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PAPER

Photophysical properties of $\{[Ag(CN)_2]^-\}_2$ complexes trapped in a supramolecular electron-acceptor organic framework

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Supporting Information

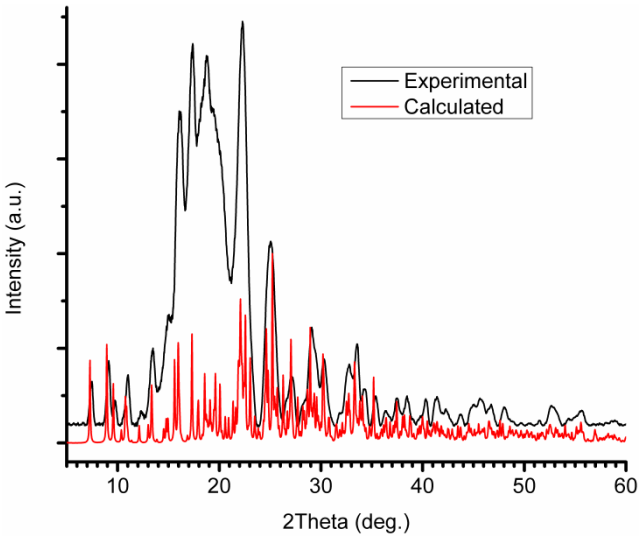

Fig. S1 Graph from PXRD analysis of powdered crystals of sample **1**.

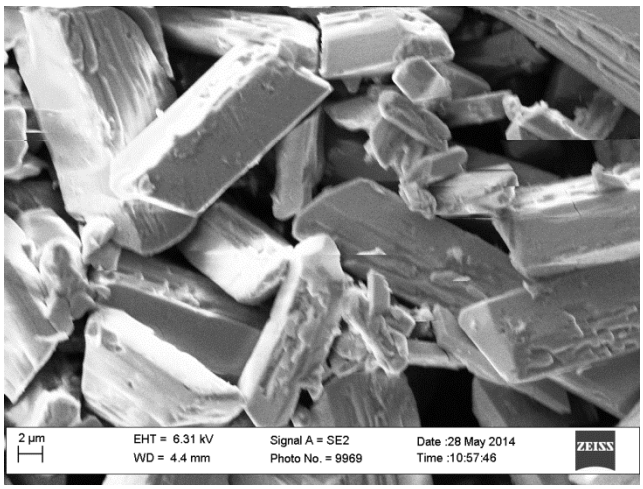

Fig. S2 SEM image of microcrystals of **1**.

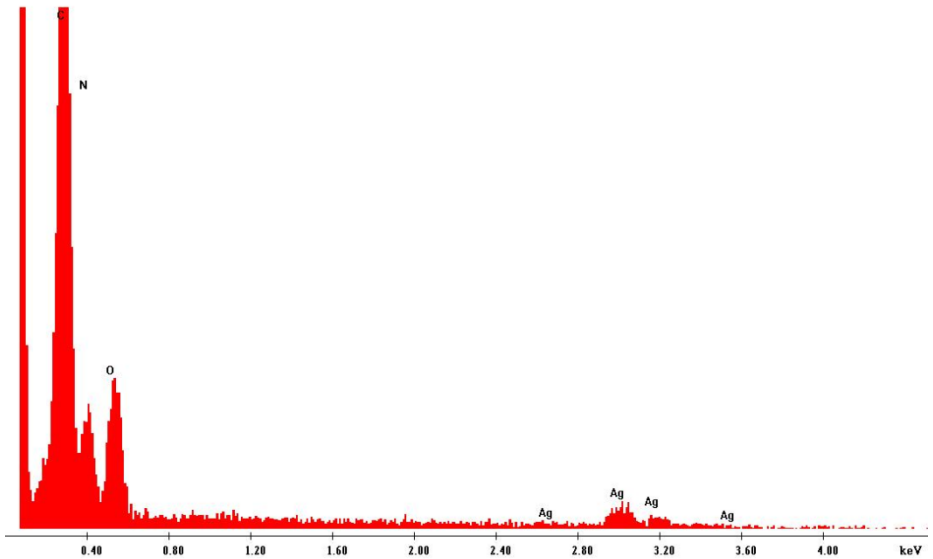

Fig. S3 SEM-EDS elemental analysis of **1**. Detection of hydrogen was not possible so its presence was extrapolated based off of the results for the other elements. Also, the carbon reading is overstated due to the carbon-based compound (DAG) used to tape the sample down.

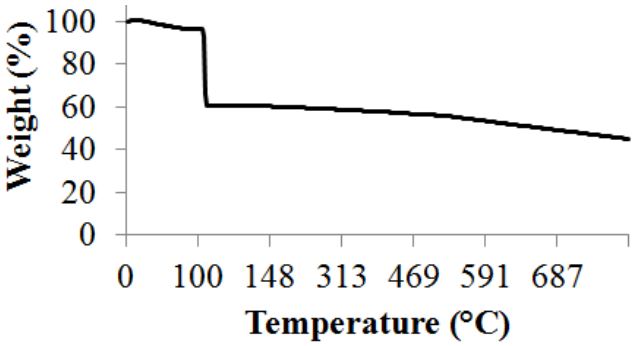

Fig. 4 TGA graph for microcrystals of **1**.

