Electronic Supplementary Information

Energetic compounds consisting of 1,2,5- and 1,3,4-oxadiazole rings

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Table S1. Crystal data and structure refinement for **1, 2**·H_2O and **5**·H_2O.

Identification code	**1**	**2**·H_2O	**5**·H_2O
CCDC number	1419914	1419915	1419916
Empirical formula	$C_4H_4N_6O_2$	$C_4H_5N_7O_5$	$C_4H_8N_8O_6$
Formula weight	168.13	231.15	264.18
Temperature/K	293(2) K	296(2) K	293(2) K
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/n$	C2/c
a/Å	7.0958(2)	6.5964(3)	26.968(2)
b/Å	8.6167(2)	7.4775(3)	4.0185(3)
c/Å	11.0839(3)	17.4904(7)	18.7676(14)
α/°	90	90	90
β/°	102.3650(10)	97.043(2)	99.579(5)
γ/°	90	90	90
Volume/Å^3	661.98(3)	856.20(6)	2005.5(3)
Z	4	4	8
ρ_{calc}g/cm^3	1.687	1.793	1.750
μ/mm^{-1}	0.140	0.163	0.161
F(000)	344	472	1088
Crystal size/mm^3	0.222 x 0.200 x 0.120	0.112 x 0.103 x 0.056	0.200 x 0.180 x 0.150
2Θ range for data collection/°	3.764 to 26.440	3.188 to 26.426	1.532 to 26.480
Index ranges	-8<=h<=8, -10<=k<=10, -13<=l<=13	-8<=h<=8, -7<=k<=9, -21<=l<=21	-33<=h<=33, -5<=k<=5, -18<=l<=23
Reflections collected	6119	7971	9159
Independent reflections	1355 [$R_{(int)}$ = 0.0144]	1763 [$R_{(int)}$ = 0.0387]	2031 [R_{int} = 0.0604]
Data/restraints/parameters	1355 / 0 / 121	1763 / 0 / 160	2031 / 5 / 181
Goodness-of-fit on F^2	1.065	1.008	1.081
Final R indexes [I>=2σ (I)]	R_1 = 0.0305, wR_2 = 0.0858	R_1 = 0.0363, wR_2 = 0.0810	R_1 = 0.0455, wR_2 = 0.1107
Final R indexes [all data]	R_1 = 0.0335, wR_2 = 0.0887	R_1 = 0.0691, wR_2 = 0.0943	R_1 = 0.0969, wR_2 = 0.1598
Largest diff. peak/hole / e Å^{-3}	0.194 and -0.225	0.221 and -0.159	0.240 and -0.259

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4865(2)	1091(1)	-1622(1)	45(1)
C(2)	5819(2)	2010(1)	-745(1)	32(1)
N(3)	6509(1)	1690(1)	420(1)	36(1)
N(4)	7392(1)	3055(1)	942(1)	35(1)
C(5)	7174(1)	4065(1)	71(1)	29(1)
O(6)	6177(1)	3506(1)	-1038(1)	31(1)
C(7)	7876(1)	5642(1)	179(1)	29(1)
N(8)	7520(2)	6652(1)	-717(1)	38(1)
O(9)	8469(1)	7980(1)	-254(1)	44(1)
N(10)	9451(2)	7769(1)	972(1)	40(1)
C(11)	9082(2)	6336(1)	1249(1)	32(1)
N(12)	9788(2)	5661(2)	2337(1)	53(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

