Supporting Information

Dancing with 5-substituted monotetrazoles, oxygen-rich ions, and silver: Towards primary explosives with positive oxygen balance and excellent energetic performance

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General methods

All reagents were purchased from Energy Chemical of analytical grade and were used as supplied, if not stated otherwise. The melting and decomposition (onset) points were obtained on a differential scanning calorimeter (Mettler Toledo DSC823e) at a scan rate of 5 °C min^{-1} in closed Al containers with a nitrogen flow of 50 ml min^{-1}. IR spectra were recorded using KBr pellets for solids on a Thermo Nicolet iS10 spectrometer. Elemental analyses were carried out on a vario EL III CHNOS elemental analyzer.

X-ray Crystallography detail

A colorless block crystal ($[Ag_7MT_4(NO_3)_3]_n$) of dimensions 0.08×0.07×0.04 mm^3, a colorless plate crystal ($[Ag_7AT_4(NO_3)_3]_n$) of dimensions 0.10×0.08×0.03 mm^3, a colorless column crystal ($[Ag_3HT_2NO_3]_n$) of dimensions 0.11×0.07×0.04 mm^3, a colorless block crystal ($[Ag_5NT_4NO_3]_n$) of dimensions 0.09×0.08×0.07 mm^3, and a colorless needle crystal ($[Ag_5NT_4ClO_4]_n$) of dimensions 0.16×0.09×0.04 mm^3 were mounted on an Enraf-Nonius CAD4 four-circle diffractometer using graphite-monochromated Mo Ka radiation (λ = 0.71073 Å) at 173 K. Corrections for Lorentz and polarization effects and for absorption (ψ scan) were applied. The structure was solved by direct methods using SHELXS-97 and refined by full-matrix least-squares calculation on F^2 with SHELXL-97. All non-hydrogen atoms were refined anisotropically. All hydrogens were placed in calculated positions and were assigned fixed isotropic thermal parameters at 1.2 times the equivalent isotropic U of the atoms to which they were attached and allowed to ride on their respective parent atoms. The contributions of these hydrogen atoms were included in the structure-factor calculations.

Table S2 Crystallographic data for four energetic CPs.

Compound	$[Ag_7MT_4(NO_3)_3]_n$	$[Ag_3HT_2NO_3]_n$	$[Ag_7AT_4(NO_3)_3]_n$	$[Ag_5NT_4NO_3]_n$	$[Ag_5NT_4ClO_4]_n$
Formula	$C_8H_{12}Ag_7N_{19}O_9$	$C_2H_2Ag_3N_9O_3$	$C_4H_8Ag_7N_{23}O_9$	$C_4Ag_5N_{21}O_{11}$	$C_4Ag_5ClN_{20}O_{12}$
M_w	1273.46	523.74	1277.42	1057.60	1095.04
Crystal system	Orthorhombic	Monoclinic	Triclinic	Monoclinic	Tetragonal
Space group	C2221	C2/c	P-1	Pn	P42/n
a [Å]	12.7239(14)	10.9448(10)	7.0494(4)	12.5704(7)	12.9865(7)
b [Å]	13.7587(16)	8.0109(9)	9.2238(5)	6.5629(4)	12.9865(7)
c [Å]	14.5684(13)	10.9401(9)	9.4011(5)	13.3028(7)	6.7777(9)
α[°]	90	90	93.300(2)	90	90
β[°]	90	98.040(3)	97.259(2)	90.303(2)	90
γ[°]	90	90	105.496(2)	90	90
V [$Å^3$]	2550.4(5)	949.77(16)	581.67(6)	1097.44(11)	1143.1(2)
Z	4	4	1	2	2
T [K]	173	173	173	173	173
λ [Å]	0.71073	0.71073	0.71073	0.71073	0.71073
ρ_{calcd}[g cm^{-3}]	3.317	3.663	3.647	3.201	3.182
μ [mm^{-1}]	5.346	6.140	5.865	4.486	4.428
F(000)	2376	968.0	594	988	1024
θ range[°]	2.96-25.99	3.16-25.36	3.16-25.30	3.06-25.12	3.74-25.29
Index ranges	-15 ≤ h ≤ 15	-13 ≤ h ≤ 13	-7 ≤ h ≤ 8	-15 ≤ h ≤ 15	-15 ≤ h ≤15
	-16 ≤ k ≤ 17	-8 ≤ k ≤ 9	-11 ≤ k ≤ 11	-7 ≤ k ≤ 7	-15≤ k ≤15
	-17 ≤ l ≤ 17	-13 ≤ l ≤ 13	-11 ≤ l ≤ 11	-15 ≤ l ≤ 16	-8≤ l ≤7
Data/restraints/ parameters	2588/60/199	872/0/79	3985/520/443	3978/121/388	1057/144/122
GOF on F2	1.033	1.089	1.165	1.056	1.037
$R[F^2 > 2\sigma(F^2)]$	0.0489	0.0275	0.0623	0.0333	0.0335
$wR(F^2)$	0.0804	0.0650	0.1799	0.0645	0.0536

Table S1 Bond lengths and angles for $[Ag_7MT_4(NO_3)_3]_n$.

