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# Single-crystal to single-crystal phase transitions of bis(*N*-phenylisonicotinamide)silver(I) nitrate reveal cooperativity properties in porous molecular materials†

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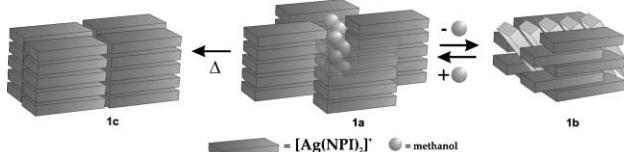
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Two single-crystal to single-crystal phase transitions in *trans*-[Ag(NPI)<sub>2</sub>](NO<sub>3</sub>)·2CH<sub>3</sub>OH (**1a**), (NPI = *N*-phenylisonicotinamide) were characterized with X-ray crystallography; the first transition is reversible and arises from a desolvation transition induced by vacuum and generated **1b**; the second transition was induced by heat at 140 °C and generated **1c**.

Recent progress in crystal engineering has expanded into understanding the relationship between single-crystal structure and structural dynamism with respect to non-covalent interactions.<sup>1–12</sup> Of particular interest are phase transitions of porous materials because of their implications to numerous applications such as separation science, catalysis, sensing, and gas storage.<sup>6–12</sup> Recently, it was demonstrated that open channels in solids are not necessarily a requirement for the solid to behave as a porous material. Dynamic cooperativity in the ensemble may transport guest molecules into the crystal matrix, even in the absence of traditional open channels.<sup>13–15</sup> This new paradigm for what is a porous material is intriguing and represents a new facet in crystal engineering that could play a role in functional materials design. Here we report two single-crystal to single-crystal phase transformations of a porous crystalline material derived from [AgL<sub>2</sub>]NO<sub>3</sub>, where L = *N*-phenylisonicotinamide (NPI), studied with single-crystal X-ray crystallography and differential scanning calorimetry (DSC). The first transition was induced by vacuum and involves a desolvation/solvation process in which the pores of the crystalline framework close and open reversibly, and the second transition was induced by heat and generated an irreversible thermodynamically stable crystal phase, Scheme 1.



Scheme 1

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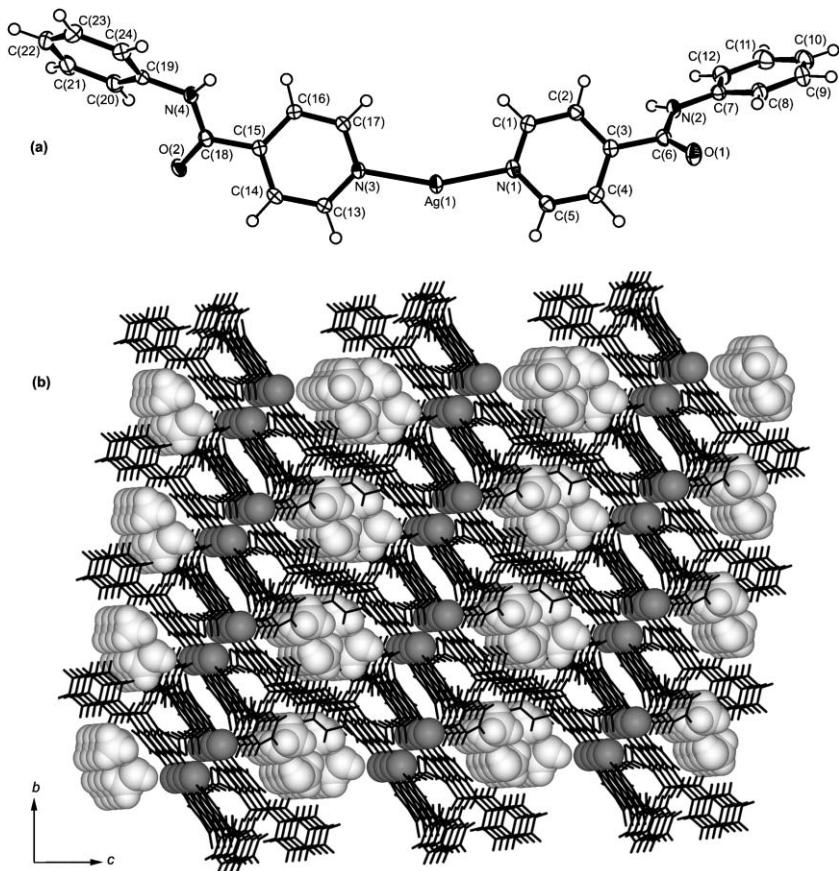
† Electronic supplementary information (ESI) available: Crystallographic data of **1a–c** and detailed experimental preparations. See DOI: 10.1039/b616502h

The NPI ligand was made by the stoichiometric reaction of isonicotinic acid chloride, aniline and triethylamine in chloroform. The Ag-complex was prepared by slow evaporation of a mixture of the nitrate salt of Ag(I) and NPI in methanol over two days to yield a crystalline batch (93%) of product. Single-crystal X-ray crystallographic studies and elemental analysis revealed structure **1a**, Scheme 1, with the molecular formulation of *trans*-[Ag(NPI)<sub>2</sub>](NO<sub>3</sub>)·2CH<sub>3</sub>OH.<sup>17a</sup>

The supramolecular structure of **1a** exhibits channels (8 Å in diameter) filled with methanol molecules along the *a*-axis, Fig. 1. There are four types of hydrogen bonds in the unit cell of which two are between the ligand and solvent in the form of N–H(amide)···O(methanol) and O=C(amide)···HO(methanol) with average distances of 2.88 and 2.86 Å, respectively, and between adjacent methanol molecules (2.73 Å), and NPI with nitrate ions via N–H(amide)···O(nitrate), 2.99 Å. The average distance between the nearest Ag centers is 3.31 Å, which is significantly longer than other crystals with suspected Ag–Ag interactions such as silver acetate (2.79 Å).<sup>18</sup> The average distance between Ag(I) and the nearest nitrate ion is 2.64 Å. The bond angle of N(1)–Ag–N(3) is 158°, which is smaller than those present in analogous Ag-complexes (169°).<sup>19</sup> Despite the expected planar structure of NPI, **1a** reveals that the ligand twist half way forming a torsion angle at C(2)–C(3)–C(6)–N(2) of 45° and its homologous in the same complex of 31°, presumably induced by the hydrogen bonds and the crystal packing forces.

