Supporting Information

for

A series of high-energy coordination polymers with 3,6-bis(4-nitroamino-1,2,5-oxadiazol-3-yl)-1,4,2,5-dioxadiazine, a ligand with multi- coordination sites, high oxygen content and detonation performance: Syntheses, structures, and performance

Cheng Shen, Yuan-gang Xu and Ming Lu [*]

(School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China)

Contents

S2 Single crystal data for compound 1

S3 Single crystal data for compound 1a

S4 Single crystal data for compound 2

S5 Single crystal data for compound 3

S9 Detonation property values comparison

S10 REFERENCES

[*] Corresponding author, E-mail: luming@mail.njust.edu.cn

Table 1. Bond lengths [Å] and angles [°] for compound (1)

Ag1 - N2	2.265(3)	N2 - Ag1 - O1	144.80(9)
Ag1 - O1	2.277(2)	N2 - Ag1 - N1	75.22(9)
Ag1 - N1	2.577(3)	N2 - Ag1 - N4	128.62(9)
Ag1 - N4	2.404(3)	O1 - Ag1 - N1	100.59(9)
O3 - N3	1.246(4)	O1 - Ag1 - N4	86.10(9)
N3 - N2	1.349(4)	N4 - Ag1 - N1	109.64(10)
N3 - O2	1.246(4)	O3 - N3 - N2	122.0(3)
N2 - C1	1.371(4)	O3 - N3 - O2	122.9(3)
O4 - N5	1.367(4)	O2 - N3 - N2	115.1(3)
O4 - N4	1.408(3)	N3 - N2 - Ag1	109.16(18)
N006 - C4	1.314(5)	N3 - N2 - C1	117.5(3)
N006 - C5	1.450(5)	C1 - N2 - Ag1	128.9(2)
N006 - C6	1.457(5)	N5 - O4 - N4	110.8(2)
O1 - C4	1.255(4)	C4 - N006 - C5	121.9(3)
C1 - C2	1.440(4)	C4 - N006 - C6	121.0(3)
C1 - N4	1.317(4)	C5 - N006 - C6	117.1(3)
C2 - N5	1.291(4)	C4 - O1 - Ag1	124.3(2)
C2 - C3	1.465(5)	N2 - C1 - C2	122.3(3)
C3 - N1	1.272(4)	N4 - C1 - N2	130.1(3)
C3 - O5	1.337(4)	N4 - C1 - C2	107.5(3)
N1 - O5	1.425(4)	C1 - C2 - C3	130.6(3)
N4 - Ag1	2.404(3)	N5 - C2 - C1	110.3(3)
O5 - N1	1.425(4)	N5 - C2 - C3	119.1(3)
C4 - H4	0.95	C2 - N5 - O4	106.0(3)
C5 - H5A	0.98	N1 - C3 - C2	121.1(3)
C5 - H5B	0.98	N1 - C3 - O5	126.8(3)
C5 - H5C	0.98	O5 - C3 - C2	112.0(3)
C6 - H6A	0.98	C3 - N1 - Ag1	125.0(2)
C6 - H6B	0.98	C3 - N1 - O5	115.3(3)
C6 - H6C	0.98	O5 - N1 - Ag1	114.58(19)
		O4 - N4 - Ag1	115.39(18)
		C1 - N4 - Ag1	126.3(2)
		C1 - N4 - O4	105.4(3)
		C3 - O5 - N1	117.9(3)
		N006 - C4 - H4	118.1
		O1 - C4 - N006	123.7(3)
		O1 - C4 - H4	118.1
		N006 - C5 - H5A	109.5
		N006 - C5 - H5B	109.5
		N006 - C5 - H5C	109.5

	H5A - C5 - H5B	109.5
	H5A - C5 - H5C	109.5
	H5B - C5 - H5C	109.5
	N006 - C6 - H6A	109.5
	N006 - C6 - H6B	109.5
	N006 - C6 - H6C	109.5
	H6A - C6 - H6B	109.5
	H6A - C6 - H6C	109.5
	H6B - C6 - H6C	109.5

Table 2. Bond lengths [Å] and angles [°] for compound (1a)