Ag1 N4 2.146(16) Ag1 N8 2.157(18) Ag2 N5 2.133(16) Ag2 N1 2.139(18) Ag3 N3 2.440(15) Ag3 N3 2.440(15) Ag3 N6 2.446(15) Ag3 N6 2.446(15) Ag3 O3 2.594(9) Ag3 O3 2.594(9) Ag4 N2 2.210(15) Ag4 O4 2.283(12) Ag4 N7 2.354(14) N2 N3 1.32(2)	C1 N1 1.34(2) C1 N4 1.35(2) C1 C2 1.48(2) C2 H2A 0.9800 C2 H2B 0.9800 C2 H2C 0.9800 C3 N5 1.33(2) C3 N8 1.34(2) C3 C4 1.46(2) C4 H4A 0.9800 C4 H4B 0.9800 C4 H4C 0.9800 N1 N2 1.37(2)	N3 N4 1.34(2) N4 Ag1 2.146(16) N5 N6 1.369(19) N6 N7 1.32(2) N6 Ag3 2.446(15) N7 N8 1.358(19) N7 Ag4 2.354(14) N9 O2 1.239(19) N9 O1 1.262(18) N9 O3 1.272(13) N10 O5 1.21(2) N10 O4 1.267(15) N10 O4 1.267(15)
N4 Ag1 N8 168.5(6) N5 Ag2 N1 165.5(6) N3 Ag3 N3 85.0(7) N3 Ag3 N6 94.0(4) N3 Ag3 N6 178.2(7) N3 Ag3 N6 178.2(7) N3 Ag3 N6 94.0(4) N6 Ag3 N6 87.0(8) N3 Ag3 O3 94.3(5) N3 Ag3 O3 94.8(5) N6 Ag3 O3 86.8(5) N6 Ag3 O3 84.3(5) N3 Ag3 O3 94.8(5) N3 Ag3 O3 94.3(5) N6 Ag3 O3 84.3(5) N6 Ag3 O3 86.8(5) O3 Ag3 O3 167.7(7) N2 Ag4 O4 154.7(5) N2 Ag4 N7 110.9(4) O4 Ag4 N7 84.8(5) O5 N10 O4 121.5(9) O4 N10 O4 117.0(19) N9 O3 Ag3 125.6(8) N7 N8 Ag1 120.0(12)	N1 C1 N4 109.8(15) N1 C1 C2 123.8(19) N4 C1 C2 126(2) C1 C2 H2A 109.5 C1 C2 H2B 109.5 H2A C2 H2B 109.5 C1 C2 H2C 109.5 H2A C2 H2C 109.5 H2B C2 H2C 109.5 N5 C3 N8 109.9(15) N5 C3 C4 126.9(19) N8 C3 C4 123.2(18) C3 C4 H4A 109.5 C3 C4 H4B 109.5 H4A C4 H4B 109.5 C3 C4 H4C 109.5 H4A C4 H4C 109.5 H4B C4 H4C 109.5 O2 N9 O3 121.3(16) O1 N9 O3 117.8(17) O5 N10 O4 121.5(9) O2 N9 O1 121.0(12) N10 O4 Ag4 111.5(10)	C1 N1 N2 106.0(15) C1 N1 Ag2 132.9(12) N2 N1 Ag2 121.0(12) N3 N2 N1 108.3(15) N3 N2 Ag4 121.3(12) N1 N2 Ag4 125.3(13) N2 N3 N4 109.3(14) N2 N3 Ag3 121.3(12) N4 N3 Ag3 128.1(11) N3 N4 C1 106.4(16) N3 N4 Ag1 121.7(11) C1 N4 Ag1 131.9(12) C3 N5 N6 106.6(15) C3 N5 Ag2 134.3(12) N6 N5 Ag2 119.0(11) N7 N6 N5 108.4(14) N7 N6 Ag3 120.9(11) N5 N6 Ag3 128.2(12) N6 N7 N8 108.3(14) N6 N7 Ag4 119.7(11) N8 N7 Ag4 130.0(12) C3 N8 N7 106.8(16) C3 N8 Ag1 133.2(12)

Table S2 Bond lengths and angles for $[Ag_7AT_4(NO_3)_3]_n$.

Ag1 N2B 2.23(3) Ag1 N2A 2.25(3) Ag2 N3B 2.22(3)	Ag7 N5C 2.53(3) C1A N5A 1.30(4) C1A N4A 1.37(4)	N2C N3C 1.28(4) N3C N4C 1.39(3) N5C Ag7 2.53(3)