N(1)-C(2)	1.3224(15)
N(1)-H(1A)	0.866(18)
N(1)-H(1B)	0.854(18)
C(2)-N(3)	1.3096(15)
C(2)-O(6)	1.3659(13)
N(3)-N(4)	1.3986(13)
N(4)-C(5)	1.2842(14)
C(5)-O(6)	1.3680(12)
C(5)-C(7)	1.4435(15)
C(7)-N(8)	1.3029(15)
C(7)-C(11)	1.4365(14)
N(8)-O(9)	1.3704(13)
O(9)-N(10)	1.3993(14)
N(10)-C(11)	1.3122(15)
C(11)-N(12)	1.3362(16)
N(12)-H(12A)	0.855(19)
N(12)-H(12B)	0.826(19)
C(2)-N(1)-H(1A)	117.0(11)
C(2)-N(1)-H(1B)	119.4(11)
H(1A)-N(1)-H(1B)	120.8(15)
N(3)-C(2)-N(1)	128.55(11)
N(3)-C(2)-O(6)	112.57(10)
N(1)-C(2)-O(6)	118.88(10)
C(2)-N(3)-N(4)	105.69(9)
C(5)-N(4)-N(3)	106.73(9)
N(4)-C(5)-O(6)	113.13(9)
N(4)-C(5)-C(7)	126.30(10)
O(6)-C(5)-C(7)	120.58(9)
C(2)-O(6)-C(5)	101.87(8)
N(8)-C(7)-C(11)	109.58(10)
N(8)-C(7)-C(5)	123.95(10)
C(11)-C(7)-C(5)	126.45(10)
C(7)-N(8)-O(9)	105.83(9)
N(8)-O(9)-N(10)	110.96(8)
C(11)-N(10)-O(9)	105.47(9)
N(10)-C(11)-N(12)	124.49(11)
N(10)-C(11)-C(7)	108.15(10)
N(12)-C(11)-C(7)	127.32(11)
C(11)-N(12)-H(12A)	118.2(12)
C(11)-N(12)-H(12B)	118.4(13)
H(12A)-N(12)-H(12B)	121.6(18)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	61(1)	38(1)	31(1)	0(1)	-6(1)	-16(1)
C(2)	33(1)	29(1)	31(1)	0(1)	2(1)	-2(1)
N(3)	42(1)	31(1)	31(1)	0(1)	-2(1)	-5(1)
N(4)	39(1)	32(1)	29(1)	-1(1)	-2(1)	-4(1)
C(5)	28(1)	31(1)	26(1)	-4(1)	1(1)	0(1)
O(6)	35(1)	30(1)	26(1)	-1(1)	-2(1)	-3(1)
C(7)	28(1)	29(1)	28(1)	-3(1)	4(1)	2(1)
N(8)	43(1)	32(1)	36(1)	0(1)	0(1)	-1(1)
O(9)	55(1)	31(1)	42(1)	2(1)	2(1)	-4(1)
N(10)	47(1)	33(1)	37(1)	-4(1)	3(1)	-4(1)
C(11)	36(1)	29(1)	31(1)	-6(1)	6(1)	0(1)
N(12)	78(1)	42(1)	29(1)	-2(1)	-8(1)	-14(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **1**.

	x	y	z	U(eq)
H(1A)	4470(20)	210(20)	-1390(16)	55
H(1B)	4370(20)	1471(19)	-2330(16)	55
H(12A)	9330(20)	4780(20)	2481(16)	63
H(12B)	10420(30)	6190(20)	2898(17)	63

Table S6. Torsion angles [°] for **1**.

N(1)-C(2)-N(3)-N(4)	179.75(12)
O(6)-C(2)-N(3)-N(4)	-0.20(12)
C(2)-N(3)-N(4)-C(5)	-0.13(12)
N(3)-N(4)-C(5)-O(6)	0.42(12)
N(3)-N(4)-C(5)-C(7)	-179.13(10)
N(3)-C(2)-O(6)-C(5)	0.42(12)
N(1)-C(2)-O(6)-C(5)	-179.53(11)
N(4)-C(5)-O(6)-C(2)	-0.52(12)
C(7)-C(5)-O(6)-C(2)	179.07(9)
N(4)-C(5)-C(7)-N(8)	-175.80(10)
O(6)-C(5)-C(7)-N(8)	4.68(16)
N(4)-C(5)-C(7)-C(11)	5.48(18)
O(6)-C(5)-C(7)-C(11)	-174.04(9)
C(11)-C(7)-N(8)-O(9)	0.17(12)
C(5)-C(7)-N(8)-O(9)	-178.74(10)
C(7)-N(8)-O(9)-N(10)	0.28(12)
N(8)-O(9)-N(10)-C(11)	-0.64(12)
O(9)-N(10)-C(11)-N(12)	178.61(12)
O(9)-N(10)-C(11)-C(7)	0.71(12)
N(8)-C(7)-C(11)-N(10)	-0.59(13)
C(5)-C(7)-C(11)-N(10)	178.29(10)
N(8)-C(7)-C(11)-N(12)	-178.41(12)
C(5)-C(7)-C(11)-N(12)	0.47(19)