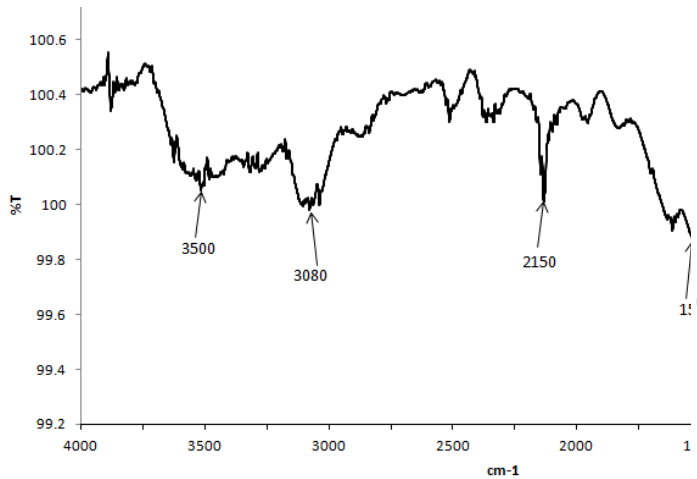

Fig. S5 Image of FT-IR results.

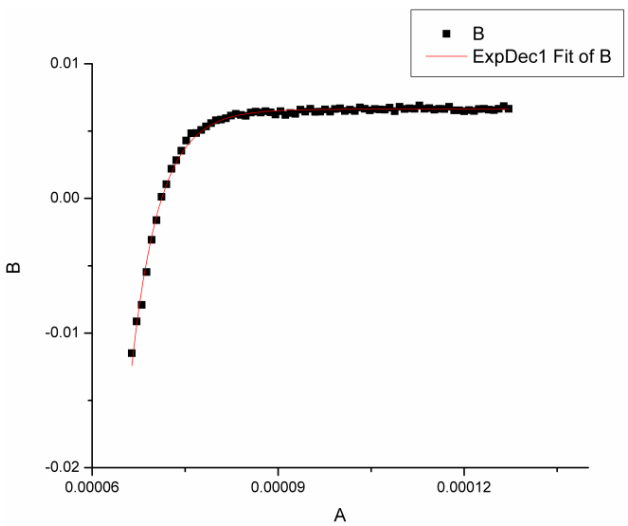

Fig. S6 Curve for luminescence lifetime determination for **1** at 78K. R^2 is 0.99599.

Table S1 Data table for luminescence lifetime determination of **1** at 78K.

y0	0.00714	4.31E-05
A1	-49742.9	10950.87
t1	4.88E-06	6.81E-08

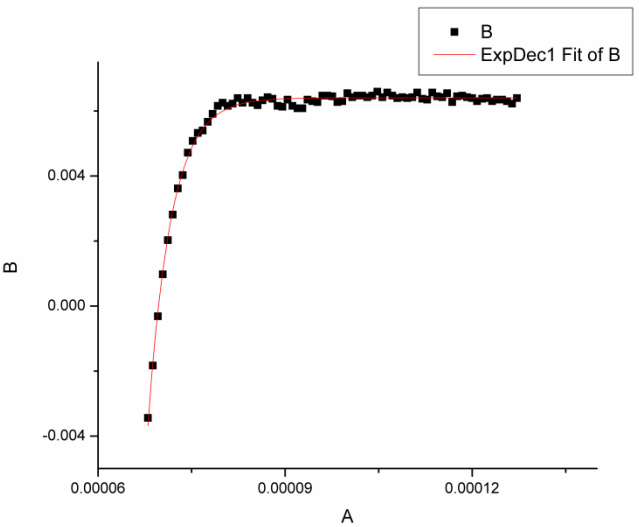

Fig. S7 Curve for luminescence lifetime determination for **1** at 298K. R^2 is 0.99547.

Table S2 Data table for luminescence lifetime determination of **1** at 298K.

	Value	Std Error
y0	0.0064	1.67E-05
A1	-798095	236149.8
t1	3.88E-06	5.97E-08

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Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)