Ag1 - N4	2.251(5)	N4 - Ag1 - N2	167.15(17)
Ag1 - N2	2.253(5)	N4 - Ag1 - O3	112.70(16)
Ag1 - O3	2.582(5)	N2 - Ag1 - O3	64.12(16)
Ag1 - N1	2.618(5)	N4 - Ag1 - N1	76.36(16)
C1 - N1	1.256(7)	N2 - Ag1 - N1	90.95(17)
C1 - O1'	1.378(15)	O3 - Ag1 - N1	88.01(15)
C1 - O1	1.397(14)	N1 - C1 - O1'	125.6(8)
C1 - C3	1.479(8)	N1 - C1 - O1	126.5(7)
C2 - N2	1.309(7)	N1 - C1 - C3	121.2(6)
C2 - N4	1.377(7)	O1' - C1 - C3	111.3(7)
C2 - C3	1.441(8)	O1 - C1 - C3	110.1(7)
C3 - N3	1.297(7)	N2 - C2 - N4	130.2(6)
N1 - O1	1.453(12)	N2 - C2 - C3	107.7(5)
N1 - O1'	1.466(15)	N4 - C2 - C3	122.1(6)
N1 - Ag1	2.618(5)	N3 - C3 - C2	109.8(5)
N2 - O2	1.393(6)	N3 - C3 - C1	118.1(6)
N3 - O2	1.363(6)	C2 - C3 - C1	132.1(6)
N4 - N5	1.361(7)	C1 - N1 - O1	115.0(6)
N4 - Ag1	2.251(5)	C1 - N1 - O1'	113.6(7)
N5 - O3	1.238(6)	C1 - N1 - Ag1	127.3(4)
N5 - O4	1.241(6)	O1 - N1 - Ag1	111.1(6)
O1 - C1	1.397(14)	O1' - N1 - Ag1	119.1(6)
O1' - C1	1.378(15)	C2 - N2 - O2	105.5(5)
		C2 - N2 - Ag1	132.3(4)
		O2 - N2 - Ag1	115.5(3)
		C3 - N3 - O2	105.6(5)
		N5 - N4 - C2	117.7(5)
		N5 - N4 - Ag1	108.1(4)
		C2 - N4 - Ag1	133.0(4)
		O3 - N5 - O4	123.1(5)

		O3 - N5 - N4	122.0(5)
		O4 - N5 - N4	114.8(5)
		N3 - O2 - N2	111.5(4)
		N5 - O3 - Ag1	127.4(4)
		C1 - O1 - N1	112.1(10)
		C1 - O1' - N1	112.4(11)

Table 3. Bond lengths [Å] and angles [°] for compound (2)

Cu1 - O5	1.9780(14)	O5 - Cu1 - O5	180.00(9)
Cu1 - O5	1.9780(14)	O5 - Cu1 - O1	95.01(6)
Cu1 - O6	1.9266(14)	O5 - Cu1 - O1	84.99(6)
Cu1 - O6	1.9265(14)	O5 - Cu1 - O1	95.01(6)
Cu1 - O1	2.3893(15)	O5 - Cu1 - O1	84.99(6)
Cu1 - O1	2.3893(15)	O6 - Cu1 - O5	88.11(6)
O5 - H5A	0.8586	O6 - Cu1 - O5	91.89(6)
O5 - H5B	0.88(2)	O6 - Cu1 - O5	91.89(6)
O6 - H6A	0.8666	O6 - Cu1 - O5	88.11(6)
O6 - H6B	0.8662	O6 - Cu1 - O6	180
O1 - N1	1.263(2)	O6 - Cu1 - O1	90.36(6)
O2 - N1	1.229(2)	O6 - Cu1 - O1	89.64(6)
O7 - H7A	0.835(16)	O6 - Cu1 - O1	90.36(6)
O7 - H7B	0.830(17)	O6 - Cu1 - O1	89.64(6)
O3 - N4	1.358(2)	O1 - Cu1 - O1	180.00(6)
O3 - N3	1.398(2)	Cu1 - O5 - H5A	109.9
O4 - N5	1.422(2)	Cu1 - O5 - H5B	125(2)
O4 - C00G	1.336(2)	H5A - O5 - H5B	110.7
N1 - N2	1.318(2)	Cu1 - O6 - H6A	110.7
N5 - O4	1.422(2)	Cu1 - O6 - H6B	110.3
N5 - C00G	1.266(2)	H6A - O6 - H6B	108.2
N2 - C00F	1.374(2)	N1 - O1 - Cu1	125.12(12)
N4 - C00E	1.302(3)	H7A - O7 - H7B	120(3)
N3 - C00F	1.310(3)	N4 - O3 - N3	111.39(15)
C00E - C00F	1.438(2)	C00G - O4 - N5	117.74(15)
C00E - C00G	1.450(3)	O1 - N1 - N2	115.56(16)
		O2 - N1 - O1	119.95(16)
		O2 - N1 - N2	124.43(17)
		C00G - N5 - O4	115.09(16)
		N1 - N2 - C00F	116.21(16)
		C00E - N4 - O3	105.68(16)
		C00F - N3 - O3	105.45(16)
		N4 - C00E - C00F	109.75(17)