Table S7. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...N(3)#1	0.866(18)	2.154(18)	3.0032(15)	166.8(15)
N(1)-H(1B)...N(8)#2	0.854(18)	2.295(18)	3.1081(15)	159.4(15)
N(12)-H(12A)...N(4)	0.855(19)	2.450(18)	3.0327(16)	126.0(15)
N(12)-H(12A)...N(10)#3	0.855(19)	2.459(18)	3.0949(16)	131.8(15)
N(12)-H(12B)...N(3)#4	0.826(19)	2.579(19)	3.3270(15)	151.3(16)
N(12)-H(12B)...N(4)#4	0.826(19)	2.402(19)	3.2035(15)	164.0(16)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z #2 -x+1,y-1/2,-z-1/2 #3 -x+2,y-1/2,-z+1/2
#4 -x+2,y+1/2,-z+1/2

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**·H_2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	13839(3)	5064(3)	7108(1)	43(1)
C(2)	12237(3)	4610(2)	6647(1)	32(1)
N(3)	11693(2)	4962(2)	5913(1)	36(1)
N(4)	9826(2)	4176(2)	5666(1)	37(1)
C(5)	9354(3)	3393(3)	6262(1)	32(1)
O(6)	10788(2)	3582(2)	6897(1)	35(1)
C(7)	7504(3)	2401(3)	6338(1)	33(1)
N(8)	7241(2)	1647(3)	6987(1)	45(1)
O(9)	5354(2)	877(2)	6861(1)	52(1)
N(10)	4431(2)	1177(2)	6104(1)	43(1)
C(11)	5761(3)	2125(3)	5774(1)	33(1)
N(12)	5683(2)	2825(2)	5045(1)	34(1)
N(13)	3970(2)	2498(2)	4576(1)	39(1)
O(14)	2548(2)	1587(2)	4772(1)	51(1)
O(15)	3855(2)	3169(2)	3919(1)	56(1)
O(1S)	9082(3)	976(3)	3640(1)	58(1)

Table S9. Bond lengths [Å] and angles [°] for **2**·H_2O.

N(1)-C(2)	1.294(2)	N(1)-H(1A)	0.89(2)
N(1)-H(1B)	0.86(2)	C(2)-N(3)	1.317(2)
C(2)-O(6)	1.341(2)	N(3)-N(4)	1.385(2)
N(3)-H(3)	0.84(2)	N(4)-C(5)	1.267(2)
C(5)-O(6)	1.375(2)	C(5)-C(7)	1.448(3)
C(7)-N(8)	1.298(2)	C(7)-C(11)	1.434(2)
N(8)-O(9)	1.364(2)	O(9)-N(10)	1.406(2)
N(10)-C(11)	1.315(2)	C(11)-N(12)	1.374(2)
N(12)-N(13)	1.334(2)	N(13)-O(14)	1.241(2)
N(13)-O(15)	1.248(2)	O(1S)-H(1S)	0.84(3)
O(1S)-H(2S)	0.77(3)		
C(2)-N(1)-H(1A)	116.5(14)	C(2)-N(1)-H(1B)	114.1(14)
H(1A)-N(1)-H(1B)	129(2)	N(1)-C(2)-N(3)	131.30(19)
N(1)-C(2)-O(6)	120.48(16)	N(3)-C(2)-O(6)	108.22(15)
C(2)-N(3)-N(4)	110.15(16)	C(2)-N(3)-H(3)	129.2(14)
N(4)-N(3)-H(3)	120.6(14)	C(5)-N(4)-N(3)	103.83(14)
N(4)-C(5)-O(6)	113.73(16)	N(4)-C(5)-C(7)	127.34(16)
O(6)-C(5)-C(7)	118.91(15)	C(2)-O(6)-C(5)	104.06(13)
N(8)-C(7)-C(11)	110.87(16)	N(8)-C(7)-C(5)	120.44(16)
C(11)-C(7)-C(5)	128.67(16)	C(7)-N(8)-O(9)	105.03(15)
N(8)-O(9)-N(10)	111.47(13)	C(11)-N(10)-O(9)	105.26(15)
N(10)-C(11)-N(12)	131.40(17)	N(10)-C(11)-C(7)	107.37(16)
N(12)-C(11)-C(7)	121.22(16)	N(13)-N(12)-C(11)	115.63(15)
O(14)-N(13)-O(15)	120.82(16)	O(14)-N(13)-N(12)	122.88(16)
O(15)-N(13)-N(12)	116.30(16)	H(1S)-O(1S)-H(2S)	108(3)