When single crystals of **1a** are placed under vacuum (0.1 Torr) for 2 h a new metastable crystal phase (**1b**) was observed via single-crystal X-ray crystallography, Fig. 2.<sup>17b</sup> The formulation of this crystal phase is *trans*-[Ag(NPI)<sub>2</sub>](NO<sub>3</sub>), which lacks solvent and the channels that once held the methanol molecules are closed, apparently, via an orchestrated rearrangement of alternate layers of the Ag-complex that rotate counter-clockwise by 63° towards the *a*-direction. Unlike **1a**, pairs of Ag-complexes in **1b** interact via two complementary N–H(amide)···O=C(amide) hydrogen bonds that have an average distance of 2.91 Å. Additionally, the nitrate ions bridge adjacent pairs of Ag-complexes via hydrogen bonds with N–H(amide)···O(nitrate) average distance 2.94 Å, and their average distances to Ag centers are 2.80 and 2.68 Å. Interestingly, there are no significant changes in the torsion angles of the NPI moieties (<2°), but the bond angle of N(1)–Ag–N(3) changed to 173°. In addition, face-edge interactions between phenyl moieties of NPI are observed. The crystal phase **1b** may be described as a metastable pseudo-polymorph of **1a**.<sup>20</sup>

The phase transition of **1a** → **1b** was examined with DSC and an endothermic  $\Delta H$  value of  $7.3 \pm 0.2$  kJ mol<sup>−1</sup> was obtained at

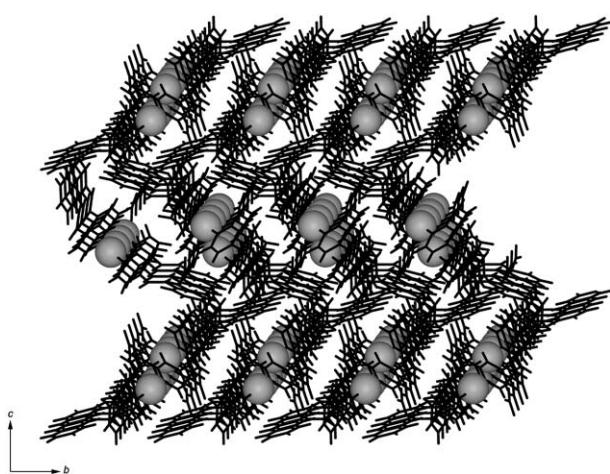


**Fig. 1** (a) Thermal ellipsoid plot (probability level 50%) of  $[\text{Ag}(\text{NPI})_2]^-$ . (b) Expanded unit cell of **1a** as viewed from the *a*-direction. Methanol and Ag shown as CPK.

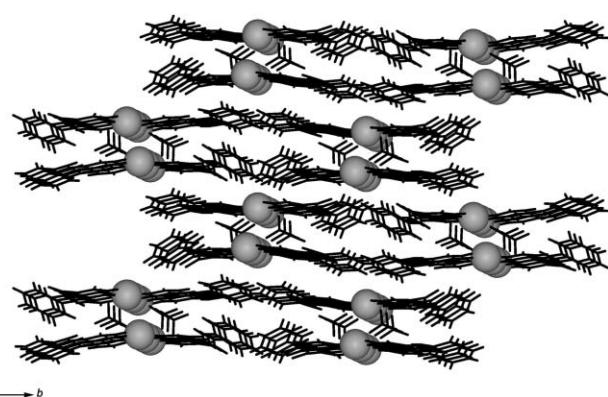
305 K. When crystals of **1b** are exposed to methanol, they revert back to phase **1a**, as indicated by X-ray powder diffraction and elemental analysis. Similar solvent-driven reversible transformations have been observed in other systems. Although the crystalline phase of **1b** lacks any imminent porosity, the fact that it can take up methanol to reconstitute **1a** suggests a well-orchestrated mechanism reminiscent of cooperativity dynamics. This behavior is consistent with other recent crystals that lack porosity, but yet

they are able to incorporate guest molecules into their lattice *via* cooperativity effects.<sup>14–16</sup>

When crystals of either **1a** or **1b** are heated slowly ( $5\text{ }^\circ\text{C min}^{-1}$ ) to higher temperatures, there is a second phase change around 453 K with an endothermic  $\Delta H$  value of  $16.5 \pm 0.3\text{ kJ mol}^{-1}$ . This new phase change also occurs with the preservation of the single-crystal quality of the material forming a new crystal phase, **1c**,<sup>17c</sup> with molecular formula *trans*-[Ag(NPI)<sub>2</sub>](NO<sub>3</sub>), Fig. 3. Single-crystal X-ray crystallography studies on **1c** revealed that the Ag-complexes interact primarily *via*  $\pi$ – $\pi$  stacking interactions and pack in columns along the *c*-axis. The nitrate ions hydrogen bond



**Fig. 2** Expanded unit cell of **1b** as viewed from the *a*-direction.



**Fig. 3** Expanded unit cell of **1c** as viewed from the *a*-direction.

to the columnar Ag-complexes *via* N–H(amide)· · · O(nitrate), (2.92 Å). The NPI ligand moieties become more planar on one side of the complex, which exhibits a torsion angle C(16)–C(15)–C(18)–N(4) of 4° (vs. 45° in **1a**), while the other side undergoes little change (33°). On the other hand, no significant changes occur in the bond angle of N(1)–Ag–N(3) (<2°). In contrast to **1b**, crystalline samples of **1c** do not uptake methanol and with further heating decompose above 270 °C.

In summary, we reported the single-crystal to single-crystal phase transformations of the Ag-complex **1a** to the pseudopolymeric phases **1b** and **1c**, which were induced by vacuum and by heat, respectively. The results indicated that each phase transition was accompanied by changes in intermolecular hydrogen bonding and π–π stacking interactions, which may have played a role in orchestrating the structural changes in the crystal lattice and maintaining single-crystal quality. The study of phase transformations in designed crystals will eventually lead to practical materials with flexible and dynamic frameworks that can switch their structure upon external stimuli with well-defined molecular motions in the solid state.