		N4 - C00E - C00G	120.22(17)
		C00F - C00E - C00G	130.03(17)
		N2 - C00F - C00E	120.59(17)
		N3 - C00F - N2	131.67(18)
		N3 - C00F - C00E	107.73(17)
		O4 - C00G - C00E	112.34(16)
		N5 - C00G - O4	127.17(18)
		N5 - C00G - C00E	120.48(17)

Table 4. Bond lengths [Å] and angles [°] for compound (3)

Co1 - O1W	2.158(6)	O1W - Co1 - N1	92.7(3)
Co1 - O2W	2.055(6)	O1W - Co1 - N2	85.6(3)
Co1 - O3W	2.091(6)	O2W - Co1 - O1W	93.8(3)
Co1 - O4W	2.147(6)	O2W - Co1 - O3W	83.5(3)
Co1 - N1	2.171(6)	O2W - Co1 - O4W	92.2(3)
Co1 - N2	2.185(7)	O2W - Co1 - N1	101.2(3)
Co2 - O5W	2.095(6)	O2W - Co1 - N2	176.4(3)
Co2 - O6W	2.070(6)	O3W - Co1 - O1W	89.3(3)
Co2 - O7W	2.091(6)	O3W - Co1 - O4W	88.7(3)
Co2 - O9W	2.071(5)	O3W - Co1 - N1	174.7(3)
Co2 - N11	2.147(6)	O3W - Co1 - N2	92.9(3)
Co2 - N12	2.151(7)	O4W - Co1 - O1W	173.5(3)
O1 - N3	1.238(8)	O4W - Co1 - N1	88.7(3)
O1W - H1WA	0.8798	O4W - Co1 - N2	88.3(3)
O1W - H1WB	0.8796	N1 - Co1 - N2	82.4(3)
O2W - H2WA	0.9177	O5W - Co2 - N11	87.9(2)
O2W - H2WB	0.9217	O5W - Co2 - N12	87.5(2)
O2 - N3	1.230(8)	O6W - Co2 - O5W	90.6(2)
O3W - H3WA	0.9172	O6W - Co2 - O7W	91.4(2)
O3W - H3WB	0.915	O6W - Co2 - O9W	86.1(2)
O3 - N4	1.414(9)	O6W - Co2 - N11	99.7(2)
O3 - N5	1.355(8)	O6W - Co2 - N12	175.5(3)
O4W - H4WA	0.872	O7W - Co2 - O5W	176.6(2)
O4W - H4WB	0.8717	O7W - Co2 - N11	94.5(2)
O4 - N6	1.442(8)	O7W - Co2 - N12	90.3(2)
O4 - C01F	1.340(10)	O9W - Co2 - O5W	92.1(2)
O5 - N2	1.429(8)	O9W - Co2 - O7W	85.4(3)
O5 - C01G	1.358(10)	O9W - Co2 - N11	174.2(3)
O5W - H5WA	0.8745	O9W - Co2 - N12	89.9(2)

