

## Supplementary Information

### Energetic Alliance of Tetrazole-1-oxides and 1,2,5-Oxadiazoles

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#### 1 X-ray Diffraction

Suitable single crystals of the described compounds (**3–6**, **11,12**, **14–17**, **20** and **23**) were measured by X-ray diffraction. For all compounds, an Oxford Xcalibur3 diffractometer with a CCD area detector was employed for data collection using Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). By using the CRYCALISPRO software<sup>[S1]</sup> the data collection and reduction were performed. The structures were solved by direct methods (SIR-92<sup>[S3]</sup>, SIR-97<sup>[S3]</sup> or SHELXS-97<sup>[S4]</sup>) and refined by full-matrix least-squares on *F*<sup>2</sup> (SHELXL <sup>[S4]</sup>) and finally checked using the PLATON software <sup>[S5]</sup> integrated in the WinGX software suite<sup>[S6]</sup>. The non-hydrogen atoms were refined anisotropically and the hydrogen atoms were located and freely refined. The absorptions were corrected by a SCALE3 ABSPACK multiscan method<sup>[S7]</sup>. In the case of chiral space groups “Friedel pairs” were merged using the SHELX command “MERG 3”. DIAMOND2 plots are shown with thermal ellipsoids at the 50% probability level.

**Table S1** Crystallographic data of **3–6**.

<b>Compound</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>
Formula	C <sub>4</sub> H <sub>6</sub> N <sub>6</sub> O <sub>3</sub>	C <sub>4</sub> H <sub>6</sub> N <sub>6</sub> O <sub>4</sub>	C <sub>4</sub> H <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>3</sub>	C <sub>4</sub> H <sub>2</sub> Cl <sub>2</sub> N <sub>4</sub> O <sub>4</sub>
FW [g mol <sup>-1</sup> ]	186.15	202.15	225.00	241.00
Crystal system	monoclinic	monoclinic	monoclinic	orthorhombic
Space Group	C2/c (No. 15)	P2 <sub>1</sub> /n (No. 14)	P2 <sub>1</sub> /n (No. 14)	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> (No. 19)
Color/Habit	colorless rod	colorless block	light-yellow block	colorless plate
Size [mm]	0.10×0.28×0.32	0.14×0.19×0.23	0.17×0.23×0.47	0.04×0.24×0.25
<i>a</i> [Å]	12.844(3)	6.9708(14)	8.2678(6)	6.9850(5)
<i>b</i> [Å]	8.919(5)	14.408(2)	11.2186(7)	8.4845(5)
<i>c</i> [Å]	6.988(4)	7.8104(13)	8.5693(5)	13.8574(9)
α [°]	90	90	90	90
β [°]	112.147(5)	105.99(2)	99.912(6)	90
γ [°]	90	90	90	90
<i>V</i> [Å <sup>3</sup> ]	741.5(6)	754.1(2)	782.97(9)	821.25(9)
<i>Z</i>	4	4	4	4
ρ <sub>calc.</sub> [g cm <sup>-3</sup> ]	1.668	1.781	1.909	1.949
μ [mm <sup>-1</sup> ]	0.143	0.158	0.807	0.785
<i>F</i> (000)	384	416	448	480
λ <sub>MoKα</sub> [Å]	0.71073	0.71073	0.71073	0.71073
<i>T</i> [K]	100	173	100	100
θ min-max [°]	4.6, 26.0	4.5, 26.5	4.2, 26.0	4.1, 26.0
Dataset <i>h</i> ; <i>k</i> ; <i>l</i>	-13:15;-10:10;-8:8	-8:7; -17:18; -9:9	-10:10;-13:13;-10:10	-8:4;-10:10;-16:17
Reflect. coll.	2426	3900	5523	4265
Independ. refl.	725	1547	1531	1607
<i>R</i> <sub>int</sub>	0.037	0.026	0.035	0.037
Reflection obs.	725	1301	1531	1607
No. parameters	72	151	126	135
<i>R</i> <sub>1</sub> (obs)	0.0388	0.0485	0.0291	0.0270
w <i>R</i> <sub>2</sub> (all data)	0.1058	0.1288	0.0736	0.0616
<i>S</i>	1.08	1.14	1.06	1.04
Resd. Dens. [e Å <sup>-3</sup> ]	-0.23, 0.22	-0.22, 0.34	-0.31, 0.31	-0.26, 0.55
Device type	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD
Solution	SHELXS-97	SIR-97	SIR-92	SIR-92
Refinement	SHELXL-97	SHELXL-97	SHELXL-97	SHELXL-97
Absorpt. corr.	multi-scan	multi-scan	multi-scan	multi-scan
CCDC	988408	988403	988407	988406

