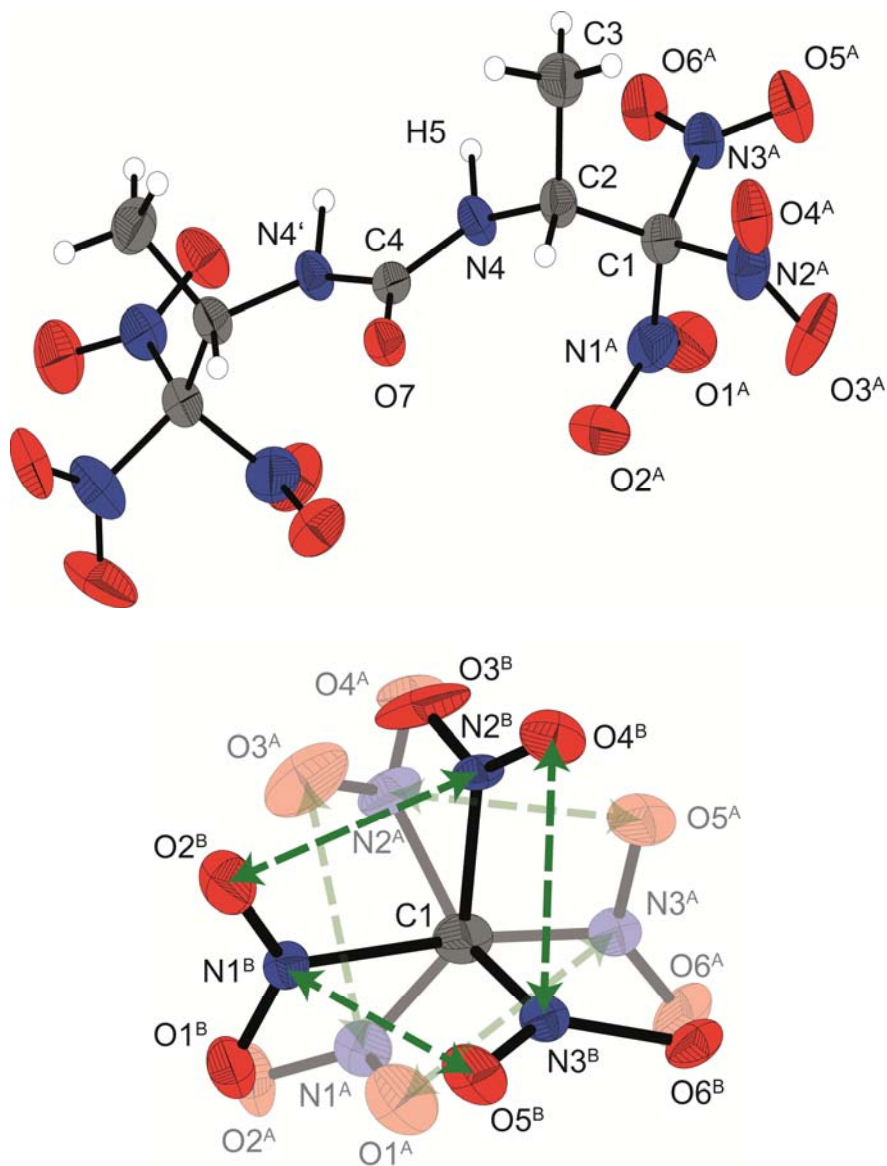
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## 1. Single crystal X-ray diffraction

### 1.1. *N,N'*-bis(1,1,1-trinitropropan-2-yl)urea (**1**)



Selected bond lengths of compound **1**:

C1–N1<sup>A</sup> 1.529(5), C1–N2<sup>A</sup> 1.495(5), C1–N3<sup>A</sup> 1.578(4), C1–C2 1.534(3), O2<sup>A</sup>–N1<sup>A</sup> 1.48(1),  
O1<sup>A</sup>–N1<sup>A</sup> 1.221(8), N2<sup>A</sup>–O3<sup>A</sup> 1.207(8), N2<sup>A</sup>–O4<sup>A</sup> 1.21(1), N3<sup>A</sup>–O5<sup>A</sup> 1.207(5), N3<sup>A</sup>–O6<sup>A</sup>  
1.23(2), C2–C3 1.520(3), C2–N4 1.441(3), C2–H1 1.00(2), C4–N4 1.360(3), C4–O7 1.231(4),  
N4–H5 0.80(2)

Selected angles of compound **1**:

N4–C4–N4 113.7, N4–C4–O7 123.1(1), C4–N4–C2 121.1(2), C2–C1–N1A 113.9(2), C2–C1–N2A 116.3(3), C2–C1–N3A 110.5(2), N2A–C1–N3A 105.0(3), N3A–C1–N1A 104.1(2), N1A–C1–N2A 106.1(3)