O5W - H5WB	0.8739	N11 - Co2 - N12	84.3(2)
O6W - H6WA	0.8976	Co1 - O1W - H1WA	110
O6W - H6WB	0.8976	Co1 - O1W - H1WB	109.8
O6 - N7	1.366(8)	H1WA - O1W - H1WB	108.9
O6 - N8	1.413(9)	Co1 - O2W - H2WA	111.5
O7 - N10	1.229(9)	Co1 - O2W - H2WB	113
O7W - H7WA	0.912	H2WA - O2W - H2WB	105.8
O7W - H7WB	0.9117	Co1 - O3W - H3WA	112.6
O8 - N10	1.286(9)	Co1 - O3W - H3WB	111.3
O9 - N20	1.259(10)	H3WA - O3W - H3WB	106.2
O9W - H9WA	0.9033	N5 - O3 - N4	112.1(5)
O9W - H9WB	0.9028	Co1 - O4W - H4WA	109.5
O10 - N20	1.244(10)	Co1 - O4W - H4WB	109.1
O11W - H11A	0.8699	H4WA - O4W - H4WB	109.3
O11W - H11B	0.8701	C01F - O4 - N6	114.3(6)
O11 - N17	1.372(9)	C01G - O5 - N2	112.9(6)
O11 - N18	1.393(10)	Co2 - O5W - H5WA	109.7
O12 - N12	1.448(8)	Co2 - O5W - H5WB	109.3
O12 - C01P	1.370(11)	H5WA - O5W - H5WB	109.2
O13 - N16	1.464(9)	Co2 - O6W - H6WA	110.9
O13 - C01L	1.337(9)	Co2 - O6W - H6WB	111
O14 - N14	1.417(8)	H6WA - O6W - H6WB	107.7
O14 - N15	1.357(8)	N7 - O6 - N8	110.8(5)
O15 - N13	1.224(8)	Co2 - O7W - H7WA	112.2
O16 - N13	1.240(8)	Co2 - O7W - H7WB	111.8
N1 - N3	1.349(9)	H7WA - O7W - H7WB	106.8
N1 - C01K	1.380(10)	Co2 - O9W - H9WA	111.7
N2 - C01F	1.271(10)	Co2 - O9W - H9WB	111.4
N4 - C01K	1.325(10)	H9WA - O9W - H9WB	107.3
N5 - C01M	1.306(10)	H11A - O11W - H11B	109.5
N6 - C01G	1.277(10)	N17 - O11 - N18	112.2(6)
N7 - C01E	1.294(10)	C01P - O12 - N12	111.9(6)
N8 - C01J	1.295(9)	C01L - O13 - N16	112.8(6)
N9 - N10	1.315(9)	N15 - O14 - N14	110.8(5)
N9 - C01J	1.387(10)	N3 - N1 - Co1	120.0(5)
N11 - N13	1.346(9)	N3 - N1 - C01K	116.3(6)
N11 - C01I	1.372(10)	C01K - N1 - Co1	119.8(5)
N12 - C01L	1.277(10)	O5 - N2 - Co1	118.1(4)
N14 - C01I	1.307(10)	C01F - N2 - Co1	127.7(6)
N15 - C01N	1.307(10)	C01F - N2 - O5	113.3(7)
N16 - C01P	1.252(10)	O1 - N3 - N1	115.4(6)
N17 - C01O	1.330(11)	O2 - N3 - O1	121.8(7)
N18 - C01Q	1.334(11)	O2 - N3 - N1	122.8(6)
N19 - N20	1.329(10)	C01K - N4 - O3	103.8(6)

N19 - C01Q	1.365(11)	C01M - N5 - O3	104.8(6)
C01Q - C01O	1.419(12)	C01G - N6 - O4	111.8(7)
C01N - C01L	1.458(10)	C01E - N7 - O6	105.8(6)
C01N - C01I	1.445(11)	C01J - N8 - O6	104.9(6)
C01E - C01G	1.452(11)	N10 - N9 - C01J	115.5(7)
C01E - C01J	1.435(11)	O7 - N10 - O8	120.6(7)
C01P - C01O	1.470(11)	O7 - N10 - N9	125.0(7)
C01F - C01M	1.455(11)	O8 - N10 - N9	114.2(7)
C01M - C01K	1.414(11)	N13 - N11 - Co2	121.0(5)
O10W - H10A	0.8701	N13 - N11 - C01I	116.2(6)
O10W - H10B	0.87	C01I - N11 - Co2	120.5(5)
O12W - H12A	0.87	O12 - N12 - Co2	119.2(4)
O12W - H12B	0.8698	C01L - N12 - Co2	128.9(5)
O8W - H8WA	0.87	C01L - N12 - O12	111.8(6)
O8W - H8WB	0.87	O15 - N13 - O16	122.6(7)
		O15 - N13 - N11	122.1(6)
		O16 - N13 - N11	115.3(6)
		C01I - N14 - O14	105.7(6)
		C01N - N15 - O14	106.1(6)
		C01P - N16 - O13	111.5(7)
		C01O - N17 - O11	104.2(7)
		C01Q - N18 - O11	105.2(7)
		N20 - N19 - C01Q	115.2(7)
		O9 - N20 - N19	115.9(7)
		O10 - N20 - O9	119.1(8)
		O10 - N20 - N19	124.9(7)
		N18 - C01Q - N19	132.2(8)
		N18 - C01Q - C01O	107.7(7)
		N19 - C01Q - C01O	120.1(8)
		N15 - C01N - C01L	120.7(7)
		N15 - C01N - C01I	109.7(7)
		C01I - C01N - C01L	129.2(7)
		O13 - C01L - C01N	114.5(6)
		N12 - C01L - O13	126.7(7)
		N12 - C01L - C01N	118.6(7)
		N7 - C01E - C01G	119.6(7)
		N7 - C01E - C01J	109.6(7)
		C01J - C01E - C01G	130.7(7)
		O12 - C01P - C01O	112.6(7)
		N16 - C01P - O12	127.0(8)
		N16 - C01P - C01O	120.4(8)
		O4 - C01F - C01M	116.1(7)
		N2 - C01F - O4	124.2(7)
		N2 - C01F - C01M	119.7(8)