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- (a) *Crystal data for 1a*:  $C_{26}H_{28}N_5O_7Ag$ ,  $M_r = 630.40$ , colorless plates of dimensions  $0.30 \times 0.25 \times 0.05$  mm, triclinic, space group  $P\bar{1}$ ,  $a = 8.72340(10)$ ,  $b = 9.6897(3)$ ,  $c = 16.9513(5)$  Å,  $\alpha = 74.6602(12)$ ,  $\beta = 76.7586(16)$ ,  $\gamma = 76.8878(16)$ °,  $V = 1323.80(6)$  Å<sup>3</sup>,  $Z = 2$ ,  $D_c = 1.582$  Mg m<sup>-3</sup>. A total of 9546 reflections were measured, of which 5982 were unique. Final residuals were  $R_1 = 0.0283$  and  $wR_2 = 0.0614$ ; (b) *Crystal data for 1b*:  $C_{24}H_{20}N_5O_5Ag$ ,  $M_r = 566.32$ , colorless plates of dimensions  $0.25 \times 0.25 \times 0.08$ , monoclinic, space group  $P2_1/c$ ,  $a = 12.7187(6)$ ,  $b = 8.4330(2)$ ,  $c = 21.2767(9)$  Å,  $\beta = 98.2743(17)$ °,  $V = 2258.32(15)$  Å<sup>3</sup>,  $Z = 4$ ,  $D_c = 1.666$  Mg m<sup>-3</sup>. A total of 9388 reflections were measured, of which 5111 were unique. Final residuals were  $R_1 = 0.0371$  and  $wR_2 = 0.0703$ ; (c) *Crystal data for 1c*:  $C_{24}H_{20}N_5O_5Ag$ ,  $M_r = 566.32$ , colorless plates of dimensions  $0.25 \times 0.10 \times 0.10$ , monoclinic, space group  $P2_1/c$ ,  $a = 8.8731(10)$ ,  $b = 36.1311(5)$ ,  $c = 13.9696(2)$  Å,  $\beta = 93.3705(5)$ °,  $V = 4470.83(10)$  Å<sup>3</sup>,  $Z = 8$ ,  $D_c = 1.683$  Mg m<sup>-3</sup>. A total of 19602 reflections were measured, of which 10777 were unique. Final residuals were  $R_1 = 0.0414$  and  $wR_2 = 0.0747$ . The data for all structures were collected at 150(1) K on a Nonius Kappa CCD diffractometer equipped with Mo-Kα radiation ( $\lambda = 0.71073$  Å). Structure refinements by full-matrix least-squares on  $F^2$  and Fourier Transform techniques and location of hydrogen atoms and their isotropically refinement was done using SHELXTL-97 (Bruker-AXS, Inc. Madison, WI). Further crystallographic data can be obtained from the ESI.† CCDC 627373–627375. For crystallographic data in CIF or other electronic format see DOI: 10.1039/b616502h.
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## Single-crystal to single-crystal phase transitions of bis(N-phenylisonicotinamide) silver (**I**) nitrate reveal cooperativity properties of porous molecular materials

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The X-ray crystallographic data was collected at 150(1) K on a Nonius Kappa CCD diffractometer equipped with Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The structure refinement was carried out by full-matrix least-squares on F<sup>2</sup> and Fourier Transform techniques and location of hydrogen atoms and their isotropically refinement was done using SHELXTL-97 (Bruker-AXS, Inc. Madison, WI). The DSC runs were performed by using a Mettler-Toledo DSC821 module. In all experiments, samples of ~5 mg were heated in open 40  $\mu\text{L}$  Al pans in a flowing atmosphere of nitrogen at a flow rate 70 mL min<sup>-1</sup> and a temperature ramp of 5 °C min<sup>-1</sup>.

**Synthesis of L (NPI).** A solution of isonicotylchloride hydrochloride (890 mg, 5 mmol) and triethylamine (1.6 mL, 11 mmol) in 50 mL of chloroform was prepared and chilled to 4 °C in an ice bath for 5 min. Then, aniline (465 mg, 5 mmol) was added slowly to the cold solution over a period of 10 min. The reaction was allowed to stir at room temperature overnight. The resulting solution was washed with NaHCO<sub>3</sub> solution thrice and the chloroform layer separated which upon concentration gave a white precipitate as the product. The solid was filtered and washed several times with ether. Yield 85 %. <sup>1</sup>H NMR spectrum (CDCl<sub>3</sub>, 300 MHz) from TMS: 8.82 (d, 2H, Py), 7.73 (d, 2H, Py), 7.65 (d, 2H, o-Bz), 7.40 (t, 2H, m-Bz), 7.20 (t, 1H, p-Bz), 10.60 (s, NH).

**Preparation of [Ag(L)<sub>2</sub>](NO<sub>3</sub>) (1a).** A solution of L (19.8 mg, 0.10 mmol) in 5 mL of methanol was added to a 5 mL methanolic solution of silver nitrate (8.45 mg, 0.050 mmol) and the mixture was stirred for 30 min in the dark. Slow evaporation of the resulting solution for 48 h generated large colorless crystals of **1a**. Yield 93%. Anal.

Calcd. for C<sub>26</sub>H<sub>28</sub>N<sub>5</sub>O<sub>7</sub>Ag (**1a**): C 49.53, H 4.45, N 11.11 %. Found: C 49.80, H 4.37, N 11.44 %. Anal. Calcd. for C<sub>24</sub>H<sub>20</sub>N<sub>5</sub>O<sub>5</sub>Ag (**1b**): C 50.89, H 3.53, N 12.36 %. Found: C 50.96, H 3.51, N 12.24%.

Table S1. Crystal data and structure refinement for **1a**.

Identification code	1a
Empirical formula	C <sub>26</sub> H <sub>28</sub> AgN <sub>5</sub> O <sub>7</sub>
Formula weight	630.40
Temperature	150(1) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P $\overline{1}$
Unit cell dimensions	a = 8.72340(10) Å $\alpha$ = 74.6602(12) $^\circ$ . b = 9.6897(3) Å $\beta$ = 76.7586(16) $^\circ$ . c = 16.9513(5) Å $\gamma$ = 76.8878(16) $^\circ$ .
Volume	1323.80(6) Å <sup>3</sup>
Z	2
Density (calculated)	1.582 Mg/m <sup>3</sup>
Absorption coefficient	0.816 mm <sup>-1</sup>
F(000)	644
Crystal size	0.30 x 0.25 x 0.05 mm <sup>3</sup>
Theta range for data collection	3.77 to 27.49 $^\circ$ .
Index ranges	-11 $\leq$ h $\leq$ 11, -12 $\leq$ k $\leq$ 12, -19 $\leq$ l $\leq$ 21
Reflections collected	9546
Independent reflections	5982 [R(int) = 0.0226]
Completeness to theta = 27.49 $^\circ$	98.6 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9603 and 0.7918
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5982 / 0 / 453
Goodness-of-fit on F <sup>2</sup>	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0285, wR2 = 0.0621
R indices (all data)	R1 = 0.0348, wR2 = 0.0657
Largest diff. peak and hole	0.396 and -0.585 e.Å <sup>-3</sup>