Selected torsion angles of compound **1**:

O7–C4–N4–H5 173(2), O7–C4–N4–C2 10.8(2), H5–N4–C2–H1 –172(2), N4–C2–C3–H3 –176(2), N4–C2–C1–N2A –160.6(3), H1–C2–C3–H2 –171(2)

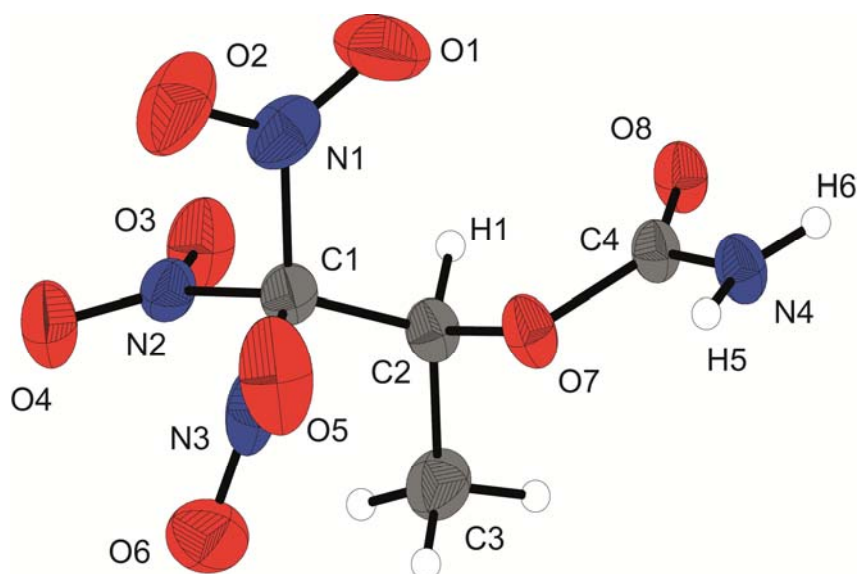
Short contact distances of compound **1**:

O3A–N1A 2.539(6), O1A–N3A 2.601(8), O5A–N2A 2.545(6), O6B–N1B 2.501(1), O4B–N3B 2.573(8), O2B–N2B 2.545(9)

**Table S1.** Hydrogen bonds of compound **1**.

D–H···A			sym. of A	H···A	D–H	D···A	∠, DHA
C2	H1	O6A	$-1/2+x,y,1.5-z$	2.738	1.00	3.640	150.6
N4	H5	O8		2.101	0.80	2.862	158.4
C6	H6A	O7	$-1/2+x,1/2-y,1/2-z$	2.706	0.98	3.683	174.4
C5	H7B	O2A	$-1/2+x,1/2-y,1.5-z$	2.561	0.99	3.329	134.3

## 1.2 1,1,1-trinitropropan-2-yl carbamate (3)



Selected bond lengths of compound **3**:

N1–O1 1.188(4), N1–O2 1.207(3), N1–C1 1.535(3), N2–O3 1.204(3), N2–O4 1.201(3), N2–C1 1.520(3), N3–O5 1.198(4), N3–O6 1.224(3), N3–C1 1.516(3), N4–C4 1.320(3), N4–H5 0.81(2), N4–H6 0.81(3), O7–C2 1.427(3), O7–C4 1.375(3), O8–C4 1.216(2), C1–C2 1.509(3), C2–C3 1.507(4), C2–H1 0.95(3), C3–H2 1.02(3), C3–H3 0.94(5), C3–H4 1.03(4)

Selected angles of compound **3**:

C2–C1–N3 111.3(2), C2–C1–N2 112.6(2), C2–C1–N1 112.8(2), O7–C2–H1 112(2), O7–C2–C3 109.6(2), H1–C2–C3 112(2), N2–C1–N1 103.5(2), N1–C1–N3 107.4(2), N3–C1–N2 108.8(2), C2–O7–C4 115.9(2), O7–C4–O8 122.4(2), O8–C4–N4 127.1(2), O7–C4–N4 110.4(2)

Selected torsion angles of compound **3**:

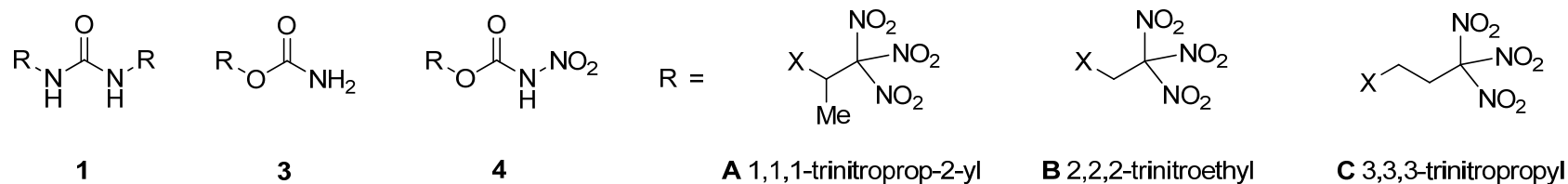
H6–N4–C4–O7 –180(2), H6–N4–C4–O8 1(2), N4–C4–O7–C2 –176.0(2), H1–C2–C3–H3 176(3), O7–C2–C3–H2 169(2), H1–C2–C1–N3 –174(2), O7–C2–C1–N2 –179.0(2)