**Table S2** Crystallographic data of **11**, **12**, **14** and **15**.

<b>Compound</b>	<b>11</b>	<b>12</b>	<b>14</b>	<b>15</b>
Formula	K <sub>2</sub> C <sub>4</sub> H <sub>4</sub> N <sub>10</sub> O <sub>5</sub>	K <sub>2</sub> C <sub>4</sub> N <sub>10</sub> O <sub>4</sub>	C <sub>4</sub> H <sub>10</sub> N <sub>12</sub> O <sub>7</sub>	C <sub>4</sub> H <sub>8</sub> N <sub>12</sub> O <sub>3</sub>
FW [g mol <sup>-1</sup> ]	350.37	330.34	338.24	272.18
Crystal system	monoclinic	triclinic	monoclinic	orthorhombic
Space Group	<i>P</i> 2 <sub>1</sub> / <i>c</i> (No. 14)	<i>P</i> -1 (No. 2)	<i>P</i> 2 <sub>1</sub> (No. 4)	<i>Pbca</i> (No. 61)
Color/Habit	colorless block	colorless rod	colorless block	colorless needles
Size [mm]	0.12×0.19×0.26	0.09×0.13×0.20	0.11×0.18×0.31	0.04×0.07×0.15
<i>a</i> [Å]	7.4337(4)	7.1412(6)	8.0286(12)	14.5573(13)
<i>b</i> [Å]	21.6146(9)	7.2056(8)	8.0668(11)	7.5523(7)
<i>c</i> [Å]	7.5901(4)	11.4980(9)	9.6666(15)	19.5093(14)
α [°]	90	89.658(7)	90	90
β [°]	97.741(5)	73.514(7)	90.004(12)	90
γ [°]	90	64.814(9)	90	90
<i>V</i> [Å <sup>3</sup> ]	1208.44(10)	508.88(9)	626.06(16)	2144.9(3)
<i>Z</i>	4	2	2	8
ρ <sub>calc.</sub> [g cm <sup>-3</sup> ]	1.926	2.156	1.794	1.686
μ [mm <sup>-1</sup> ]	0.830	0.972	0.165	0.143
<i>F</i> (000)	704	328	348	1120
λ <sub>MoKα</sub> [Å]	0.71073	0.71073	0.71073	0.71073
<i>T</i> [K]	400	100	173	293
θ min-max [°]	4.2, 26.0	4.2, 26.0	4.2, 27.5	4.2, 27.0
Dataset <i>h</i> ; <i>k</i> ; <i>l</i>	-9:9; -25:26; -8:9	-8:8; -8:8; -14:14	-9:10; -10:9; -12:9	-11:18; -9:4; -21:24
Reflect. coll.	9113	7459	3674	5832
Independ. refl.	2362	1985	1544	2335
<i>R</i> <sub>int</sub>	0.031	0.037	0.036	0.047
Reflection obs.	2093	1985	1544	1518
No. parameters	206	181	248	204
<i>R</i> <sub>1</sub> (obs)	0.0254	0.0255	0.0346	0.0465
<i>wR</i> <sub>2</sub> (all data)	0.0610	0.0595	0.0635	0.0959
<i>S</i>	1.05	1.07	1.04	1.01
Resd. Dens. [e Å <sup>-3</sup> ]	-0.28, 0.27	-0.23, 0.32	-0.22, 0.23	-0.24, 0.21
Device type	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD
Solution	SIR-92	SIR-92	SIR-92	SHELXS-97
Refinement	SHELXL-97	SHELXL-97	SHELXL-97	SHELXL-97
Absorpt. corr.	multi-scan	multi-scan	multi-scan	multi-scan
CCDC	988412	988409	988405	988414