Ag2 N5D 2.40(3)	C1A N1A 1.38(4)	N6C O2C 1.20(4)
Ag2 O2C 2.42(2)	C1B N4B 1.32(5)	N6C O1C 1.27(4)
Ag2 N3C 2.58(3)	C1B N5B 1.33(4)	N6C O3C 1.28(4)
Ag3 N4C 2.13(3)	C1B N1B 1.37(5)	N1D N2D 1.39(4)
Ag3 N1B 2.17(3)	C1C N4C 1.30(4)	N1D Ag5 2.15(3)
Ag3 O2C 2.57(3)	C1C N1C 1.33(4)	N2D N3D 1.34(4)
Ag3 Ag5 3.322(4)	C1C N5C 1.47(4)	N3D N4D 1.34(4)
Ag4 N4B 2.15(3)	C1D N1D 1.25(4)	N4D Ag6 2.15(3)
Ag4 N1C 2.17(3)	C1D N4D 1.39(5)	N5D Ag2 2.40(3)
Ag4 O3Y 2.39(9)	C1D N5D 1.40(4)	O2C Ag2 2.42(2)
Ag5 N1D 2.15(3)	N1A N2A 1.35(4)	O2C Ag3 2.57(3)
Ag5 N4A 2.19(3)	N2A N3A 1.31(4)	N6A O1A 1.23(3)
Ag5 Ag3 3.322(4)	N3A N4A 1.29(4)	N6A O2A 1.23(3)
Ag6 N1A 2.11(3)	N1B N2B 1.35(4)	N6A O3A 1.24(3)
Ag6 N4D 2.15(3)	N1B Ag3 2.17(3)	N6Z O2Z 1.23(3)
Ag7 N3D 2.19(3)	N2B N3B 1.29(4)	N6Z O1Z 1.24(3)
Ag7 N3A 2.28(3)	N3B N4B 1.42(4)	N6Z O3Z 1.24(3)
Ag7 O1C 2.29(3)	N1C N2C 1.35(4)	N6B O2B 1.26(2)
N6Y O3Y 1.27(2)	N1C Ag4 2.17(3)	N6B O3B 1.27(2)
N6Y O2Y 1.27(2)	N6Y O1Y 1.27(2)	N6B O1B 1.28(2)
N2B Ag1 N2A 176.1(10)	N3A Ag7 N5C 134.1(9)	N2B N1B C1B 109(3)
N3B Ag2 N5D 163.2(10)	O1C Ag7 N5C 86.6(10)	N2B N1B Ag3 117.7(19)
N3B Ag2 O2C 110.7(9)	N5A C1A N4A 126(3)	C1B N1B Ag3 133(2)
N5D Ag2 O2C 83.4(9)	N5A C1A N1A 128(3)	N3B N2B N1B 107(3)
N3B Ag2 N3C 91.8(10)	N4A C1A N1A 106(3)	N3B N2B Ag1 116(2)
N5D Ag2 N3C 101.4(9)	N4B C1B N5B 126(3)	N1B N2B Ag1 137(2)
O2C Ag2 N3C 72.9(8)	N4B C1B N1B 108(3)	N2B N3B N4B 110(3)
N4C Ag3 N1B 166.9(10)	N5B C1B N1B 126(3)	N2B N3B Ag2 121(2)
N4C Ag3 O2C 83.2(8)	N4C C1C N1C 117(3)	N4B N3B Ag2 127(2)
N1B Ag3 O2C 103.8(9)	N4C C1C N5C 120(3)	C1B N4B N3B 105(3)
N4C Ag3 Ag5 97.6(8)	N1C C1C N5C 122(3)	C1B N4B Ag4 132(3)
N1B Ag3 Ag5 89.2(7)	N1D C1D N4D 112(3)	N3B N4B Ag4 122(2)
O2C Ag3 Ag5 117.1(6)	N1D C1D N5D 131(3)	C1C N1C N2C 102(3)
N4B Ag4 N1C 165.7(10)	N4D C1D N5D 118(3)	C1C N1C Ag4 137(2)
N4B Ag4 O3Y 107(3)	N2A N1A C1A 105(3)	N2C N1C Ag4 120.3(19)
N1C Ag4 O3Y 87(3)	N2A N1A Ag6 123(2)	N3C N2C N1C 110(3)
N1D Ag5 N4A 166.8(10)	C1A N1A Ag6 132(2)	N2C N3C N4C 111(2)
N1D Ag5 Ag3 88.3(8)	N3A N2A N1A 111(3)	N2C N3C Ag2 112.7(19)
N4A Ag5 Ag3 104.2(7)	N3A N2A Ag1 121(2)	N4C N3C Ag2 129(2)
N1A Ag6 N4D 168.4(11)	N1A N2A Ag1 127(2)	C1C N4C N3C 100(2)
N3D Ag7 N3A 111.7(10)	N4A N3A N2A 108(3)	C1C N4C Ag3 136(2)
N3D Ag7 O1C 152.9(10)	N4A N3A Ag7 133(2)	N3C N4C Ag3 124(2)

N3A Ag7 O1C 80.9(10)	N2A N3A Ag7 119(2)	C1C N5C Ag7 110(2)
N3D Ag7 N5C 99.3(10)	N3A N4A C1A 110(3)	O2C N6C O1C 125(3)
C1D N4D Ag6 135(2)	N3A N4A Ag5 119(2)	O2C N6C O3C 117(3)
C1D N5D Ag2 110(2)	C1A N4A Ag5 130(2)	O1C N6C O3C 117(3)
N6C O1C Ag7 112(2)	O2A N6A O3A 119(2)	C1D N1D N2D 107(3)
N6C O2C Ag2 114(2)	O2Z N6Z O1Z 120(2)	C1D N1D Ag5 140(2)
N6C O2C Ag3 120(2)	O2Z N6Z O3Z 120(2)	N2D N1D Ag5 113(2)
Ag2 O2C Ag3 120.7(9)	O1Z N6Z O3Z 120(2)	N3D N2D N1D 107(3)
O1A N6A O2A 121(2)	O2B N6B O3B 121.8(18)	N4D N3D N2D 109(3)
O1A N6A O3A 120(2)	O2B N6B O1B 119.8(17)	N4D N3D Ag7 130(2)
O3Y N6Y O1Y 120(2)	O3B N6B O1B 118.4(17)	N2D N3D Ag7 119(2)
O2Y N6Y O1Y 120(2)	O3Y N6Y O2Y 120(2)	N3D N4D C1D 105(3)
N6Y O3Y Ag4 157(7)	N3D N4D Ag6 120(2)	

Table S3 Bond lengths and angles for $[Ag_3HT_2NO_3]_n$.