Short contact distances of compound **3**:

O7–N3 2.749(3), O5–N1 2.625(3), O2–N2 2.796(3), O4–N3 2.664(3)

**Table S2.** Hydrogen bonds of compound **3**.

D–H···A			sym. of A	H···A	D–H	D···A	∠, DHA
N4	H6	O8	$1-x, 1-y, 1-z$	2.214	0.81	2.969	156.3
C3	H2	O4	$2-x, -y, 1-z$	2.796	1.02	3.761	159.0
N4	H5	O8	$x, 1/2-y, -1/2+z$	2.328	0.81	3.124	167.7
C3	H4	O5	$x, 1/2-y, -1/2+z$	2.735	1.03	3.603	142.3



**Table S3.** Calculated detonation and combustion parameters (using EXPLO5 V6.02 EOS BKWG-S).

	1A	3A	4A	1B	3B	4B	1C	3C	4C
	C <sub>7</sub> H <sub>10</sub> N <sub>8</sub> O <sub>13</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	C <sub>4</sub> H <sub>5</sub> N <sub>5</sub> O <sub>10</sub>	C <sub>5</sub> H <sub>6</sub> N <sub>8</sub> O <sub>13</sub>	C <sub>3</sub> H <sub>4</sub> N <sub>4</sub> O <sub>8</sub>	C <sub>3</sub> H <sub>3</sub> N <sub>5</sub> O <sub>10</sub>	C <sub>7</sub> H <sub>10</sub> N <sub>8</sub> O <sub>13</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O <sub>8</sub>	C <sub>4</sub> H <sub>5</sub> N <sub>5</sub> O <sub>10</sub>
density RT	1.82	1.73	1.58	1.86	1.82	1.72	1.71	1.73	1.70
<i>T<sub>m</sub></i> /°C (onset)	142	81	(liquid)	185	91	109	-	78	68
<i>T<sub>dec</sub></i> /°C (onset)	144	154	133	187	169	153	160	152	134
<i>IS</i> /J	8	40	15	3	40	10	20	> 40	30
<i>FS</i> /N	360	360	>360	160	64	96	120	> 360	360
<i>ESD</i> /J	0.20	0.15	-	0.30	0.15	0.10	0.40	0.30	0.20
<i>N</i> /%	27.1	23.5	24.7	29.0	25.0	26.0	27.1	23.5	24.7
<i>O</i> /%	50.2	53.8	56.5	53.9	57.1	59.5	50.2	53.8	56.5
<i>N+O</i> /%	77.3	77.3	81.2	82.9	82.1	85.5	77.3	77.3	81.2
<i>Ω<sub>CO</sub></i> /%	+3.9	+6.7	+19.8	+20.7	+21.4	+32.7	+3.9	+6.7	+19.8
<i>Ω<sub>CO2</sub></i> /%	-20.2	-20.2	-2.8	0.00	+0.0	+14.9	-20.2	-20.2	-2.8
<i>ΔH<sub>f</sub></i> /kJ mol <sup>-1</sup>	-367	-500	-368	-307	-459	-366	-522	-504	-402
<i>ΔU<sub>f</sub></i> /kJ kg <sup>-1</sup>	-793	-2005	-1213	-708	-1961	-1277	-1092	-2021	-1331
<i>Q<sub>v</sub></i> /kJ kg <sup>-1</sup>	-5390	-4675	-5878	-5970	-5286	-4456	-5095	-4662	-5809
<i>T<sub>ex</sub></i> /K	3631	3334	4332	4181	3780	3618	3605	3328	4175
<i>V<sub>0</sub></i> /L kg <sup>-1</sup>	724	744	762	755	761	750	732	724	755
<i>P<sub>Cl</sub></i> /kbar	321	266	228	343	302	232	268	265	269
<i>v<sub>Det</sub></i> /m s <sup>-1</sup>	8469	7900	7680	8915	8530	7704	7937	7896	8134
<i>I<sub>s</sub></i> /s	253	236	257	257	246	232	245	237	256
<i>I<sub>s</sub></i> /s (15 % Al)	267	255	262	263	254	251	263	256	261
<i>I<sub>s</sub></i> /s (15 % Al, 14 % binder)	249	240	254	256	247	261	245	240	253