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**·H_2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	42(1)	52(1)	33(1)	0(1)	-3(1)	-12(1)
C(2)	32(1)	32(1)	30(1)	-4(1)	0(1)	1(1)
N(3)	33(1)	43(1)	30(1)	4(1)	-2(1)	-7(1)
N(4)	32(1)	46(1)	33(1)	5(1)	-2(1)	-5(1)
C(5)	30(1)	39(1)	26(1)	0(1)	-2(1)	5(1)
O(6)	32(1)	44(1)	27(1)	1(1)	-1(1)	-3(1)
C(7)	31(1)	37(1)	32(1)	3(1)	3(1)	3(1)
N(8)	36(1)	60(1)	41(1)	12(1)	4(1)	-4(1)
O(9)	42(1)	70(1)	43(1)	19(1)	4(1)	-10(1)
N(10)	37(1)	50(1)	42(1)	8(1)	2(1)	-6(1)
C(11)	30(1)	32(1)	36(1)	3(1)	6(1)	1(1)
N(12)	27(1)	41(1)	33(1)	0(1)	-4(1)	-4(1)
N(13)	33(1)	47(1)	37(1)	-6(1)	2(1)	-2(1)
O(14)	34(1)	68(1)	49(1)	-3(1)	0(1)	-17(1)
O(15)	48(1)	83(1)	33(1)	7(1)	-6(1)	-7(1)
O(1S)	43(1)	86(1)	45(1)	-13(1)	-2(1)	-15(1)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2**·H_2O.

	x	y	z	U(eq)
H(1A)	13900(30)	4690(30)	7592(13)	51
H(1B)	14680(30)	5740(30)	6900(13)	51
H(3)	12300(30)	5580(30)	5607(12)	43
H(1S)	8300(50)	400(40)	3889(17)	88
H(2S)	10050(50)	1200(40)	3914(17)	88

Table S12. Torsion angles [°] for **2**·H_2O.

N(1)-C(2)-N(3)-N(4)	180.0(2)
O(6)-C(2)-N(3)-N(4)	0.9(2)
C(2)-N(3)-N(4)-C(5)	-0.2(2)
N(3)-N(4)-C(5)-O(6)	-0.5(2)
N(3)-N(4)-C(5)-C(7)	177.87(18)
N(1)-C(2)-O(6)-C(5)	179.68(18)
N(3)-C(2)-O(6)-C(5)	-1.14(19)
N(4)-C(5)-O(6)-C(2)	1.1(2)
C(7)-C(5)-O(6)-C(2)	-177.47(17)
N(4)-C(5)-C(7)-N(8)	179.2(2)
O(6)-C(5)-C(7)-N(8)	-2.5(3)
N(4)-C(5)-C(7)-C(11)	-2.4(3)
O(6)-C(5)-C(7)-C(11)	175.87(18)
C(11)-C(7)-N(8)-O(9)	0.1(2)
C(5)-C(7)-N(8)-O(9)	178.69(17)
C(7)-N(8)-O(9)-N(10)	-0.1(2)
N(8)-O(9)-N(10)-C(11)	0.0(2)
O(9)-N(10)-C(11)-N(12)	-178.97(19)
O(9)-N(10)-C(11)-C(7)	0.0(2)
N(8)-C(7)-C(11)-N(10)	-0.1(2)
C(5)-C(7)-C(11)-N(10)	-178.5(2)
N(8)-C(7)-C(11)-N(12)	179.05(17)
C(5)-C(7)-C(11)-N(12)	0.6(3)
N(10)-C(11)-N(12)-N(13)	-0.3(3)
C(7)-C(11)-N(12)-N(13)	-179.13(17)
C(11)-N(12)-N(13)-O(14)	-1.6(3)
C(11)-N(12)-N(13)-O(15)	178.02(16)