for P1bar.res. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	6302(1)	335(1)	3898(1)	30(1)
Ag(2)	3401(1)	4309(1)	4631(1)	28(1)
Ag(3)	2737(1)	1056(1)	902(1)	32(1)
O(1)	-318(3)	9527(2)	5874(2)	37(1)
O(2)	-2545(3)	10170(2)	6167(2)	38(1)
O(3)	-4297(3)	6140(2)	7939(1)	31(1)
O(4)	-5196(3)	7871(2)	7690(2)	34(1)
O(5)	9320(3)	6010(2)	333(1)	27(1)
O(6)	9423(3)	7745(2)	303(1)	28(1)
O(7)	5984(3)	9985(2)	1614(1)	30(1)
O(8)	4601(3)	9304(2)	2395(1)	32(1)
O(9)	7670(3)	3591(2)	1936(1)	26(1)
O(10)	8608(4)	2537(3)	2788(1)	47(1)
O(11)	11562(4)	-853(3)	2510(2)	59(1)
O(12)	11069(4)	-1829(3)	1757(2)	53(1)
O(13)	-208(3)	6480(2)	2749(2)	31(1)
O(14)	3908(3)	6392(3)	1217(1)	32(1)
O(15)	1232(3)	5734(3)	1559(2)	37(1)
N(1)	3952(4)	1762(3)	4762(2)	29(1)
N(2)	8399(4)	-1260(3)	2970(2)	31(1)
N(3)	5636(5)	4471(3)	3418(2)	37(1)
N(4)	1238(4)	4232(3)	5932(2)	38(1)
N(5)	1311(4)	3400(4)	1344(2)	39(1)
N(6)	3815(5)	-1325(4)	487(2)	49(1)
N(7)	-1525(3)	9421(2)	6123(2)	24(1)
N(8)	-4266(3)	7044(3)	7630(2)	26(1)
N(9)	8977(3)	6907(2)	548(2)	22(1)
N(10)	5577(3)	9211(2)	1959(2)	22(1)
N(11)	8276(3)	2715(2)	2199(2)	22(1)
N(12)	10948(4)	-971(3)	2017(2)	39(1)
N(13)	144(3)	7415(2)	5590(1)	17(1)
N(14)	5065(3)	7161(2)	2824(1)	17(1)
N(15)	7261(3)	2759(2)	811(1)	16(1)
C(1)	4791(5)	1311(3)	4473(2)	31(1)
C(2)	7707(4)	-667(3)	3294(2)	27(1)
C(3)	4906(5)	4442(3)	3813(2)	26(1)
C(4)	1956(4)	4278(3)	5459(2)	30(1)
C(5)	1851(5)	2584(4)	1197(2)	32(1)
C(6)	3494(5)	-514(4)	615(2)	36(1)
C(7)	2089(4)	7368(3)	4499(2)	17(1)
C(8)	2548(4)	7042(3)	5155(2)	20(1)
C(9)	1566(4)	7062(3)	5693(2)	19(1)
C(10)	-337(4)	7761(3)	4963(2)	20(1)
C(11)	612(4)	7737(3)	4415(2)	19(1)
C(12)	-913(4)	7367(3)	6155(2)	18(1)
C(13)	-1754(4)	8304(3)	6387(2)	19(1)
C(14)	-2847(4)	8211(3)	6876(2)	20(1)
C(15)	-3051(4)	7164(3)	7138(2)	21(1)
C(16)	-2185(4)	6220(3)	6944(2)	22(1)
C(17)	-1105(4)	6325(3)	6438(2)	21(1)
C(18)	3138(4)	7280(3)	3914(2)	17(1)
C(19)	2747(4)	6997(3)	3308(2)	18(1)
C(20)	3727(4)	6943(3)	2767(2)	18(1)
C(21)	5501(4)	7386(3)	3414(2)	20(1)
C(22)	4557(4)	7456(3)	3964(2)	20(1)
C(23)	6059(3)	7134(3)	2236(2)	17(1)
C(24)	6765(4)	6110(3)	2084(2)	20(1)
C(25)	7729(4)	6032(3)	1526(2)	21(1)
C(26)	7946(4)	6984(3)	1139(2)	20(1)
C(27)	7253(4)	8024(3)	1273(2)	20(1)
C(28)	6298(4)	8093(3)	1831(2)	18(1)
C(29)	5840(4)	2737(3)	801(2)	23(1)
C(30)	4932(4)	3619(3)	490(2)	26(1)
C(31)	5482(4)	4522(3)	172(2)	17(1)
C(32)	6975(4)	4493(3)	180(2)	23(1)
C(33)	7836(4)	3620(3)	506(2)	22(1)
C(34)	8208(3)	1816(3)	1140(2)	17(1)
C(35)	8658(4)	1786(3)	1792(2)	18(1)
C(36)	9544(4)	863(3)	2080(2)	24(1)
C(37)	9964(4)	-9(3)	1704(2)	26(1)
C(38)	9542(4)	-4(3)	1060(2)	28(1)
C(39)	8633(4)	924(3)	777(2)	21(1)

Table S4. Bond lengths [Å] and angles [°] for P1bar.res.