	N5 - C01M - C01F	119.7(7)
	N5 - C01M - C01K	110.9(7)
	C01K - C01M - C01F	129.3(7)
	O5 - C01G - C01E	114.7(7)
	N6 - C01G - O5	124.9(7)
	N6 - C01G - C01E	120.4(7)
	N17 - C01O - C01Q	110.7(7)
	N17 - C01O - C01P	117.7(8)
	C01Q - C01O - C01P	131.6(8)
	N11 - C01I - C01N	121.7(7)
	N14 - C01I - N11	130.6(8)
	N14 - C01I - C01N	107.7(7)
	N1 - C01K - C01M	121.9(7)
	N4 - C01K - N1	129.7(7)
	N4 - C01K - C01M	108.4(6)
	N8 - C01J - N9	131.0(7)
	N8 - C01J - C01E	108.9(7)
	N9 - C01J - C01E	120.1(7)
	H10A - O10W - H10B	109.5
	H12A - O12W - H12B	109.5
	H8WA - O8W - H8WB	109.5

Table 5. Detonation property values comparison with methods in this work, EXPLO5_V6.01, and literature values.

Compound	Density (g/cm^3)	Q (kcal/g)	P (GPa)	D (m/s)
2	1.937	1.21[a]/1.21[b]	28.99[a]/31.30[b]	7913[a]/8006[b]
TNT[1]	1.654	1.44[a]/1.30[b]/1.22[c]	21.95[a]/22.75[b]/20.50[c]	7220[a]/7465[b]/7178[c]
HMX[1]	1.910	1.62[a]/1.49[b]/1.32[c]	40.36[a]/41.25[b]/38.39[c]	9374[a]/9310[b]/8900[c]
RDX[1]	1.806	1.59[a]/1.46[b]/1.44[c]	35.77[a]/36.6b/33.92[c]	8971[a]/8937[b]/8600[c]
$[Cu(tztr)]_n$[2]	2.216	2.78[a]/3.40[b,c]	31.15[a]/40.02b,[c]	7909[a]/8429b,[c]
$\{[Cu(tztr)]\ H_2O\}$[3]	2.316	1.32[a]/1.79[b]/1.32[c]	26.80[a]/39.15[b]/31.99[c]	7254[a]/8406[b]/7920[c]
$[Pb(Htztr)_2(H_2O)]_n$[4]	2.519	1.73[a]/0.47[b]/1.36[c]	20.11[a]/17.15[b]/31.57[c]	6432[a]/5755[b]/7715[c]
$[Cu(ntz)]_n$[5]	2.428	1.82[a]/1.47[b,c]	31.07[a]/33.10[b,c]	7721[a]/7970[b,c]
$[Cu(ntz)(N_3)(^AMF)]_n$[5]	1.801	1.99[a]/1.81[b,c]	23.29[a]/16.04[b,c]	7245[a]/6080[b,c]
$[Cu(ntz)(N_3)(H_2O)]_n$[5]	2.218	0.09[a]/0.02[b,c]	7.75[a]/4.46[b,c]	3943[a]/2220[b,c]

[a] calculation method in this work. [b] calculated with EXPLO5_V6.01[6]. [c] literature values.

REFERENCES

1 C. Shen, P. Wang, and M. Lu, J. Phys. Chem. A, 2015, 119 (29), 8250-8255.

2 Y. Zhang, S. Zhang, L. Sun, Q. Yang, J. Han, Q. Wei, G. Xie, S. Chen, and S. Gao, Chem. Commun., 2017, 53, 3034-3037.

3 X. Liu, W. Gao, P. Sun, Z. Su, S. Chen, Q. Wei, G. Xie, and S. Gao, Green Chem., 2015, 17, 831-836.

4 W. Gao, X. Liu, Z. Su, S. Zhang, Q. Yang, Q. Wei, S. Chen, G. Xie, X. Yanga, and S. Gao, J. Mater. Chem. A, 2014, 2, 11958-11965.

5 X. Qu, L. Zhai, B. Wang, Q. Wei, G. Xie, S. Chen, and S. Gao, Dalton Trans., 2016, 45, 17304-17311.

6 M. Sućeska, *EXPLO5 6.01*, Brodarski Institute, Zagreb, Croatia, 2013