Table S13. Hydrogen bonds for **2**·H_2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(1S)#1	0.89(2)	1.89(2)	2.774(2)	177(2)
N(1)-H(1B)...O(15)#2	0.86(2)	2.00(2)	2.821(3)	159(2)
N(3)-H(3)...N(12)#2	0.84(2)	2.21(2)	3.041(2)	170.7(19)
O(1S)-H(1S)...N(10)#3	0.84(3)	2.15(3)	2.901(2)	149(3)
O(1S)-H(2S)...O(14)#4	0.77(3)	2.11(3)	2.872(2)	172(3)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y+1/2,z+1/2 #2 -x+2,-y+1,-z+1 #3 -x+1,-y,-z+1
#4 x+1,y,z

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**·H_2O. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3775(1)	723(7)	4498(1)	32(1)
N(2)	3853(1)	725(7)	5252(1)	34(1)
C(3)	4243(1)	-1148(8)	5453(2)	29(1)
O(4)	4439(1)	-2391(6)	4886(1)	30(1)
C(5)	4121(1)	-1113(8)	4307(2)	26(1)
C(6)	4200(1)	-1949(8)	3583(2)	27(1)
N(7)	4562(1)	-3888(7)	3465(1)	34(1)
O(8)	4518(1)	-4080(6)	2726(1)	42(1)
N(9)	4117(1)	-2144(7)	2376(2)	35(1)
C(10)	3915(1)	-838(8)	2903(2)	26(1)
N(11)	4463(1)	-1884(8)	6111(2)	47(1)
N(12)	3505(1)	1208(7)	2897(1)	29(1)
N(13)	3264(1)	2106(7)	2259(1)	28(1)
O(14)	2883(1)	3924(6)	2261(1)	39(1)
O(15)	3397(1)	1271(6)	1681(1)	40(1)
O(1S)	2825(1)	6398(6)	4210(2)	45(1)
N(2S)	2770(1)	3514(7)	3786(2)	31(1)
O(3S)	3033(1)	5711(6)	557(1)	33(1)

Table S15. Bond lengths [Å] and angles [°] for **5**·H_2O.

N(1)-C(5)	1.285(4)	N(1)-N(2)	1.396(4)
N(2)-C(3)	1.297(4)	C(3)-N(11)	1.311(4)
C(3)-O(4)	1.359(4)	O(4)-C(5)	1.369(4)
C(5)-C(6)	1.448(4)	C(6)-N(7)	1.297(4)
C(6)-C(10)	1.446(4)	N(7)-O(8)	1.374(3)
O(8)-N(9)	1.403(3)	N(9)-C(10)	1.317(4)
C(10)-N(12)	1.375(4)	N(11)-H(11A)	0.8600
N(11)-H(11B)	0.8600	N(12)-N(13)	1.315(3)
N(13)-O(15)	1.244(3)	N(13)-O(14)	1.260(3)
O(1S)-N(2S)	1.400(4)	O(1S)-H(1S)	0.98(4)
N(2S)-H(2SA)	0.8800(11)	N(2S)-H(2SB)	0.8801(11)
N(2S)-H(2SC)	0.8801(11)	O(3S)-H(3SA)	0.8402(11)
O(3S)-H(3SB)	0.8402(11)		

C(5)-N(1)-N(2)	106.8(2)	C(3)-N(2)-N(1)	105.8(2)
N(2)-C(3)-N(11)	128.5(3)	N(2)-C(3)-O(4)	112.8(3)
N(11)-C(3)-O(4)	118.7(3)	C(3)-O(4)-C(5)	102.1(2)
N(1)-C(5)-O(4)	112.4(3)	N(1)-C(5)-C(6)	128.4(3)
O(4)-C(5)-C(6)	119.2(3)	N(7)-C(6)-C(10)	109.9(3)
N(7)-C(6)-C(5)	122.1(3)	C(10)-C(6)-C(5)	128.0(3)
C(6)-N(7)-O(8)	105.3(2)	N(7)-O(8)-N(9)	112.0(2)
C(10)-N(9)-O(8)	104.5(2)	N(9)-C(10)-N(12)	131.6(3)
N(9)-C(10)-C(6)	108.4(3)	N(12)-C(10)-C(6)	120.0(3)
C(3)-N(11)-H(11A)	120.0	C(3)-N(11)-H(11B)	120.0
H(11A)-N(11)-H(11B)	120.0	N(13)-N(12)-C(10)	116.6(3)
O(15)-N(13)-O(14)	120.9(2)	O(15)-N(13)-N(12)	123.3(3)
O(14)-N(13)-N(12)	115.9(3)	N(2S)-O(1S)-H(1S)	106(2)
O(1S)-N(2S)-H(2SA)	112(2)	O(1S)-N(2S)-H(2SB)	107(2)
H(2SA)-N(2S)-H(2SB)	120(3)	O(1S)-N(2S)-H(2SC)	105(2)
H(2SA)-N(2S)-H(2SC)	113(3)	H(2SB)-N(2S)-H(2SC)	97(3)
H(3SA)-O(3S)-H(3SB)	81(3)		