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

	x	y	z	U(eq)
Ag(1)	5738(1)	3704(1)	4478(1)	23(1)
O(1)	8139(2)	10271(2)	1954(1)	27(1)
O(2)	2057(2)	-2441(1)	6696(1)	22(1)
O(3)	7713(2)	4353(2)	5573(1)	45(1)
O(4)	8485(2)	2420(2)	6474(1)	33(1)
O(5)	8050(2)	2240(2)	5304(1)	36(1)
O(6)	7375(2)	6726(2)	583(1)	29(1)
O(7)	8382(2)	4196(2)	1651(1)	45(1)
N(1)	6405(2)	5613(2)	3561(1)	19(1)
N(2)	7524(2)	9436(2)	934(1)	22(1)
N(3)	4295(2)	2064(2)	5176(1)	17(1)
N(4)	-200(2)	-727(2)	6528(1)	20(1)
N(5)	8092(2)	3019(2)	5783(1)	22(1)
C(1)	5490(2)	6317(2)	2987(1)	21(1)
C(2)	5886(2)	7491(2)	2365(1)	20(1)
C(3)	7276(2)	7999(2)	2332(1)	18(1)
C(4)	8221(2)	7280(2)	2929(1)	20(1)
C(5)	7760(2)	6096(2)	3522(1)	19(1)
C(6)	7708(2)	9349(2)	1720(1)	20(1)
C(7)	7818(2)	10568(2)	231(1)	21(1)
C(8)	7922(2)	11956(2)	285(2)	26(1)
C(9)	8221(3)	13007(3)	-440(2)	33(1)
C(10)	8402(3)	12714(3)	-1211(2)	34(1)
C(11)	8277(3)	11344(3)	-1264(2)	33(1)
C(12)	7987(3)	10277(3)	-552(1)	27(1)
C(13)	4786(2)	917(2)	5770(1)	18(1)
C(14)	3872(2)	-141(2)	6183(1)	18(1)
C(15)	2383(2)	-32(2)	5982(1)	16(1)
C(16)	1886(2)	1124(2)	5357(1)	18(1)
C(17)	2861(2)	2152(2)	4978(1)	18(1)
C(18)	1401(2)	-1183(2)	6439(1)	18(1)

C(19)	-1356(2)	-1638(2)	6913(1)	20(1)
C(20)	-1147(3)	-3022(2)	6769(1)	25(1)
C(21)	-2317(3)	-3875(3)	7149(2)	31(1)
C(22)	-3676(3)	-3354(3)	7665(2)	37(1)
C(23)	-3880(3)	-1976(3)	7799(2)	35(1)
C(24)	-2730(2)	-1105(2)	7423(1)	27(1)
C(25)	5978(3)	6581(3)	343(2)	45(1)
C(26)	9908(3)	3513(3)	1299(2)	31(1)

Table S3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 1a.

Ag(1)-N(1)	2.1746(17)
Ag(1)-N(3)	2.1773(16)
Ag(1)-O(5)	2.6436(16)
Ag(1)-Ag(1)#1	3.3090(3)
O(1)-C(6)	1.227(2)
O(2)-C(18)	1.233(2)
O(3)-N(5)	1.235(2)
O(4)-N(5)	1.248(2)
O(5)-N(5)	1.257(2)
O(6)-C(25)	1.415(3)
O(6)-H(6A)	0.75(3)
O(7)-C(26)	1.419(3)
O(7)-H(7A)	0.75(3)
N(1)-C(1)	1.344(3)
N(1)-C(5)	1.349(2)
N(2)-C(6)	1.357(3)
N(2)-C(7)	1.409(3)
N(2)-H(2N)	0.82(3)
N(3)-C(17)	1.347(2)
N(3)-C(13)	1.349(3)
N(4)-C(18)	1.351(2)
N(4)-C(19)	1.421(2)
N(4)-H(4N)	0.82(2)
C(1)-C(2)	1.379(3)

C(1)-H(1)	0.95(2)
C(2)-C(3)	1.393(3)
C(2)-H(2)	0.93(2)
C(3)-C(4)	1.391(3)
C(3)-C(6)	1.502(3)
C(4)-C(5)	1.380(3)
C(4)-H(4)	0.97(2)
C(5)-H(5)	0.96(2)
C(7)-C(8)	1.396(3)
C(7)-C(12)	1.397(3)
C(8)-C(9)	1.388(3)
C(8)-H(8)	0.94(3)
C(9)-C(10)	1.377(4)
C(9)-H(9)	0.94(3)
C(10)-C(11)	1.384(4)
C(10)-H(10)	0.94(3)
C(11)-C(12)	1.382(3)
C(11)-H(11)	0.95(3)
C(12)-H(12)	0.91(3)
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.95(2)
C(14)-C(15)	1.391(3)
C(14)-H(14)	0.92(2)
C(15)-C(16)	1.389(3)
C(15)-C(18)	1.500(3)
C(16)-C(17)	1.386(3)
C(16)-H(16)	0.93(2)
C(17)-H(17)	0.91(3)
C(19)-C(20)	1.390(3)
C(19)-C(24)	1.391(3)
C(20)-C(21)	1.393(3)
C(20)-H(20)	0.97(2)
C(21)-C(22)	1.383(4)
C(21)-H(21)	0.92(3)
C(22)-C(23)	1.379(4)
C(22)-H(22)	0.93(3)

C(23)-C(24)	1.389(3)
C(23)-H(23)	0.94(3)
C(24)-H(24)	0.93(2)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.99(3)
C(26)-H(26B)	0.98(3)
C(26)-H(26C)	0.99(3)
N(1)-Ag(1)-N(3)	158.69(6)
N(1)-Ag(1)-O(5)	112.85(6)
N(3)-Ag(1)-O(5)	88.39(6)
N(1)-Ag(1)-Ag(1)#1	78.25(4)
N(3)-Ag(1)-Ag(1)#1	100.77(4)
O(5)-Ag(1)-Ag(1)#1	99.50(3)
N(5)-O(5)-Ag(1)	104.58(11)
C(25)-O(6)-H(6A)	109(2)
C(26)-O(7)-H(7A)	109(2)
C(1)-N(1)-C(5)	117.78(17)
C(1)-N(1)-Ag(1)	120.03(13)
C(5)-N(1)-Ag(1)	122.14(13)
C(6)-N(2)-C(7)	127.23(18)
C(6)-N(2)-H(2N)	114.7(18)
C(7)-N(2)-H(2N)	116.5(18)
C(17)-N(3)-C(13)	117.67(16)
C(17)-N(3)-Ag(1)	118.40(13)
C(13)-N(3)-Ag(1)	123.84(12)
C(18)-N(4)-C(19)	124.67(17)
C(18)-N(4)-H(4N)	117.8(16)
C(19)-N(4)-H(4N)	116.5(16)
O(3)-N(5)-O(4)	121.19(18)
O(3)-N(5)-O(5)	119.77(18)
O(4)-N(5)-O(5)	119.02(17)
N(1)-C(1)-C(2)	122.85(18)
N(1)-C(1)-H(1)	115.9(14)