Ag1 N1 2.157(5)	C1 N1 1.328(8)	N3 N4 1.357(7)
Ag1 N1 2.157(5)	C1 N4 1.333(8)	N3 Ag2 2.255(5)
Ag2 N4 2.237(5)	C1 H1 0.9500	N5 O1 1.239(10)
Ag2 N3 2.255(5)	N1 N2 1.349(7)	N5 O2 1.260(6)
Ag2 N2 2.363(5)	N2 N3 1.315(6)	N5 O2 1.260(6)
Ag2 O1 2.623(2)	N2 Ag2 2.363(5)	
N1 Ag1 N1 167.9(3)	N1 C1 H1 124.7	N2 N3 Ag2 118.0(4)
N4 Ag2 N3 144.95(19)	N4 C1 H1 124.7	N4 N3 Ag2 129.7(4)
N4 Ag2 N2 110.11(18)	C1 N1 N2 106.3(5)	C1 N4 N3 105.6(5)
N3 Ag2 N2 104.42(18)	C1 N1 Ag1 130.2(4)	C1 N4 Ag2 124.6(4)
N4 Ag2 O1 79.46(14)	N2 N1 Ag1 123.1(4)	N3 N4 Ag2 129.7(4)
N3 Ag2 O1 92.39(18)	N3 N2 N1 108.8(5)	O1 N5 O2 120.0(4)
N2 Ag2 O1 94.21(15)	N3 N2 Ag2 130.3(4)	O1 N5 O2 120.0(4)
N1 C1 N4 110.5(5)	N1 N2 Ag2 119.2(3)	O2 N5 O2 119.9(7)
N5 O1 Ag2 109.54(14)	N2 N3 N4 108.8(5)	

Table S4 Bond lengths and angles for $[Ag_5NT_4NO_3]_n$.

Ag1 N1A 2.228(11)	C1A N1A 1.344(16)	N5B O1B 1.210(14)
Ag1 N4B 2.361(11)	C1A N5A 1.436(17)	N1C N2C 1.316(15)
Ag1 O4' 2.44(4)	C1B N4B 1.333(16)	N2C N3C 1.317(15)
Ag1 N2D 2.470(12)	C1B N1B 1.340(17)	N3C N4C 1.346(15)
Ag2 N1D 2.237(11)	C1B N5B 1.421(17)	N3C Ag3 2.403(11)
Ag2 N4C 2.245(10)	C1C N4C 1.305(16)	N4C Ag2 2.245(10)
Ag2 N2A 2.414(13)	C1C N1C 1.332(17)	N5C O1C 1.196(15)
Ag2 O5 2.425(15)	C1C N5C 1.458(17)	N5C O2C 1.198(16)
Ag2 O5' 2.59(3)	C1D N1D 1.310(16)	N1D N2D 1.338(15)
Ag3 N3A 2.342(11)	C1D N4D 1.318(16)	N2D N3D 1.310(15)

Ag3 N3D 2.352(11)	C1D N5D 1.455(17)	N3D N4D 1.353(15)
Ag3 N3C 2.403(11)	N1A N2A 1.369(17)	N3D Ag3 2.352(11)
Ag3 N3B 2.408(11)	N2A N3A 1.297(16)	N4D Ag5 2.278(10)
Ag4 N1C 2.223(11)	N3A N4A 1.343(15)	N5D O2D 1.211(16)
Ag4 N4A 2.232(10)	N5A O2A 1.218(15)	N5D O1D 1.220(15)
Ag4 N2B 2.393(12)	N5A O1A 1.231(16)	N6 O5 1.241(16)
Ag4 O3' 2.43(4)	N1B N2B 1.338(15)	N6 O3 1.243(16)
Ag4 O3 2.56(2)	N2B N3B 1.294(16)	N6 O4 1.250(16)
Ag5 N1B 2.223(10)	N3B N4B 1.375(16)	O3 Ag4 2.56(2)
Ag5 N4D 2.278(10)	N4B Ag1 2.361(11)	O5 Ag2 2.425(15)
Ag5 N2C 2.487(11)	N5B O2B 1.199(15)	N6' O5' 1.245(19)
C1A N4A 1.314(16)	O3' Ag4 2.43(4)	N6' O3' 1.246(19)
N6' O4' 1.247(19)	O5' Ag2 2.59(3)	
N1A Ag1 N4B 117.4(4)	N2B Ag4 O3 86.0(5)	N2A N3A Ag3 124.8(9)
N1A Ag1 O4' 143.9(16)	N1B Ag5 N4D 145.9(4)	N4A N3A Ag3 122.6(8)
N4B Ag1 O4' 96.7(15)	N1B Ag5 N2C 102.4(4)	C1A N4A N3A 103.6(10)
N1A Ag1 N2D 103.5(4)	N4D Ag5 N2C 95.1(4)	C1A N4A Ag4 139.7(9)
N4B Ag1 N2D 94.5(4)	N4A C1A N1A 113.4(12)	N3A N4A Ag4 116.6(8)
O4' Ag1 N2D 84.2(10)	N4A C1A N5A 124.8(12)	O2A N5A O1A 125.2(12)
N1D Ag2 N4C 143.1(4)	N1A C1A N5A 121.8(12)	O2A N5A C1A 117.2(12)
N1D Ag2 N2A 102.1(4)	N4B C1B N1B 112.8(11)	O1A N5A C1A 117.6(12)
N4C Ag2 N2A 95.0(4)	N4B C1B N5B 123.4(13)	N2B N1B C1B 104.0(10)
N1D Ag2 O5 107.9(5)	N1B C1B N5B 123.7(12)	N2B N1B Ag5 124.5(8)
N4C Ag2 O5 102.6(5)	N4C C1C N1C 112.8(12)	C1B N1B Ag5 129.5(8)
N2A Ag2 O5 95.4(8)	N4C C1C N5C 124.5(12)	N3B N2B N1B 110.7(11)
N1D Ag2 O5' 108.8(6)	N1C C1C N5C 122.5(12)	N3B N2B Ag4 116.3(9)
N4C Ag2 O5' 95.0(7)	N1D C1D N4D 113.5(11)	N1B N2B Ag4 132.9(8)
N2A Ag2 O5' 110.5(8)	N1D C1D N5D 123.3(11)	N2B N3B N4B 109.5(11)
N3A Ag3 N3D 162.4(4)	N4D C1D N5D 123.1(11)	N2B N3B Ag3 122.5(9)
N3A Ag3 N3C 91.8(4)	C1A N1A N2A 103.0(11)	N4B N3B Ag3 127.7(8)
N3D Ag3 N3C 86.1(3)	C1A N1A Ag1 131.3(9)	C1B N4B N3B 103.0(11)
N3A Ag3 N3B 93.7(4)	N2A N1A Ag1 123.3(9)	C1B N4B Ag1 142.5(9)
N3D Ag3 N3B 92.5(4)	N3A N2A N1A 108.7(11)	N3B N4B Ag1 111.5(8)
N3C Ag3 N3B 165.8(4)	N3A N2A Ag2 118.4(10)	O2B N5B O1B 125.5(13)
N1C Ag4 N4A 139.8(4)	N1A N2A Ag2 132.6(9)	O2B N5B C1B 117.5(12)
N1C Ag4 N2B 102.6(4)	N2A N3A N4A 111.3(12)	O1B N5B C1B 116.8(12)
N4A Ag4 N2B 103.2(4)	N2C N1C C1C 103.7(10)	N2C N3C N4C 107.8(10)
N1C Ag4 O3' 111.3(9)	N2C N1C Ag4 126.1(9)	N2C N3C Ag3 129.8(8)
N4A Ag4 O3' 98.6(8)	C1C N1C Ag4 126.1(9)	N4C N3C Ag3 122.4(8)
N2B Ag4 O3' 90.8(9)	N3C N2C N1C 110.8(11)	C1C N4C N3C 104.8(10)
N1C Ag4 O3 117.1(6)	N3C N2C Ag5 119.9(8)	C1C N4C Ag2 130.7(9)
N4A Ag4 O3 95.0(5)	N1C N2C Ag5 129.3(8)	N3C N4C Ag2 121.1(8)
O2D N5D C1D 116.8(12)	O1C N5C O2C 125.1(13)	C1D N4D Ag5 132.1(8)