Table S16. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**·H_2O. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	33(2)	41(2)	22(2)	2(1)	6(1)	9(1)
N(2)	34(2)	46(2)	21(1)	0(1)	4(1)	10(1)
C(3)	29(2)	36(2)	22(2)	-1(2)	4(1)	4(1)
O(4)	27(1)	41(1)	21(1)	2(1)	2(1)	11(1)
C(5)	23(2)	30(2)	23(2)	0(1)	1(1)	2(1)
C(6)	26(2)	30(2)	27(2)	4(1)	5(1)	0(1)
N(7)	33(2)	45(2)	26(2)	0(1)	9(1)	10(1)
O(8)	40(1)	56(2)	32(1)	2(1)	15(1)	19(1)
N(9)	39(2)	44(2)	25(2)	0(1)	11(1)	12(1)
C(10)	28(2)	30(2)	21(2)	1(1)	8(1)	-3(1)
N(11)	43(2)	70(2)	24(2)	-2(2)	-2(1)	24(2)
N(12)	28(1)	37(2)	20(1)	4(1)	2(1)	9(1)
N(13)	31(2)	34(2)	20(2)	1(1)	2(1)	2(1)
O(14)	35(1)	52(2)	29(1)	6(1)	0(1)	14(1)
O(15)	52(2)	51(2)	18(1)	1(1)	6(1)	12(1)
O(1S)	69(2)	27(1)	36(2)	-2(1)	-1(1)	3(1)
N(2S)	29(2)	31(2)	34(2)	-4(1)	4(1)	5(1)
O(3S)	31(1)	42(1)	26(1)	5(1)	2(1)	-5(1)

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2 x\ 10^3$) for **5**·H_2O.

	x	y	z	U(eq)
H(11A)	4348	-1083	6476	56
H(11B)	4722	-3166	6177	56
H(1S)	2910(14)	5630(100)	4710(20)	54
H(2SA)	3049(6)	2340(60)	3836(18)	38
H(2SB)	2486(6)	2560(70)	3846(18)	38
H(2SC)	2670(12)	4220(80)	3341(6)	38
H(3SA)	3316(5)	6630(70)	650(20)	40
H(3SB)	3166(12)	4500(60)	901(11)	40

Table S18. Torsion angles [°] for **5**·H_2O.