C(2)-C(1)-H(1)	121.3(14)
C(1)-C(2)-C(3)	119.26(19)
C(1)-C(2)-H(2)	119.3(14)
C(3)-C(2)-H(2)	121.4(14)
C(4)-C(3)-C(2)	118.09(19)
C(4)-C(3)-C(6)	119.56(17)
C(2)-C(3)-C(6)	122.18(18)
C(5)-C(4)-C(3)	119.26(18)
C(5)-C(4)-H(4)	119.0(14)
C(3)-C(4)-H(4)	121.7(14)
N(1)-C(5)-C(4)	122.74(19)
N(1)-C(5)-H(5)	115.4(12)
C(4)-C(5)-H(5)	121.8(12)
O(1)-C(6)-N(2)	125.81(19)
O(1)-C(6)-C(3)	120.14(18)
N(2)-C(6)-C(3)	114.02(17)
C(8)-C(7)-C(12)	119.2(2)
C(8)-C(7)-N(2)	123.06(19)
C(12)-C(7)-N(2)	117.72(18)
C(9)-C(8)-C(7)	119.3(2)
C(9)-C(8)-H(8)	122.2(16)
C(7)-C(8)-H(8)	118.5(16)
C(10)-C(9)-C(8)	121.4(2)
C(10)-C(9)-H(9)	118.9(17)
C(8)-C(9)-H(9)	119.7(17)
C(9)-C(10)-C(11)	119.2(2)
C(9)-C(10)-H(10)	120.1(16)
C(11)-C(10)-H(10)	120.6(16)
C(12)-C(11)-C(10)	120.5(2)
C(12)-C(11)-H(11)	117.3(17)
C(10)-C(11)-H(11)	122.2(17)
C(11)-C(12)-C(7)	120.4(2)
C(11)-C(12)-H(12)	122.4(17)
C(7)-C(12)-H(12)	117.2(17)
N(3)-C(13)-C(14)	122.79(17)
N(3)-C(13)-H(13)	116.5(14)

C(14)-C(13)-H(13)	120.7(14)
C(13)-C(14)-C(15)	119.16(18)
C(13)-C(14)-H(14)	121.0(14)
C(15)-C(14)-H(14)	119.9(14)
C(16)-C(15)-C(14)	118.46(17)
C(16)-C(15)-C(18)	122.93(16)
C(14)-C(15)-C(18)	118.60(17)
C(17)-C(16)-C(15)	118.98(17)
C(17)-C(16)-H(16)	117.7(15)
C(15)-C(16)-H(16)	123.4(15)
N(3)-C(17)-C(16)	122.89(18)
N(3)-C(17)-H(17)	116.9(15)
C(16)-C(17)-H(17)	120.2(15)
O(2)-C(18)-N(4)	124.58(18)
O(2)-C(18)-C(15)	120.40(16)
N(4)-C(18)-C(15)	115.01(16)
C(20)-C(19)-C(24)	120.22(19)
C(20)-C(19)-N(4)	121.10(18)
C(24)-C(19)-N(4)	118.66(18)
C(19)-C(20)-C(21)	119.4(2)
C(19)-C(20)-H(20)	119.9(15)
C(21)-C(20)-H(20)	120.6(15)
C(22)-C(21)-C(20)	120.4(2)
C(22)-C(21)-H(21)	120.6(16)
C(20)-C(21)-H(21)	118.8(16)
C(23)-C(22)-C(21)	119.8(2)
C(23)-C(22)-H(22)	120.7(17)
C(21)-C(22)-H(22)	119.5(17)
C(22)-C(23)-C(24)	120.7(2)
C(22)-C(23)-H(23)	121.6(17)
C(24)-C(23)-H(23)	117.7(17)
C(23)-C(24)-C(19)	119.4(2)
C(23)-C(24)-H(24)	121.6(14)
C(19)-C(24)-H(24)	119.0(15)
O(6)-C(25)-H(25A)	109.5
O(6)-C(25)-H(25B)	109.5

H(25A)-C(25)-H(25B)	109.5
O(6)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(7)-C(26)-H(26A)	110.4(15)
O(7)-C(26)-H(26B)	106.8(15)
H(26A)-C(26)-H(26B)	108(2)
O(7)-C(26)-H(26C)	111.3(15)
H(26A)-C(26)-H(26C)	110(2)
H(26B)-C(26)-H(26C)	110(2)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

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

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Ag(1)	25(1)	18(1)	22(1)	1(1)	-2(1)	-8(1)
O(1)	40(1)	22(1)	21(1)	-5(1)	-4(1)	-14(1)
O(2)	24(1)	14(1)	22(1)	0(1)	-2(1)	-2(1)
O(3)	64(1)	19(1)	42(1)	3(1)	-5(1)	1(1)
O(4)	34(1)	35(1)	27(1)	-1(1)	-11(1)	1(1)
O(5)	28(1)	44(1)	46(1)	-24(1)	-14(1)	-2(1)
O(6)	35(1)	23(1)	29(1)	-1(1)	-11(1)	-6(1)
O(7)	54(1)	35(1)	27(1)	8(1)	0(1)	8(1)
N(1)	23(1)	15(1)	18(1)	-3(1)	-1(1)	-4(1)
N(2)	30(1)	17(1)	20(1)	-1(1)	-5(1)	-8(1)
N(3)	19(1)	16(1)	15(1)	-2(1)	-1(1)	-5(1)
N(4)	19(1)	13(1)	27(1)	-1(1)	-3(1)	-3(1)
N(5)	19(1)	22(1)	23(1)	-2(1)	-4(1)	-2(1)
C(1)	22(1)	20(1)	21(1)	-5(1)	-2(1)	-7(1)
C(2)	22(1)	20(1)	18(1)	-3(1)	-5(1)	-3(1)
C(3)	22(1)	18(1)	15(1)	-5(1)	0(1)	-4(1)
C(4)	20(1)	21(1)	20(1)	-7(1)	-2(1)	-5(1)

C(5)	21(1)	18(1)	18(1)	-4(1)	-2(1)	-1(1)
C(6)	21(1)	19(1)	18(1)	-2(1)	-2(1)	-4(1)
C(7)	19(1)	21(1)	19(1)	1(1)	-3(1)	-4(1)
C(8)	31(1)	22(1)	24(1)	1(1)	-6(1)	-8(1)
C(9)	36(1)	23(1)	35(1)	6(1)	-7(1)	-10(1)
C(10)	28(1)	36(1)	27(1)	10(1)	-1(1)	-7(1)
C(11)	32(1)	41(1)	18(1)	-1(1)	-2(1)	-2(1)
C(12)	30(1)	27(1)	22(1)	-4(1)	-2(1)	-5(1)
C(13)	18(1)	17(1)	18(1)	-4(1)	-4(1)	-2(1)
C(14)	22(1)	16(1)	15(1)	-2(1)	-4(1)	0(1)
C(15)	18(1)	14(1)	15(1)	-5(1)	-1(1)	-2(1)
C(16)	17(1)	19(1)	20(1)	-3(1)	-4(1)	-3(1)
C(17)	20(1)	16(1)	15(1)	-1(1)	-4(1)	-2(1)
C(18)	24(1)	17(1)	13(1)	-3(1)	-2(1)	-5(1)
C(19)	20(1)	21(1)	19(1)	2(1)	-8(1)	-6(1)
C(20)	31(1)	24(1)	23(1)	0(1)	-10(1)	-10(1)
C(21)	44(1)	27(1)	28(1)	5(1)	-19(1)	-18(1)
C(22)	33(1)	42(1)	36(1)	14(1)	-16(1)	-23(1)
C(23)	21(1)	42(1)	35(1)	5(1)	-5(1)	-8(1)
C(24)	22(1)	27(1)	29(1)	-1(1)	-6(1)	-4(1)
C(25)	37(1)	47(2)	57(2)	-17(1)	-17(1)	-6(1)
C(26)	35(1)	32(1)	26(1)	-2(1)	-9(1)	-8(1)