Ag(1)-C(1)	2.073(5)
Ag(1)-C(2)	2.073(4)
Ag(2)-C(4)	2.067(4)
Ag(2)-C(3)	2.097(5)
Ag(3)-C(5)	2.067(5)
Ag(3)-C(6)	2.085(6)
O(1)-N(7)	1.227(4)
O(2)-N(7)	1.216(4)
O(3)-N(8)	1.218(4)
O(4)-N(8)	1.234(4)
O(5)-N(9)	1.224(4)
O(6)-N(9)	1.225(4)
O(7)-N(10)	1.217(4)
O(8)-N(10)	1.219(4)
O(9)-N(11)	1.210(4)
O(10)-N(11)	1.224(4)
O(11)-N(12)	1.212(6)
O(12)-N(12)	1.224(6)
O(13)-H(13A)	0.871(19)
O(13)-H(13B)	0.883(19)
O(14)-H(14A)	0.889(19)
O(14)-H(14B)	0.898(19)
O(15)-H(15A)	0.875(19)
O(15)-H(15B)	0.885(19)
N(1)-C(1)	1.060(5)
N(2)-C(2)	1.126(5)
N(3)-C(3)	1.011(6)
N(4)-C(4)	1.124(6)
N(5)-C(5)	1.111(6)
N(6)-C(6)	1.054(7)
N(7)-C(13)	1.471(4)
N(8)-C(15)	1.470(5)
N(9)-C(26)	1.476(4)
N(10)-C(28)	1.474(4)
N(11)-C(35)	1.468(4)
N(12)-C(37)	1.476(5)
N(13)-C(9)	1.351(4)
N(13)-C(10)	1.356(4)
N(13)-C(12)	1.454(4)
N(14)-C(20)	1.348(4)
N(14)-C(21)	1.350(5)
N(14)-C(23)	1.450(4)
N(15)-C(29)	1.341(5)
N(15)-C(33)	1.347(5)
N(15)-C(34)	1.454(4)
C(7)-C(11)	1.395(5)
C(7)-C(8)	1.399(5)
C(7)-C(18)	1.477(5)
C(8)-C(9)	1.367(5)
C(8)-H(8)	0.9500
C(9)-H(9)	0.9500
C(10)-C(11)	1.363(5)
C(10)-H(10)	0.9500
C(11)-H(11)	0.9500
C(12)-C(17)	1.385(5)
C(12)-C(13)	1.393(5)
C(13)-C(14)	1.378(5)
C(14)-C(15)	1.382(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.381(5)
C(16)-C(17)	1.393(5)
C(16)-H(16)	0.9500
C(17)-H(17)	0.9500
C(18)-C(19)	1.391(5)
C(18)-C(22)	1.402(5)
C(19)-C(20)	1.371(5)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(22)	1.364(5)
C(21)-H(21)	0.9500
C(22)-H(22)	0.9500
C(23)-C(24)	1.382(5)
C(23)-C(28)	1.401(5)
C(24)-C(25)	1.388(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.372(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.385(5)
C(27)-C(28)	1.383(5)
C(27)-H(27)	0.9500
C(29)-C(30)	1.373(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.385(5)
C(30)-H(30)	0.9500
C(31)-C(32)	1.396(5)
C(31)-C(31)#1	1.485(7)
C(32)-C(33)	1.357(5)
C(32)-H(32)	0.9500
C(33)-H(33)	0.9500
C(34)-C(39)	1.380(5)
C(34)-C(35)	1.393(5)
C(35)-C(36)	1.378(5)
C(36)-C(37)	1.376(6)
C(36)-H(36)	0.9500
C(37)-C(38)	1.372(6)
C(38)-C(39)	1.390(5)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500
C(1)-Ag(1)-C(2)	176.46(15)
C(4)-Ag(2)-C(3)	175.95(15)
C(5)-Ag(3)-C(6)	176.20(16)
H(13A)-O(13)-H(13B)	98(4)
H(14A)-O(14)-H(14B)	111(4)
H(15A)-O(15)-H(15B)	116(4)
O(2)-N(7)-O(1)	125.0(3)
O(2)-N(7)-C(13)	117.5(3)
O(1)-N(7)-C(13)	117.5(3)
O(3)-N(8)-O(4)	124.8(3)
O(3)-N(8)-C(15)	118.1(3)
O(4)-N(8)-C(15)	117.0(3)
O(5)-N(9)-O(6)	124.5(3)
O(5)-N(9)-C(26)	117.5(3)
O(6)-N(9)-C(26)	118.0(3)
O(7)-N(10)-O(8)	124.1(3)
O(7)-N(10)-C(28)	117.5(3)
O(8)-N(10)-C(28)	118.3(3)
O(9)-N(11)-O(10)	124.7(3)
O(9)-N(11)-C(35)	118.9(3)
O(10)-N(11)-C(35)	116.5(3)
O(11)-N(12)-O(12)	125.4(4)
O(11)-N(12)-C(37)	117.8(4)
O(12)-N(12)-C(37)	116.8(4)
C(9)-N(13)-C(10)	121.5(3)
C(9)-N(13)-C(12)	119.7(3)
C(10)-N(13)-C(12)	118.7(3)
C(20)-N(14)-C(21)	121.7(3)
C(20)-N(14)-C(23)	118.5(3)
C(21)-N(14)-C(23)	119.7(3)
C(29)-N(15)-C(33)	121.4(3)
C(29)-N(15)-C(34)	119.3(3)
C(33)-N(15)-C(34)	119.3(3)
N(1)-C(1)-Ag(1)	174.8(4)
N(2)-C(2)-Ag(1)	175.0(3)
N(3)-C(3)-Ag(2)	177.5(4)
N(4)-C(4)-Ag(2)	175.9(4)
N(5)-C(5)-Ag(3)	176.5(4)
N(6)-C(6)-Ag(3)	176.2(5)
C(11)-C(7)-C(8)	118.1(3)
C(11)-C(7)-C(18)	121.3(3)
C(8)-C(7)-C(18)	120.6(3)
C(9)-C(8)-C(7)	120.6(3)
C(9)-C(8)-H(8)	119.7
C(7)-C(8)-H(8)	119.7