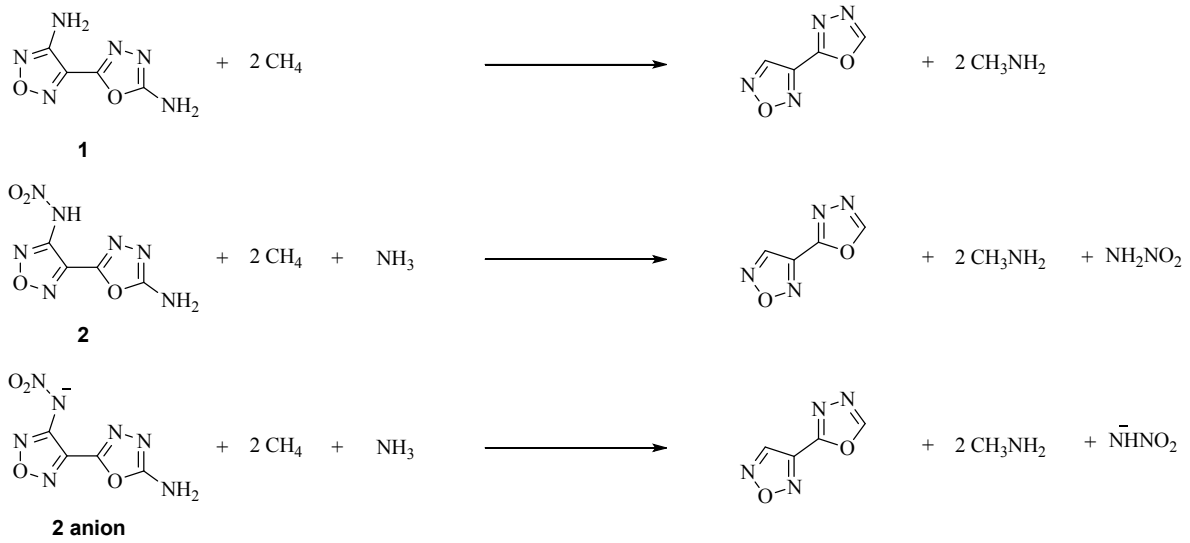
C(5)-N(1)-N(2)-C(3)	-0.2(4)
N(1)-N(2)-C(3)-N(11)	179.4(4)
N(1)-N(2)-C(3)-O(4)	0.7(4)
N(2)-C(3)-O(4)-C(5)	-0.9(3)
N(11)-C(3)-O(4)-C(5)	-179.7(3)
N(2)-N(1)-C(5)-O(4)	-0.3(4)
N(2)-N(1)-C(5)-C(6)	179.0(3)
C(3)-O(4)-C(5)-N(1)	0.7(4)
C(3)-O(4)-C(5)-C(6)	-178.7(3)
N(1)-C(5)-C(6)-N(7)	-178.9(3)
O(4)-C(5)-C(6)-N(7)	0.3(5)
N(1)-C(5)-C(6)-C(10)	1.8(6)
O(4)-C(5)-C(6)-C(10)	-179.0(3)
C(10)-C(6)-N(7)-O(8)	-0.4(4)
C(5)-C(6)-N(7)-O(8)	-179.8(3)
C(6)-N(7)-O(8)-N(9)	1.0(3)
N(7)-O(8)-N(9)-C(10)	-1.2(3)
O(8)-N(9)-C(10)-N(12)	-178.2(3)
O(8)-N(9)-C(10)-C(6)	0.9(3)
N(7)-C(6)-C(10)-N(9)	-0.3(4)
C(5)-C(6)-C(10)-N(9)	179.0(3)
N(7)-C(6)-C(10)-N(12)	178.9(3)
C(5)-C(6)-C(10)-N(12)	-1.8(5)
N(9)-C(10)-N(12)-N(13)	-0.7(5)
C(6)-C(10)-N(12)-N(13)	-179.8(3)
C(10)-N(12)-N(13)-O(15)	-2.0(4)
C(10)-N(12)-N(13)-O(14)	178.6(3)

Table S19. Hydrogen bonds for **5**·H_2O [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(11)-H(11A)...N(9)#1	0.86	2.30	3.140(4)	167.2
N(11)-H(11B)...N(7)#2	0.86	2.27	3.121(4)	170.3
O(1S)-H(1S)...O(3S)#3	0.98(4)	1.65(5)	2.637(3)	178(4)
N(2S)-H(2SA)...N(1)	0.8800(11)	2.234(17)	3.031(4)	150(3)
N(2S)-H(2SB)...O(3S)#4	0.8801(11)	2.071(15)	2.892(4)	155(3)
N(2S)-H(2SC)...O(14)	0.8801(11)	2.20(2)	2.933(4)	140(3)
O(3S)-H(3SA)...N(2)#5	0.8402(11)	2.04(2)	2.773(3)	146(3)
O(3S)-H(3SB)...O(15)	0.8402(11)	1.977(5)	2.812(3)	172(3)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y,z+1/2 #2 -x+1,-y-1,-z+1 #3 x,-y+1,z+1/2
#4 -x+1/2,y-1/2,-z+1/2 #5 x,-y+1,z-1/2

Computational Details



Scheme S1. Isodesmic reactions for **1**, **2** and **2** anion