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Table S5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )  
 for 1a.

	x	y	z	U(eq)
H(25A)	6242	5812	32	67
H(25B)	5552	7502	-8	67
H(25C)	5174	6328	841	67
H(1)	4540(30)	5950(20)	3032(14)	22(6)
H(2)	5200(30)	7950(20)	1992(15)	20(5)
H(2N)	7430(30)	8670(30)	845(16)	28(6)
H(4)	9190(30)	7600(20)	2945(15)	24(6)
H(4N)	-530(30)	150(30)	6432(15)	23(6)
H(5)	8380(20)	5570(20)	3940(13)	11(5)
H(6A)	7600(30)	6070(30)	921(19)	41(9)
H(7A)	8220(40)	3860(40)	2100(20)	51(10)
H(8)	7780(30)	12150(30)	812(17)	33(7)
H(9)	8330(30)	13930(30)	-407(17)	35(7)
H(10)	8650(30)	13430(30)	-1697(18)	42(7)
H(11)	8430(30)	11080(30)	-1782(18)	40(7)
H(12)	7910(30)	9360(30)	-567(16)	32(7)
H(13)	5800(30)	870(20)	5903(14)	22(6)
H(14)	4250(30)	-930(30)	6577(15)	20(5)
H(16)	920(30)	1250(20)	5175(15)	24(6)
H(17)	2560(30)	2920(30)	4563(16)	29(6)
H(20)	-200(30)	-3380(30)	6405(16)	31(6)
H(21)	-2200(30)	-4760(30)	7024(17)	34(7)
H(22)	-4430(30)	-3940(30)	7927(18)	44(7)
H(23)	-4800(30)	-1580(30)	8137(18)	44(8)
H(24)	-2870(30)	-160(30)	7495(15)	27(6)
H(26A)	10760(30)	3780(30)	1493(17)	38(7)
H(26B)	10030(30)	3880(30)	697(19)	40(7)
H(26C)	10000(30)	2440(30)	1436(17)	40(7)

Table S6. Torsion angles [°] for 1a.

N(1)-Ag(1)-O(5)-N(5)	72.80(13)
N(3)-Ag(1)-O(5)-N(5)	-109.02(13)
Ag(1)#1-Ag(1)-O(5)-N(5)	-8.38(13)
N(3)-Ag(1)-N(1)-C(1)	-7.3(2)
O(5)-Ag(1)-N(1)-C(1)	167.66(13)
Ag(1)#1-Ag(1)-N(1)-C(1)	-96.87(14)
N(3)-Ag(1)-N(1)-C(5)	175.42(14)
O(5)-Ag(1)-N(1)-C(5)	-9.59(15)
Ag(1)#1-Ag(1)-N(1)-C(5)	85.88(14)
N(1)-Ag(1)-N(3)-C(17)	0.3(2)
O(5)-Ag(1)-N(3)-C(17)	-175.09(13)
Ag(1)#1-Ag(1)-N(3)-C(17)	85.55(13)
N(1)-Ag(1)-N(3)-C(13)	176.82(15)
O(5)-Ag(1)-N(3)-C(13)	1.43(15)
Ag(1)#1-Ag(1)-N(3)-C(13)	-97.93(14)
Ag(1)-O(5)-N(5)-O(3)	-30.3(2)
Ag(1)-O(5)-N(5)-O(4)	148.15(14)
C(5)-N(1)-C(1)-C(2)	0.5(3)
Ag(1)-N(1)-C(1)-C(2)	-176.85(14)
N(1)-C(1)-C(2)-C(3)	-1.3(3)
C(1)-C(2)-C(3)-C(4)	0.7(3)
C(1)-C(2)-C(3)-C(6)	-174.51(17)
C(2)-C(3)-C(4)-C(5)	0.5(3)
C(6)-C(3)-C(4)-C(5)	175.84(17)
C(1)-N(1)-C(5)-C(4)	0.8(3)
Ag(1)-N(1)-C(5)-C(4)	178.08(14)
C(3)-C(4)-C(5)-N(1)	-1.3(3)
C(7)-N(2)-C(6)-O(1)	1.5(3)
C(7)-N(2)-C(6)-C(3)	179.44(17)
C(4)-C(3)-C(6)-O(1)	-42.5(3)
C(2)-C(3)-C(6)-O(1)	132.7(2)
C(4)-C(3)-C(6)-N(2)	139.43(18)
C(2)-C(3)-C(6)-N(2)	-45.4(2)
C(6)-N(2)-C(7)-C(8)	-18.5(3)

C(6)-N(2)-C(7)-C(12)	162.47(19)
C(12)-C(7)-C(8)-C(9)	-1.2(3)
N(2)-C(7)-C(8)-C(9)	179.74(19)
C(7)-C(8)-C(9)-C(10)	0.6(3)
C(8)-C(9)-C(10)-C(11)	0.3(3)
C(9)-C(10)-C(11)-C(12)	-0.5(3)
C(10)-C(11)-C(12)-C(7)	-0.1(3)
C(8)-C(7)-C(12)-C(11)	1.0(3)
N(2)-C(7)-C(12)-C(11)	-179.94(19)
C(17)-N(3)-C(13)-C(14)	-1.0(3)
Ag(1)-N(3)-C(13)-C(14)	-177.51(13)
N(3)-C(13)-C(14)-C(15)	0.2(3)
C(13)-C(14)-C(15)-C(16)	1.4(3)
C(13)-C(14)-C(15)-C(18)	-179.70(17)
C(14)-C(15)-C(16)-C(17)	-2.3(3)
C(18)-C(15)-C(16)-C(17)	178.94(17)
C(13)-N(3)-C(17)-C(16)	0.1(3)
Ag(1)-N(3)-C(17)-C(16)	176.83(14)
C(15)-C(16)-C(17)-N(3)	1.5(3)
C(19)-N(4)-C(18)-O(2)	-1.5(3)
C(19)-N(4)-C(18)-C(15)	177.77(17)
C(16)-C(15)-C(18)-O(2)	147.97(19)
C(14)-C(15)-C(18)-O(2)	-30.8(3)
C(16)-C(15)-C(18)-N(4)	-31.4(3)
C(14)-C(15)-C(18)-N(4)	149.83(17)
C(18)-N(4)-C(19)-C(20)	-41.6(3)
C(18)-N(4)-C(19)-C(24)	140.1(2)
C(24)-C(19)-C(20)-C(21)	-0.8(3)
N(4)-C(19)-C(20)-C(21)	-179.14(19)
C(19)-C(20)-C(21)-C(22)	0.0(3)
C(20)-C(21)-C(22)-C(23)	0.6(3)
C(21)-C(22)-C(23)-C(24)	-0.3(4)
C(22)-C(23)-C(24)-C(19)	-0.5(3)
C(20)-C(19)-C(24)-C(23)	1.1(3)
N(4)-C(19)-C(24)-C(23)	179.42(19)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