N(13)-C(9)-C(8)	119.5(3)
N(13)-C(9)-H(9)	120.2
C(8)-C(9)-H(9)	120.2
N(13)-C(10)-C(11)	120.3(3)
N(13)-C(10)-H(10)	119.8
C(11)-C(10)-H(10)	119.8
C(10)-C(11)-C(7)	119.9(3)
C(10)-C(11)-H(11)	120.0
C(7)-C(11)-H(11)	120.0
C(17)-C(12)-C(13)	120.6(3)
C(17)-C(12)-N(13)	116.4(3)
C(13)-C(12)-N(13)	122.9(3)
C(14)-C(13)-C(12)	120.5(3)
C(14)-C(13)-N(7)	117.5(3)
C(12)-C(13)-N(7)	122.0(3)
C(13)-C(14)-C(15)	117.9(3)
C(13)-C(14)-H(14)	121.0
C(15)-C(14)-H(14)	121.0
C(16)-C(15)-C(14)	122.9(3)
C(16)-C(15)-N(8)	118.3(3)
C(14)-C(15)-N(8)	118.8(3)
C(15)-C(16)-C(17)	118.7(3)
C(15)-C(16)-H(16)	120.7
C(17)-C(16)-H(16)	120.7
C(12)-C(17)-C(16)	119.3(3)
C(12)-C(17)-H(17)	120.4
C(16)-C(17)-H(17)	120.4
C(19)-C(18)-C(22)	118.7(3)
C(19)-C(18)-C(7)	120.8(3)
C(22)-C(18)-C(7)	120.5(3)
C(20)-C(19)-C(18)	119.8(3)
C(20)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
N(14)-C(20)-C(19)	119.9(3)
N(14)-C(20)-H(20)	120.1
C(19)-C(20)-H(20)	120.1
N(14)-C(21)-C(22)	120.2(3)
N(14)-C(21)-H(21)	119.9
C(22)-C(21)-H(21)	119.9
C(21)-C(22)-C(18)	119.5(3)
C(21)-C(22)-H(22)	120.3
C(18)-C(22)-H(22)	120.3
C(24)-C(23)-C(28)	120.8(3)
C(24)-C(23)-N(14)	117.0(3)
C(28)-C(23)-N(14)	122.2(3)
C(23)-C(24)-C(25)	119.6(3)
C(23)-C(24)-H(24)	120.2
C(25)-C(24)-H(24)	120.2
C(26)-C(25)-C(24)	118.5(3)
C(26)-C(25)-H(25)	120.7
C(24)-C(25)-H(25)	120.7
C(25)-C(26)-C(27)	123.6(3)
C(25)-C(26)-N(9)	118.7(3)
C(27)-C(26)-N(9)	117.7(3)
C(28)-C(27)-C(26)	117.5(3)
C(28)-C(27)-H(27)	121.3
C(26)-C(27)-H(27)	121.3
C(27)-C(28)-C(23)	120.1(3)
C(27)-C(28)-N(10)	116.1(3)
C(23)-C(28)-N(10)	123.8(3)
N(15)-C(29)-C(30)	120.0(3)
N(15)-C(29)-H(29)	120.0
C(30)-C(29)-H(29)	120.0
C(29)-C(30)-C(31)	120.3(3)
C(29)-C(30)-H(30)	119.9
C(31)-C(30)-H(30)	119.9
C(30)-C(31)-C(32)	117.6(3)
C(30)-C(31)-C(31)#1	120.9(4)
C(32)-C(31)-C(31)#1	121.4(4)
C(33)-C(32)-C(31)	120.6(3)
C(33)-C(32)-H(32)	119.7
C(31)-C(32)-H(32)	119.7
N(15)-C(33)-C(32)	120.1(3)
N(15)-C(33)-H(33)	120.0
C(32)-C(33)-H(33)	120.0
C(39)-C(34)-C(35)	120.6(3)
C(39)-C(34)-N(15)	116.7(3)
C(35)-C(34)-N(15)	122.7(3)
C(36)-C(35)-C(34)	120.0(3)
C(36)-C(35)-N(11)	116.6(3)
C(34)-C(35)-N(11)	123.3(3)
C(37)-C(36)-C(35)	118.1(3)
C(37)-C(36)-H(36)	120.9
C(35)-C(36)-H(36)	120.9
C(38)-C(37)-C(36)	123.3(3)
C(38)-C(37)-N(12)	119.9(4)
C(36)-C(37)-N(12)	116.8(4)
C(37)-C(38)-C(39)	118.2(3)
C(37)-C(38)-H(38)	120.9
C(39)-C(38)-H(38)	120.9
C(34)-C(39)-C(38)	119.8(3)
C(34)-C(39)-H(39)	120.1
C(38)-C(39)-H(39)	120.1