O1D N5D C1D 116.6(12)	O1C N5C C1C 118.7(12)	N3D N4D Ag5 119.5(8)
O5 N6 O3 120.5(16)	O2C N5C C1C 116.1(12)	O2D N5D O1D 126.5(13)
O5 N6 O4 119.8(16)	N2D N3D Ag3 120.2(8)	C1D N1D N2D 104.1(10)
O3 N6 O4 119.7(16)	N4D N3D Ag3 130.8(8)	C1D N1D Ag2 128.5(9)
N6 O3 Ag4 109.0(14)	C1D N4D N3D 103.8(10)	N2D N1D Ag2 125.8(8)
N6 O5 Ag2 129.2(13)	N6' O3' Ag4 125(2)	N3D N2D N1D 109.9(11)
O5' N6' O3' 120(2)	N6' O4' Ag1 100(2)	N3D N2D Ag1 119.6(8)
O5' N6' O4' 121(2)	N6' O5' Ag2 124(2)	N1D N2D Ag1 129.9(8)
O3' N6' O4' 119(2)	N2D N3D N4D 108.7(10)	

Table S5 Bond lengths (Å) and bond angles (°) for $[Ag_5NT_4ClO_4]_n$.

Ag1 N1 2.204(5)	C1 N1 1.318(7)	N1 N2 1.348(6)
Ag1 N4 2.249(4)	C1 N4 1.324(7)	N2 N3 1.323(6)
Ag1 N2 2.445(5)	C1 N5Z 1.46(3)	N2 Ag1 2.445(5)
Ag1 O1 2.581(4)	C1 N5 1.46(2)	N3 N4 1.341(6)
Ag2 N3 2.408(5)	C1 N5A 1.47(2)	N4 Ag1 2.249(4)
Ag2 N3 2.408(5)	Cl1 O1 1.442(4)	N5 O2 1.220(11)
Ag2 N3 2.408(5)	Cl1 O1 1.442(4)	N5 O3 1.234(12)
Ag2 N3 2.408(5)	Cl1 O1 1.442(4)	N5A O2A 1.228(13)
N5Z O2Z 1.222(15)	Cl1 O1 1.442(4)	N5A O3A 1.232(14)
N5Z O3Z 1.232(15)		
N1 Ag1 N4 141.68(17)	N4 C1 N5Z 120.7(9)	N2 N3 N4 109.8(4)
N1 Ag1 N2 108.08(16)	N1 C1 N5 122.8(7)	N2 N3 Ag2 123.8(3)
N4 Ag1 N2 99.26(16)	N4 C1 N5 122.8(7)	N4 N3 Ag2 126.4(3)
N1 Ag1 O1 119.03(15)	N1 C1 N5A 120.5(8)	C1 N4 N3 103.2(4)
N4 Ag1 O1 92.00(15)	N4 C1 N5A 123.6(8)	C1 N4 Ag1 134.1(4)
N2 Ag1 O1 78.49(14)	O1 Cl1 O1 108.98(17)	N3 N4 Ag1 118.8(3)
N3 Ag2 N3 91.49(4)	O1 Cl1 O1 110.5(3)	Cl1 O1 Ag1 111.8(2)
N3 Ag2 N3 91.49(4)	O1 Cl1 O1 108.98(17)	O2 N5 O3 125.4(18)
N3 Ag2 N3 161.5(2)	O1 Cl1 O1 108.98(17)	O2 N5 C1 117.6(13)
N3 Ag2 N3 161.5(2)	O1 Cl1 O1 110.5(3)	O3 N5 C1 116.9(12)
N3 Ag2 N3 91.49(4)	O1 Cl1 O1 108.98(17)	O2A N5A O3A 126(2)
N3 Ag2 N3 91.49(4)	C1 N1 N2 103.3(4)	O2A N5A C1 115.9(15)
N1 C1 N4 114.5(5)	C1 N1 Ag1 131.6(4)	O3A N5A C1 117.8(14)
N1 C1 N5Z 124.7(9)	N2 N1 Ag1 120.1(4)	O2Z N5Z O3Z 125(3)
N3 N2 Ag1 120.5(3)	N3 N2 N1 109.2(4)	O2Z N5Z C1 118.0(17)
N1 N2 Ag1 130.1(4)	O3Z N5Z C1 116.8(17)	