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

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle$ (DHA)
N(2)-H(2N)...O(6)	0.82(3)	2.06(3)	2.878(2)	176(2)
N(4)-H(4N)...O(4)#2	0.82(2)	2.19(2)	2.989(2)	167(2)
O(6)-H(6A)...O(7)	0.75(3)	1.99(3)	2.732(3)	170(3)
O(7)-H(7A)...O(2)#3	0.75(3)	2.13(4)	2.859(2)	167(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x-1,y,z #3 -x+1,-y,-z+1

Table S8. Crystal data and structure refinement for **1b**.

Identification code	1b		
Empirical formula	C24 H20 Ag N5 O5		
Formula weight	566.32		
Temperature	150(1) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	<i>P</i> 2 <sub>1</sub> /n		
Unit cell dimensions	a = 12.7187(6) Å	$\alpha$ = 90°.	
	b = 8.4330(2) Å	$\beta$ = 98.274(2)°.	
	c = 21.2767(9) Å	$\gamma$ = 90°.	
Volume	2258.32(15) Å <sup>3</sup>		
Z	4		
Density (calculated)	1.666 Mg/m <sup>3</sup>		
Absorption coefficient	0.940 mm <sup>-1</sup>		
F(000)	1144		
Crystal size	0.25 x 0.25 x 0.08 mm <sup>3</sup>		
Theta range for data collection	3.62 to 27.48°.		
Index ranges	-16≤h≤16, -10≤k≤10, -27≤l≤27		
Reflections collected	9388		

Independent reflections	5111 [R(int) = 0.0328]
Completeness to theta = 27.48°	98.7 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9286 and 0.7989
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5111 / 2 / 396
Goodness-of-fit on F <sup>2</sup>	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0371, wR2 = 0.0703
R indices (all data)	R1 = 0.0660, wR2 = 0.0796
Largest diff. peak and hole	0.567 and -0.552 e.Å <sup>-3</sup>

Table S9. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1b. U(eq) is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
Ag(1)	8901(1)	4457(1)	4540(1)	33(1)
O(1)	4094(2)	8466(2)	4910(1)	35(1)
O(2)	13456(2)	1567(2)	3314(1)	28(1)
O(3)	10921(2)	7431(3)	4368(1)	44(1)
O(4)	9298(2)	7091(2)	3906(1)	44(1)
O(5)	10507(2)	7929(3)	3366(1)	47(1)
N(1)	7498(2)	5573(3)	4797(1)	26(1)
N(2)	4537(2)	7580(3)	5930(1)	30(1)
N(3)	10186(2)	3217(3)	4196(1)	28(1)
N(4)	12688(2)	-815(2)	3498(1)	25(1)
N(5)	10239(2)	7490(3)	3878(1)	32(1)
C(1)	7064(2)	6879(3)	4499(2)	30(1)
C(2)	6172(2)	7607(3)	4663(1)	29(1)
C(3)	5698(2)	7011(3)	5160(1)	23(1)
C(4)	6142(2)	5664(3)	5470(1)	25(1)
C(5)	7034(2)	5000(3)	5277(1)	25(1)
C(6)	4696(2)	7774(3)	5319(1)	24(1)
C(7)	3696(2)	8178(3)	6231(2)	29(1)
C(8)	2743(2)	8720(3)	5891(2)	35(1)
C(9)	1978(3)	9346(4)	6222(2)	49(1)

C(10)	2135(3)	9412(4)	6874(2)	59(1)
C(11)	3063(3)	8823(4)	7214(2)	53(1)
C(12)	3847(3)	8217(4)	6891(2)	36(1)
C(13)	10557(2)	3679(3)	3665(1)	27(1)
C(14)	11387(2)	2929(3)	3437(1)	26(1)
C(15)	11840(2)	1599(3)	3751(1)	23(1)
C(16)	11455(2)	1100(3)	4292(1)	28(1)
C(17)	10643(2)	1945(3)	4503(2)	30(1)
C(18)	12746(2)	784(3)	3499(1)	24(1)
C(19)	13409(2)	-1900(3)	3284(1)	25(1)
C(20)	14458(2)	-1507(4)	3244(1)	32(1)
C(21)	15120(3)	-2641(4)	3031(2)	36(1)
C(22)	14753(3)	-4152(3)	2873(2)	34(1)
C(23)	13709(3)	-4538(3)	2917(1)	31(1)
C(24)	13031(2)	-3414(3)	3119(1)	28(1)

Table S10. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 1b.

Ag(1)-N(3)	2.156(2)
Ag(1)-N(1)	2.156(2)
Ag(1)-O(4)	2.685(2)
Ag(1)-Ag(1)#1	3.3021(5)
O(1)-C(6)	1.222(3)
O(2)-C(18)	1.229(3)
O(3)-N(5)	1.257(3)
O(4)-N(5)	1.253(3)
O(5)-N(5)	1.244(3)
N(1)-C(5)	1.340(4)
N(1)-C(1)	1.349(3)
N(2)-C(6)	1.354(4)
N(2)-C(7)	1.416(4)
N(2)-H(2N)	0.814(10)
N(3)-C(13)	1.343(4)
N(3)-C(17)	1.344(4)
N(4)-C(18)	1.351(3)