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

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for P1bar.res. 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}
Ag(1)	27(1)	28(1)	35(1)	-8(1)	-6(1)	-2(1)
Ag(2)	25(1)	26(1)	31(1)	1(1)	-2(1)	-1(1)
Ag(3)	29(1)	37(1)	33(1)	3(1)	-4(1)	-15(1)
O(1)	34(2)	24(1)	54(2)	-6(1)	13(1)	-10(1)
O(2)	36(2)	18(1)	55(2)	-3(1)	7(1)	2(1)
O(3)	31(1)	32(1)	28(1)	2(1)	5(1)	-9(1)
O(4)	28(1)	30(1)	43(2)	-7(1)	12(1)	-1(1)
O(5)	30(1)	24(1)	27(1)	-8(1)	8(1)	-10(1)
O(6)	35(1)	24(1)	26(1)	-1(1)	8(1)	-13(1)
O(7)	36(2)	17(1)	34(1)	2(1)	7(1)	-5(1)
O(8)	28(1)	23(1)	38(2)	0(1)	15(1)	3(1)
O(9)	37(2)	18(1)	23(1)	-3(1)	1(1)	-2(1)
O(10)	61(2)	55(2)	21(1)	-11(1)	-17(1)	13(2)
O(11)	32(2)	36(2)	104(3)	27(2)	-36(2)	-6(1)
O(12)	49(2)	21(2)	74(2)	11(2)	21(2)	10(1)
O(13)	30(1)	32(1)	32(1)	-6(1)	-4(1)	-7(1)
O(14)	33(2)	39(2)	26(1)	-8(1)	-2(1)	-6(1)
O(15)	31(2)	34(2)	44(2)	-6(1)	3(1)	-4(1)
N(1)	25(2)	43(2)	24(2)	-4(2)	-11(1)	-12(2)
N(2)	30(2)	30(2)	32(2)	0(1)	-4(2)	-8(2)
N(3)	42(2)	29(2)	40(2)	3(2)	-21(2)	-1(2)
N(4)	41(2)	26(2)	45(2)	-6(2)	2(2)	-2(2)
N(5)	38(2)	48(2)	36(2)	-2(2)	-2(2)	-20(2)
N(6)	47(2)	61(3)	41(2)	-2(2)	-10(2)	-9(2)
N(7)	27(2)	19(1)	25(2)	-4(1)	1(1)	-5(1)
N(8)	23(2)	30(2)	25(2)	-4(1)	3(1)	-6(1)
N(9)	23(2)	23(2)	20(1)	-2(1)	2(1)	-7(1)
N(10)	21(2)	20(1)	24(1)	0(1)	-2(1)	-3(1)
N(11)	21(1)	25(2)	19(1)	-2(1)	-2(1)	-6(1)
N(12)	18(2)	24(2)	68(3)	14(2)	4(2)	0(1)
N(13)	16(1)	16(1)	18(1)	-2(1)	1(1)	-2(1)
N(14)	16(1)	16(1)	18(1)	1(1)	0(1)	-2(1)
N(15)	16(1)	18(1)	13(1)	-2(1)	0(1)	-1(1)
C(1)	33(2)	27(2)	35(2)	-1(2)	-14(2)	-8(2)
C(2)	26(2)	24(2)	32(2)	-2(2)	-5(2)	-6(2)
C(3)	25(2)	17(2)	37(2)	7(2)	-16(2)	-5(2)
C(4)	29(2)	22(2)	38(2)	-4(2)	3(2)	0(2)
C(5)	30(2)	42(2)	30(2)	2(2)	-3(2)	-22(2)
C(6)	30(2)	48(3)	31(2)	6(2)	-10(2)	-12(2)
C(7)	18(2)	11(1)	21(2)	-1(1)	-1(1)	-2(1)
C(8)	14(2)	21(2)	22(2)	-2(1)	-2(1)	1(1)
C(9)	20(2)	20(2)	16(2)	-1(1)	-4(1)	-2(1)
C(10)	16(2)	22(2)	20(2)	0(1)	-5(1)	-2(1)
C(11)	17(2)	19(2)	19(2)	1(1)	-4(1)	-1(1)
C(12)	16(2)	23(2)	16(2)	-2(1)	-2(1)	-2(1)
C(13)	22(2)	18(2)	18(2)	-2(1)	-5(1)	-3(1)
C(14)	17(2)	22(2)	21(2)	-6(1)	-5(1)	0(1)
C(15)	16(2)	27(2)	18(2)	-3(1)	0(1)	-2(1)
C(16)	21(2)	20(2)	24(2)	0(1)	-1(1)	-4(1)
C(17)	19(2)	20(2)	22(2)	-3(1)	0(1)	1(1)
C(18)	18(2)	12(1)	18(2)	2(1)	-4(1)	-1(1)
C(19)	15(2)	18(2)	19(2)	2(1)	-4(1)	-2(1)
C(20)	20(2)	18(2)	15(2)	1(1)	-4(1)	-3(1)
C(21)	17(2)	22(2)	22(2)	-2(1)	-3(1)	-4(1)
C(22)	19(2)	23(2)	18(2)	-4(1)	-3(1)	-3(1)
C(23)	14(2)	21(2)	16(2)	0(1)	-1(1)	-2(1)
C(24)	20(2)	19(2)	21(2)	0(1)	-1(1)	-5(1)
C(25)	20(2)	19(2)	23(2)	-4(1)	-1(1)	-4(1)
C(26)	19(2)	23(2)	18(2)	-4(1)	-1(1)	-6(1)
C(27)	21(2)	19(2)	21(2)	2(1)	-3(1)	-7(1)
C(28)	14(2)	19(2)	22(2)	-1(1)	-3(1)	-3(1)
C(29)	16(2)	26(2)	26(2)	7(1)	-1(1)	-7(1)
C(30)	13(2)	30(2)	31(2)	10(2)	0(1)	-5(1)
C(31)	16(2)	22(2)	13(1)	-3(1)	1(1)	-5(1)
C(32)	19(2)	24(2)	26(2)	6(1)	-5(1)	-9(1)
C(33)	15(2)	26(2)	26(2)	3(1)	-2(1)	-8(1)
C(34)	13(2)	17(2)	20(2)	1(1)	0(1)	-4(1)
C(35)	16(2)	18(2)	21(2)	0(1)	-1(1)	-6(1)
C(36)	16(2)	26(2)	27(2)	8(1)	-3(1)	-5(1)
C(37)	15(2)	17(2)	44(2)	8(2)	1(2)	-2(1)
C(38)	23(2)	17(2)	44(2)	-5(2)	9(2)	-4(1)
C(39)	19(2)	22(2)	24(2)	-4(1)	3(1)	-7(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3})
for P1bar.res.