Packing styles of five ECPs without metal nodes

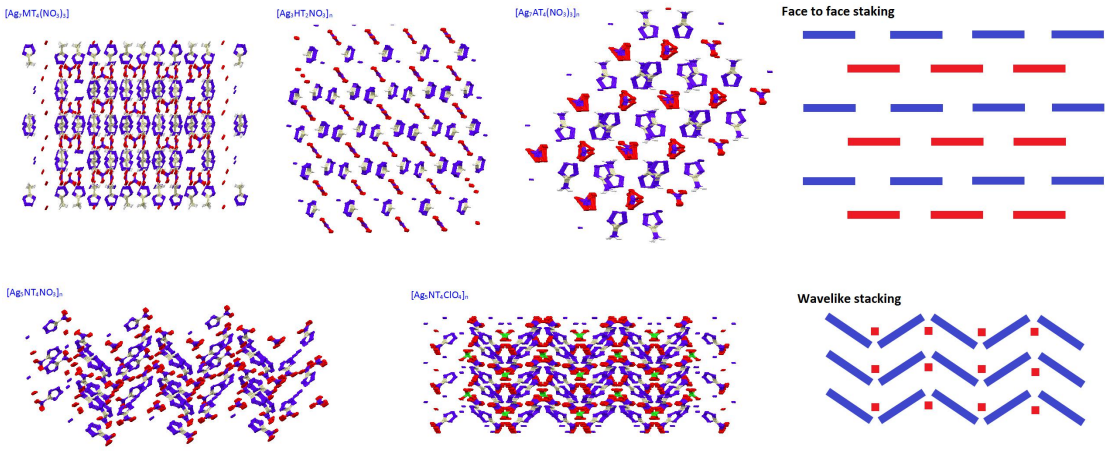

Figure S1 Packing styles of five ECPs without metal nodes.

Electronic surfaces of four tetrazole ligands

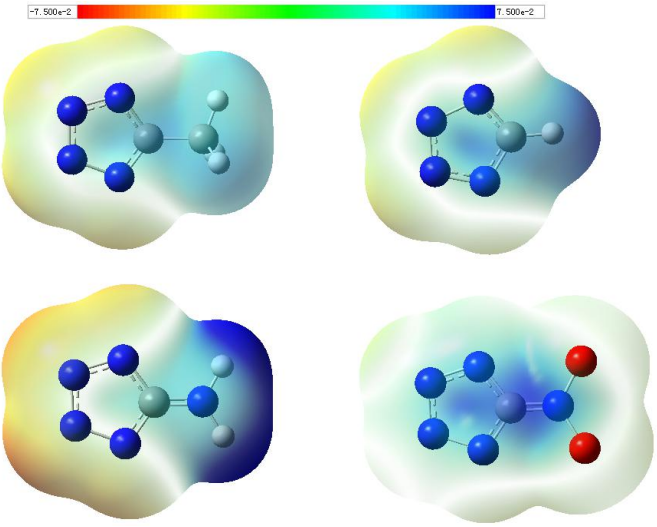

Figure S2 Electronic surfaces of four ligands in the same range.

IR Spectra

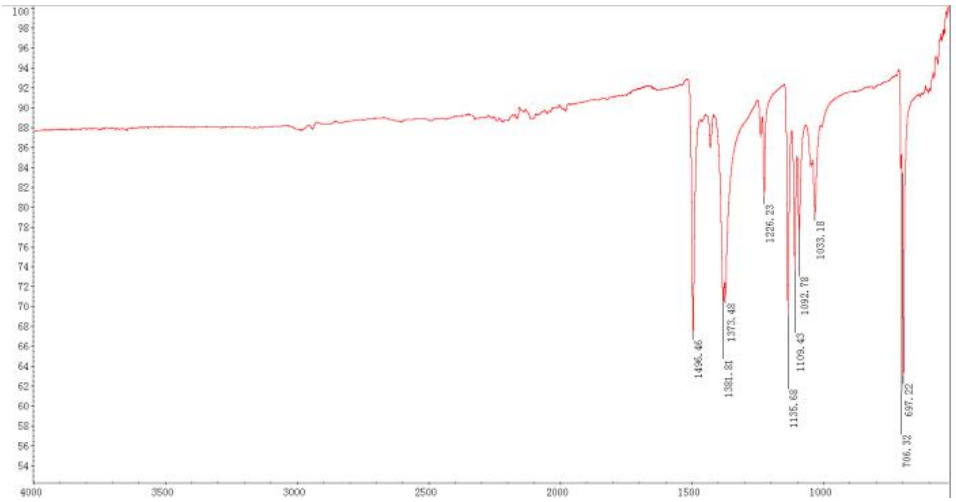

Figure S3 IR spectra for $[Ag_7MT_4(NO_3)_3]_n$.