**Table S3** Crystallographic data of **16**, **17**, **20** and **23**.

Compound	16	17	20	23
Formula	C <sub>4</sub> H <sub>8</sub> N <sub>12</sub> O <sub>4</sub>	C <sub>4</sub> H <sub>10</sub> N <sub>14</sub> O <sub>3</sub>	C <sub>6</sub> H <sub>12</sub> N <sub>16</sub> O <sub>4</sub>	C <sub>6</sub> H <sub>14</sub> N <sub>18</sub> O <sub>4</sub>
FW [g mol <sup>-1</sup> ]	288.22	302.26	372.32	402.35
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space Group	<i>P</i> 2 <sub>1</sub> / <i>n</i> (No. 14)	<i>P</i> -1 (No. 2)	<i>C</i> 2/ <i>c</i> (No. 15)	<i>P</i> 2 <sub>1</sub> / <i>n</i> (No. 14)
Color/Habit	colorless rod	colorless plate	colorless block	colorless block
Size [mm]	0.10x0.15x0.20	0.05x0.12x0.36	0.13x0.21x0.29	0.20x0.23x0.25
<i>a</i> [Å]	7.5509(13)	3.7659(3)	14.7455(8)	7.0135(7)
<i>b</i> [Å]	7.8440(15)	11.0046(14)	11.7557(6)	31.347(2)
<i>c</i> [Å]	18.562(3)	14.3912(16)	10.6941(6)	7.9795(7)
α [°]	90	97.056(10)	90	90
β [°]	94.987(16)	95.040(8)	129.904(5)	115.793(12)
γ [°]	90	98.978(9)	90	90
<i>V</i> [Å <sup>3</sup> ]	1095.3(3)	581.14(11)	1422.05(17)	1579.5(3)
<i>Z</i>	4	2	4	4
ρ <sub>calc.</sub> [g cm <sup>-3</sup> ]	1.748	1.727	1.739	1.692
μ [mm <sup>-1</sup> ]	0.152	0.146	0.146	0.142
<i>F</i> (000)	592	312	768	832
λ <sub>MoKα</sub> [Å]	0.71073	0.71073	0.71073	0.71073
<i>T</i> [K]	293	236	100	100
θ min-max [°]	4.4, 26.0	4.3, 27.0	4.3, 26.7	4.2, 26.3
Dataset <i>h</i> ; <i>k</i> ; <i>l</i>	-9:9; -9:9; -22:14	-4:4; -14:13, -15:18	-13:18; -14:14; -13:13	-6:8; -38:39; -9:9
Reflect. coll.	5459	4048	5356	8257
Independ. refl.	2140	2518	1503	3158
<i>R</i> <sub>int</sub>	0.036	0.027	0.031	0.034
Reflection obs.	1624	1735	1503	3158
No. parameters	213	230	147	309
<i>R</i> <sub>1</sub> (obs)	0.0386	0.0446	0.0366	0.0374
w <i>R</i> <sub>2</sub> (all data)	0.1018	0.0970	0.0876	0.0874
<i>S</i>	1.03	0.98	1.06	1.02
Resd. Dens. [e Å <sup>-3</sup> ]	-0.22, 0.29	-0.24, 0.22	-0.22, 0.33	-0.22, 0.28
Device type	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD	Oxford Xcalibur3 CCD
Solution	SIR-92	SIR-92	SHELXS-97	SIR-92
Refinement	SHELXL-97	SHELXL-97	SHELXL-97	SHELXL-97
Absorpt. corr.	multi-scan	multi-scan	multi-scan	multi-scan
CCDC	988404	988413	988410	988411

## 2 Computations

### 2.1 Heat of Formation

All calculations were carried out using the Gaussian G09 program package<sup>[S8]</sup>. The enthalpies (H) and free energies (G) were calculated using the complete basis set (CBS) method of Petersson and coworkers in order to obtain very accurate energies. The CBS models use the known asymptotic convergence of pair natural orbital expressions to extrapolate from calculations using a finite basis set to the estimated CBS limit. CBS-4 begins with an HF/3-21G(d) geometry optimization; the zero point energy is computed at the same level. It then uses a large basis set SCF calculation as a base energy, and an MP2/6-31+G calculation with a CBS extrapolation to correct the energy through second order. An MP4(SDQ)/6-31+ (d,p) calculation is used to approximate higher order contributions. In this study, we applied the modified CBS-4M method (**M** referring to the use of Minimal Population localization) which is a re-parametrized version of the original CBS-4 method and also includes some additional empirical corrections<sup>[S9,S10]</sup>.

The calculated gas phase enthalpies of formation  $\Delta_f H^\circ(\text{g})$  were converted into the solid state enthalpies of formation ( $\Delta H_m(\text{s})$ ) by (i) for neutrals: subtraction of sublimation enthalpy, calculated by the "Troutons' rule" ( $\Delta H_{sub} [\text{kJ mol}] = 188 \cdot T_m[\text{K}]$ )<sup>[S11]</sup> (ii) for ionics: using the Jenkins and Glasser equations<sup>[S12]</sup> based on the molecular volumes  $V_M$  (taken from X-ray structures) in order to calculate the lattice energies ( $\Delta E_L$ ) and enthalpies ( $\Delta H_L$ ).

$$\Delta_f H^\circ_{(\text{g, M, 298})} = H_{(\text{Molecule, 298})} - \sum H^\circ_{(\text{Atoms, 298})} + \sum \Delta_f H^\circ_{(\text{Atoms, 298})} \quad (1)$$

Lastly, the molar standard enthalpies of formation ( $\Delta_f H_m$ ) were used to calculate the molar solid state energies of formation ( $\Delta U_m$ ) according to equation (2).