	x	y	z	U(eq)
H(8)	3550	6805	5227	23
H(9)	1882	6829	6137	23
H(10)	-1340	8021	4906	23
H(11)	269	7972	3976	23
H(14)	-3443	8846	7029	24
H(16)	-2322	5514	7151	26
H(17)	-507	5689	6289	25
H(19)	1803	6842	3270	21
H(20)	3463	6752	2352	21
H(21)	6468	7496	3446	24
H(22)	4861	7622	4378	24
H(24)	6591	5463	2359	24
H(25)	8228	5336	1415	25
H(27)	7429	8666	993	24
H(29)	5461	2113	1010	28
H(30)	3922	3609	492	31
H(32)	7390	5090	-45	27
H(33)	8846	3617	519	26
H(36)	9856	829	2525	28
H(38)	9863	-619	813	34
H(39)	8305	945	336	26
H(13A)	-580(50)	6230(40)	3137(14)	26
H(13B)	-610(50)	7180(19)	2750(20)	26
H(14A)	3060(30)	6180(40)	1330(20)	26
H(14B)	3790(50)	7070(20)	990(20)	26
H(15A)	870(50)	5970(40)	1941(14)	26
H(15B)	1250(50)	5027(18)	1520(20)	26

Table S7. Torsion angles [°] for P1bar.res.