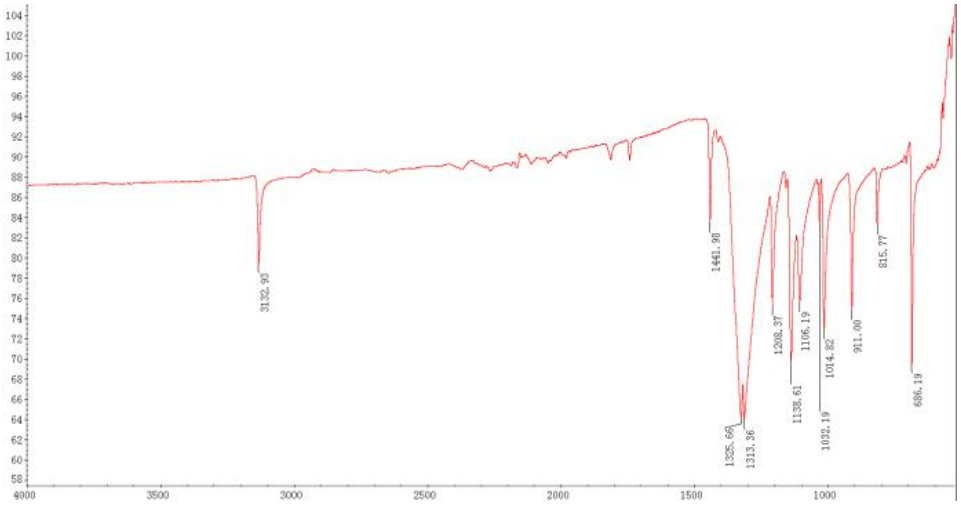

Figure S4 IR spectra for $[Ag_3HT_2NO_3]_n$.

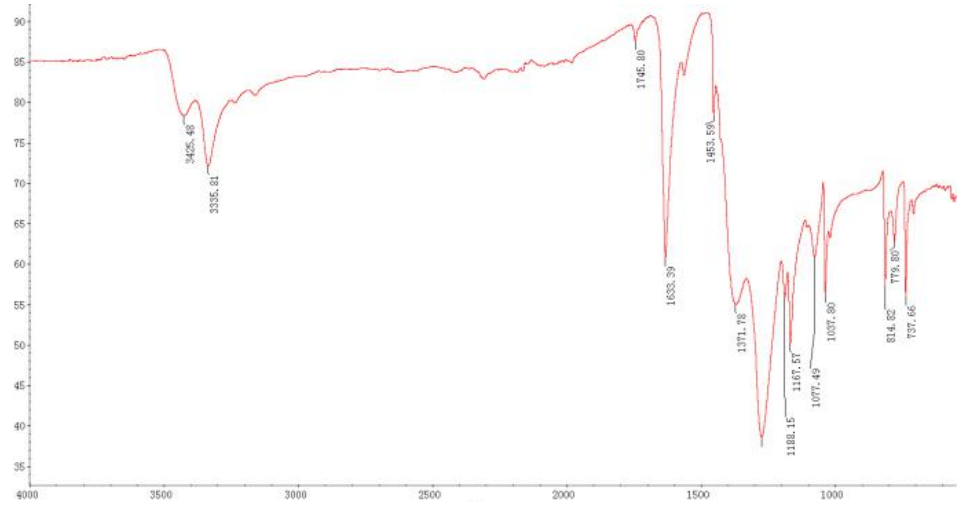

Figure S5 IR spectra for $[Ag_7AT_4(NO_3)_3]_n$.

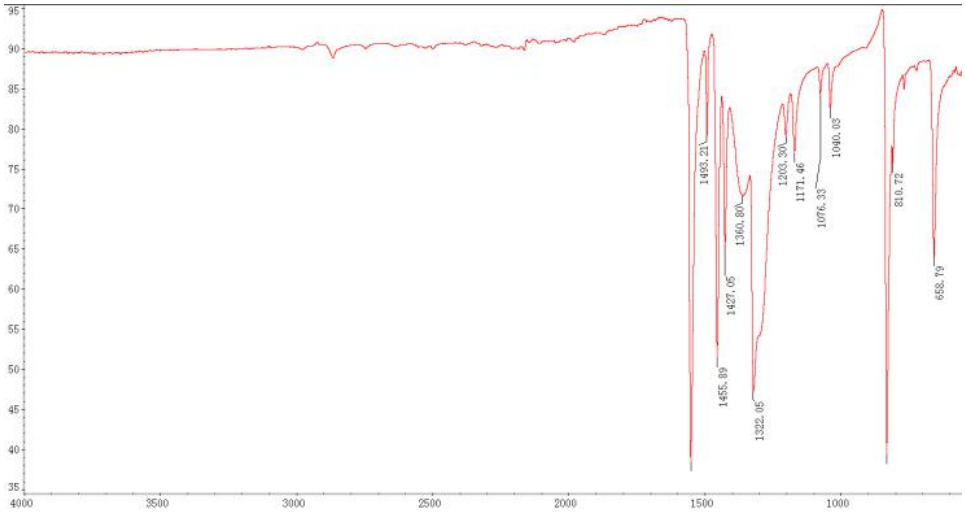

Figure S6 IR spectra for $[Ag_5NT_4NO_3]_n$.