$$\Delta U_m = \Delta H_m - \Delta n RT \quad (2)$$

( $\Delta n$  being the change of moles of gaseous components)

**Table S4.** CBS-4M calculation results, molecular volumes taken from X-ray solution and calculated lattice enthalpy.

M	$-H^{298}$ / a.u.	$\Delta_f H^\circ(\text{g,M})$ / kJ mol <sup>-1</sup>	$V_M$ / nm <sup>3</sup>	$\Delta E_L, \Delta H_L$ ( <b>15–17, 20, 23</b> ); $\Delta H_{sub}$ ( <b>3,4</b> ) / kJ mol <sup>-1</sup>	$\Delta n$
<b>3</b>	709.121081	238.8		88.6	7.5
<b>4</b>	784.204956	244.5		85.2	8
<b>BOTFAZ</b> <b>dianion</b>	924.24619	720.7			
<b>BOTFOX</b> <b>dianion</b>	999.336611	709.6			
<b>NH<sub>4</sub><sup>+</sup></b>	56.796608	645.8			
<b>NH<sub>4</sub>O<sup>+</sup></b>	131.863249	687.2			
<b>N<sub>2</sub>H<sub>5</sub><sup>+</sup></b>	112.030523	774.1			
<b>G<sup>+</sup></b>	205.453192	571.9			
<b>AG<sup>+</sup></b>	260.701802	671.6			
<b>15</b>		1992.4	0.2681	1359.3, 1366.7	11.5
<b>16</b>		1981.2	0.2738	1348.6, 1359.5	12
<b>17</b>		2269.0	0.2933	1314.0, 1321.4	13.5
<b>20</b>		1853.4	0.366	1207.6, 1215.1	16
<b>23</b>		2052.8	0.4067	1160.0, 1167.4	18

## 2.2 Detonation Parameters

The calculation of the detonation parameters was performed with the program package EXPLO5 (version 5.05)<sup>[S13]</sup>. The program is based on the chemical equilibrium, steady-state model of detonation. It uses the Becker–Kistiakowsky–Wilson's equation of state (BKW EOS) for gaseous detonation products and Cowan–Fickett's equation of state for solid carbon. The calculation of the equilibrium composition of the detonation products is done by applying modified White, Johnson and Dantzig's free energy minimization technique. The program is designed to enable the calculation of detonation parameters at the CJ point. The BKW equation in the following form was used with the BKWN set of parameters ( $\alpha$ ,  $\beta$ ,  $\kappa$ ,  $\theta$ ) as stated below the equations and  $X_i$  being the mol fraction of  $i$ -th gaseous product,  $k_i$  is the molar covolume of the  $i$ -th gaseous product:<sup>[S14]</sup>

$$pV/RT = 1 + xe^{\beta x} \quad x = (\kappa \sum X_i k_i) / [V(T + \theta)]^{\alpha}$$

$$\alpha = 0.5, \beta = 0.176, \kappa = 14.71, \theta = 6620.$$

## 3 Experimental Procedures

Raman spectra were recorded with a Bruker MultiRAM FT-Raman instrument fitted with a liquid-nitrogen-cooled germanium detector and a Nd:YAG laser ( $\lambda = 1064$  nm), infrared spectra were measured with a Perkin–Elmer Spectrum BX-FTIR spectrometer equipped with a Smiths DuraSamplIR II ATR device. All spectra were recorded at ambient temperature; the samples were neat solids. NMR spectra were recorded with a JEOL Eclipse 400 ECX instrument, all samples were measured at 25 °C. Mass spectrometric data were obtained with a JEOL MStation JMS 700 spectrometer (DEI<sup>+</sup> / FAB<sup>+/-</sup>). C/H/N analysis was carried out by the department's internal micro analytical laboratory on a *Elementar Vario el* by pyrolysis of the sample and subsequent analysis of the formed gases. Differential Scanning Calorimetry (DSC) was performed on a *LINSEIS DSC PT10* with about 1 mg substance in a perforated aluminum vessel and a heating rate of 5 K min<sup>-1</sup> and a nitrogen steam of 5 L h<sup>-1</sup>. Melting points were determined in the same way. The sensitivities of the compounds were determined according to the BAM (German: Bundesanstalt für Materialforschung und Prüfung) standard for friction and impact<sup>[S15]</sup>. The impact sensitivities were tested according to STANAG 4489 modified instruction using a

BAM drophammer. The friction sensitivities were tested according to STANAG 4487 modified instructions using a BAM friction tester. The tested compounds were classified from the results by the “UN Recommendations on the Transport of Dangerous Goods”. Additionally all compounds were tested for sensitivity towards electrical discharge using an Electric Spark Tester ESD 2010 EN<sup>[S16]</sup>.

## 4

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