C(11)-C(7)-C(8)-C(9)	1.6(5)
C(18)-C(7)-C(8)-C(9)	-176.1(3)
C(10)-N(13)-C(9)-C(8)	-0.6(5)
C(12)-N(13)-C(9)-C(8)	175.9(3)
C(7)-C(8)-C(9)-N(13)	-1.0(5)
C(9)-N(13)-C(10)-C(11)	1.4(5)
C(12)-N(13)-C(10)-C(11)	-175.0(3)
N(13)-C(10)-C(11)-C(7)	-0.8(5)
C(8)-C(7)-C(11)-C(10)	-0.7(5)
C(18)-C(7)-C(11)-C(10)	176.9(3)
C(9)-N(13)-C(12)-C(17)	-68.0(4)
C(10)-N(13)-C(12)-C(17)	108.5(4)
C(9)-N(13)-C(12)-C(13)	115.2(4)
C(10)-N(13)-C(12)-C(13)	-68.3(4)
C(17)-C(12)-C(13)-C(14)	-3.7(5)
N(13)-C(12)-C(13)-C(14)	173.0(3)
C(17)-C(12)-C(13)-N(7)	176.7(3)
N(13)-C(12)-C(13)-N(7)	-6.6(5)
O(2)-N(7)-C(13)-C(14)	-24.0(5)
O(1)-N(7)-C(13)-C(14)	156.1(3)
O(2)-N(7)-C(13)-C(12)	155.6(3)
O(1)-N(7)-C(13)-C(12)	-24.3(5)
C(12)-C(13)-C(14)-C(15)	1.7(5)
N(7)-C(13)-C(14)-C(15)	-178.7(3)
C(13)-C(14)-C(15)-C(16)	1.8(5)
C(13)-C(14)-C(15)-N(8)	-176.3(3)
O(3)-N(8)-C(15)-C(16)	13.7(5)
O(4)-N(8)-C(15)-C(16)	-165.2(3)
O(3)-N(8)-C(15)-C(14)	-168.1(3)
O(4)-N(8)-C(15)-C(14)	13.0(5)
C(14)-C(15)-C(16)-C(17)	-3.3(5)
N(8)-C(15)-C(16)-C(17)	174.8(3)
C(13)-C(12)-C(17)-C(16)	2.2(5)
N(13)-C(12)-C(17)-C(16)	-174.7(3)
C(15)-C(16)-C(17)-C(12)	1.3(5)
C(11)-C(7)-C(18)-C(19)	-33.6(5)
C(8)-C(7)-C(18)-C(19)	144.0(3)
C(11)-C(7)-C(18)-C(22)	147.9(3)
C(8)-C(7)-C(18)-C(22)	-34.6(5)
C(22)-C(18)-C(19)-C(20)	-2.8(5)
C(7)-C(18)-C(19)-C(20)	178.6(3)
C(21)-N(14)-C(20)-C(19)	3.1(5)
C(23)-N(14)-C(20)-C(19)	-177.9(3)
C(18)-C(19)-C(20)-N(14)	0.1(5)
C(20)-N(14)-C(21)-C(22)	-3.5(5)
C(23)-N(14)-C(21)-C(22)	177.5(3)
N(14)-C(21)-C(22)-C(18)	0.7(5)
C(19)-C(18)-C(22)-C(21)	2.4(5)
C(7)-C(18)-C(22)-C(21)	-179.0(3)
C(20)-N(14)-C(23)-C(24)	-79.9(4)
C(21)-N(14)-C(23)-C(24)	99.1(4)
C(20)-N(14)-C(23)-C(28)	99.5(4)
C(21)-N(14)-C(23)-C(28)	-81.5(4)
C(28)-C(23)-C(24)-C(25)	0.5(5)
N(14)-C(23)-C(24)-C(25)	180.0(3)
C(23)-C(24)-C(25)-C(26)	-0.4(5)
C(24)-C(25)-C(26)-C(27)	0.0(5)
C(24)-C(25)-C(26)-N(9)	179.6(3)
O(5)-N(9)-C(26)-C(25)	17.5(5)
O(6)-N(9)-C(26)-C(25)	-163.0(3)
O(5)-N(9)-C(26)-C(27)	-162.9(3)
O(6)-N(9)-C(26)-C(27)	16.6(5)
C(25)-C(26)-C(27)-C(28)	0.1(5)
N(9)-C(26)-C(27)-C(28)	-179.4(3)
C(26)-C(27)-C(28)-C(23)	0.0(5)
C(26)-C(27)-C(28)-N(10)	-179.9(3)
C(24)-C(23)-C(28)-C(27)	-0.4(5)
N(14)-C(23)-C(28)-C(27)	-179.8(3)
C(24)-C(23)-C(28)-N(10)	179.5(3)
N(14)-C(23)-C(28)-N(10)	0.1(5)
O(7)-N(10)-C(28)-C(27)	-7.6(5)
O(8)-N(10)-C(28)-C(27)	171.3(3)
O(7)-N(10)-C(28)-C(23)	172.6(3)
O(8)-N(10)-C(28)-C(23)	-8.6(5)
C(33)-N(15)-C(29)-C(30)	-1.7(5)
C(34)-N(15)-C(29)-C(30)	-179.7(3)
N(15)-C(29)-C(30)-C(31)	1.4(6)
C(29)-C(30)-C(31)-C(32)	0.4(6)
C(29)-C(30)-C(31)-C(31)#1	179.4(4)
C(30)-C(31)-C(32)-C(33)	-1.9(5)
C(31)#1-C(31)-C(32)-C(33)	179.0(4)
C(29)-N(15)-C(33)-C(32)	0.1(5)
C(34)-N(15)-C(33)-C(32)	178.1(3)
C(31)-C(32)-C(33)-N(15)	1.7(6)
C(29)-N(15)-C(34)-C(39)	79.9(4)
C(33)-N(15)-C(34)-C(39)	-98.1(4)
C(29)-N(15)-C(34)-C(35)	-99.0(4)
C(33)-N(15)-C(34)-C(35)	83.0(4)
C(39)-C(34)-C(35)-C(36)	0.4(5)
N(15)-C(34)-C(35)-C(36)	179.3(3)
C(39)-C(34)-C(35)-N(11)	178.4(3)
N(15)-C(34)-C(35)-N(11)	-2.8(5)
O(9)-N(11)-C(35)-C(36)	170.0(3)
O(10)-N(11)-C(35)-C(36)	-9.8(5)
O(9)-N(11)-C(35)-C(34)	-8.0(5)
O(10)-N(11)-C(35)-C(34)	172.2(4)
C(34)-C(35)-C(36)-C(37)	0.3(5)
N(11)-C(35)-C(36)-C(37)	-177.8(3)
C(35)-C(36)-C(37)-C(38)	-0.1(5)
C(35)-C(36)-C(37)-N(12)	178.2(3)
O(11)-N(12)-C(37)-C(38)	163.1(4)
O(12)-N(12)-C(37)-C(38)	-17.3(5)
O(11)-N(12)-C(37)-C(36)	-15.3(5)
O(12)-N(12)-C(37)-C(36)	164.3(3)
C(36)-C(37)-C(38)-C(39)	-0.7(5)
N(12)-C(37)-C(38)-C(39)	-179.0(3)
C(35)-C(34)-C(39)-C(38)	-1.3(5)
N(15)-C(34)-C(39)-C(38)	179.8(3)
C(37)-C(38)-C(39)-C(34)	1.4(5)

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

Table S8. Hydrogen bonds for P1bar.res [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	
O(13)-H(13A)...N(4)#2		0.871(19)	1.97(2)	2.840(5)	173(4)
O(13)-H(13B)...N(2)#3		0.883(19)	2.08(2)	2.946(5)	169(4)
O(14)-H(14B)...N(6)#4		0.898(19)	2.13(2)	3.017(6)	172(4)
O(14)-H(14A)...O(15)		0.889(19)	1.91(2)	2.795(4)	179(5)
O(15)-H(15A)...O(13)		0.875(19)	1.96(2)	2.825(4)	172(4)
O(15)-H(15B)...N(5)	0.885(19)	2.08(2)	2.966(5)	175(4)	

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

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