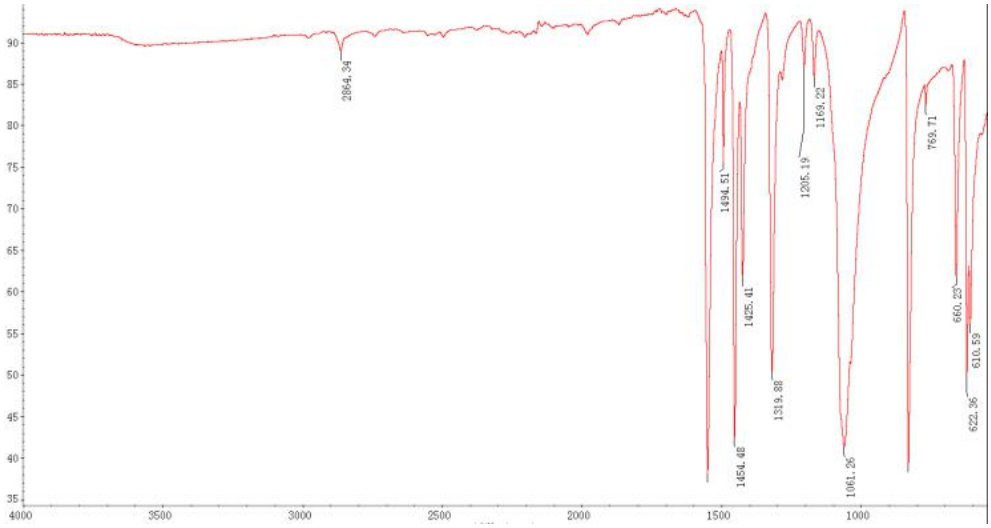

Figure S7 IR spectra for $[Ag_5NT_4ClO_4]_n$.

DSC and TGA plots

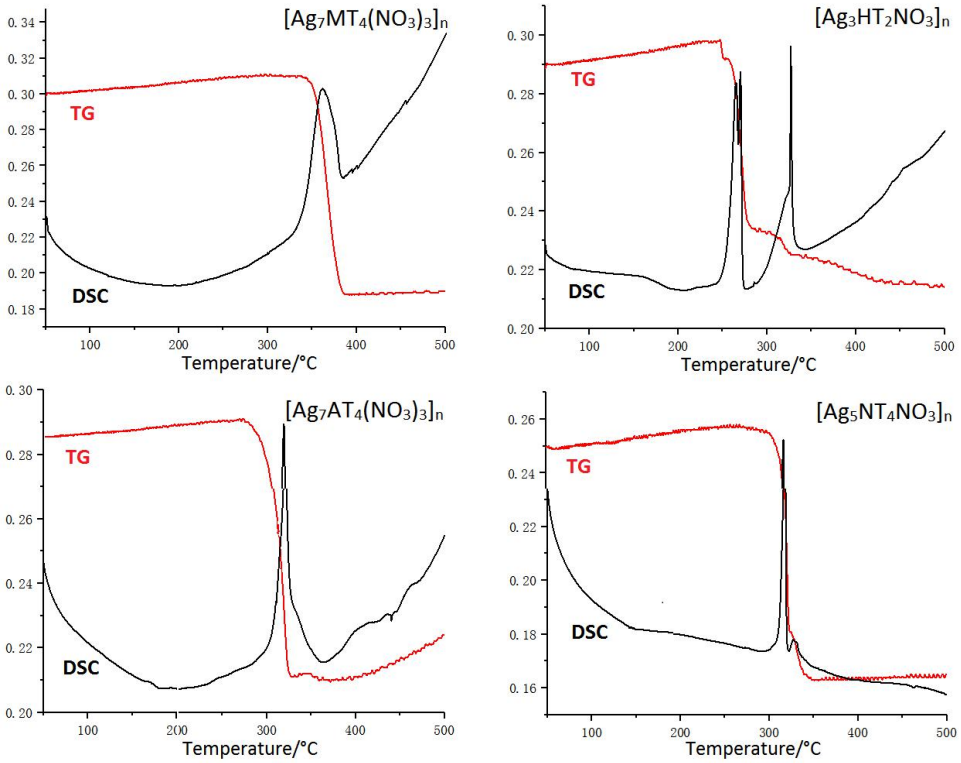

Figure S8 DSC and TGA plots for $[Ag_7MT_4(NO_3)_3]_n$, $[Ag_3HT_2NO_3]_n$, $[Ag_7AT_4(NO_3)_3]_n$, and $[Ag_5NT_4NO_3]_n$.

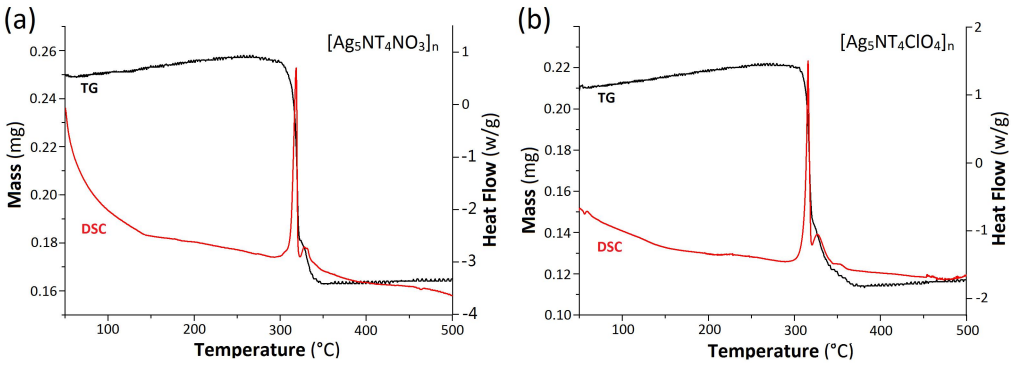

Figure S9 IR spectra for $[Ag_5NT_4NO_3]_n$ and $[Ag_5NT_4ClO_4]_n$.

Bond dissociation energy

Table s6 BDEs of four ligand

Compd	5-MT	5-HT	5-AT	5-NT
BDEs/kJ mol^{-1}	363.4	298.1	348.7	234.5