N(4)-C(19)	1.417(3)
N(4)-H(4N)	0.817(10)
C(1)-C(2)	1.378(4)
C(1)-H(1)	0.91(3)
C(2)-C(3)	1.385(4)
C(2)-H(2)	0.91(3)
C(3)-C(4)	1.392(4)
C(3)-C(6)	1.510(4)
C(4)-C(5)	1.380(4)
C(4)-H(4)	0.93(3)
C(5)-H(5)	0.81(3)
C(7)-C(12)	1.389(4)
C(7)-C(8)	1.396(4)
C(8)-C(9)	1.384(5)
C(8)-H(8)	0.93(3)
C(9)-C(10)	1.375(6)
C(9)-H(9)	0.92(4)
C(10)-C(11)	1.385(6)
C(10)-H(10)	0.91(4)
C(11)-C(12)	1.388(5)
C(11)-H(11)	0.88(3)
C(12)-H(12)	0.93(3)
C(13)-C(14)	1.377(4)
C(13)-H(13)	0.91(3)
C(14)-C(15)	1.387(4)
C(14)-H(14)	0.94(3)
C(15)-C(16)	1.381(4)
C(15)-C(18)	1.504(4)
C(16)-C(17)	1.383(4)
C(16)-H(16)	0.94(3)
C(17)-H(17)	0.91(3)
C(19)-C(20)	1.388(4)
C(19)-C(24)	1.391(4)
C(20)-C(21)	1.393(4)
C(20)-H(20)	0.93(3)
C(21)-C(22)	1.381(4)

C(21)-H(21)	0.96(3)
C(22)-C(23)	1.383(5)
C(22)-H(22)	0.96(3)
C(23)-C(24)	1.391(4)
C(23)-H(23)	0.96(3)
C(24)-H(24)	0.92(3)

N(3)-Ag(1)-N(1)	173.46(9)
N(3)-Ag(1)-O(4)	91.37(8)
N(1)-Ag(1)-O(4)	89.36(7)
N(3)-Ag(1)-Ag(1)#1	73.58(6)
N(1)-Ag(1)-Ag(1)#1	112.95(6)
O(4)-Ag(1)-Ag(1)#1	82.20(5)
N(5)-O(4)-Ag(1)	119.70(17)
C(5)-N(1)-C(1)	117.2(2)
C(5)-N(1)-Ag(1)	120.45(19)
C(1)-N(1)-Ag(1)	122.35(19)
C(6)-N(2)-C(7)	128.2(2)
C(6)-N(2)-H(2N)	115(3)
C(7)-N(2)-H(2N)	112(2)
C(13)-N(3)-C(17)	117.5(2)
C(13)-N(3)-Ag(1)	121.33(18)
C(17)-N(3)-Ag(1)	121.17(19)
C(18)-N(4)-C(19)	127.5(2)
C(18)-N(4)-H(4N)	116.6(19)
C(19)-N(4)-H(4N)	115.4(19)
O(5)-N(5)-O(4)	120.3(3)
O(5)-N(5)-O(3)	119.6(3)
O(4)-N(5)-O(3)	120.1(3)
N(1)-C(1)-C(2)	122.8(3)
N(1)-C(1)-H(1)	117.3(19)
C(2)-C(1)-H(1)	119.9(18)
C(1)-C(2)-C(3)	119.7(3)
C(1)-C(2)-H(2)	118.4(17)
C(3)-C(2)-H(2)	121.9(17)
C(2)-C(3)-C(4)	117.8(2)

C(2)-C(3)-C(6)	119.4(2)
C(4)-C(3)-C(6)	122.7(2)
C(5)-C(4)-C(3)	119.0(3)
C(5)-C(4)-H(4)	120.2(18)
C(3)-C(4)-H(4)	120.8(18)
N(1)-C(5)-C(4)	123.5(3)
N(1)-C(5)-H(5)	116(2)
C(4)-C(5)-H(5)	120(2)
O(1)-C(6)-N(2)	125.2(3)
O(1)-C(6)-C(3)	120.4(3)
N(2)-C(6)-C(3)	114.3(2)
C(12)-C(7)-C(8)	120.0(3)
C(12)-C(7)-N(2)	117.5(3)
C(8)-C(7)-N(2)	122.6(3)
C(9)-C(8)-C(7)	118.9(3)
C(9)-C(8)-H(8)	121(2)
C(7)-C(8)-H(8)	120(2)
C(10)-C(9)-C(8)	121.2(4)
C(10)-C(9)-H(9)	118(2)
C(8)-C(9)-H(9)	121(2)
C(9)-C(10)-C(11)	120.1(3)
C(9)-C(10)-H(10)	123(3)
C(11)-C(10)-H(10)	117(3)
C(10)-C(11)-C(12)	119.5(4)
C(10)-C(11)-H(11)	124(2)
C(12)-C(11)-H(11)	117(2)
C(11)-C(12)-C(7)	120.3(3)
C(11)-C(12)-H(12)	121.7(19)
C(7)-C(12)-H(12)	118.0(19)
N(3)-C(13)-C(14)	122.8(3)
N(3)-C(13)-H(13)	116.7(18)
C(14)-C(13)-H(13)	120.5(18)
C(13)-C(14)-C(15)	119.3(3)
C(13)-C(14)-H(14)	120.0(17)
C(15)-C(14)-H(14)	120.7(17)
C(16)-C(15)-C(14)	118.4(3)

C(16)-C(15)-C(18)	122.6(2)
C(14)-C(15)-C(18)	119.0(2)
C(15)-C(16)-C(17)	119.0(3)
C(15)-C(16)-H(16)	123(2)
C(17)-C(16)-H(16)	118(2)
N(3)-C(17)-C(16)	123.0(3)
N(3)-C(17)-H(17)	116.2(18)
C(16)-C(17)-H(17)	120.8(18)
O(2)-C(18)-N(4)	125.3(3)
O(2)-C(18)-C(15)	120.3(2)
N(4)-C(18)-C(15)	114.4(2)
C(20)-C(19)-C(24)	120.3(3)
C(20)-C(19)-N(4)	122.5(2)
C(24)-C(19)-N(4)	117.2(2)
C(19)-C(20)-C(21)	119.1(3)
C(19)-C(20)-H(20)	122(2)
C(21)-C(20)-H(20)	119(2)
C(22)-C(21)-C(20)	120.9(3)
C(22)-C(21)-H(21)	119(2)
C(20)-C(21)-H(21)	120(2)
C(21)-C(22)-C(23)	119.7(3)
C(21)-C(22)-H(22)	121.5(19)
C(23)-C(22)-H(22)	118.6(19)
C(22)-C(23)-C(24)	120.3(3)
C(22)-C(23)-H(23)	119.4(18)
C(24)-C(23)-H(23)	120.3(18)
C(23)-C(24)-C(19)	119.7(3)
C(23)-C(24)-H(24)	123.3(19)
C(19)-C(24)-H(24)	116.9(19)

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Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1

Table S11. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1b. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^{*} b^{*} U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
Ag(1)	29(1)	29(1)	43(1)	-2(1)	14(1)	6(1)
O(1)	29(1)	35(1)	41(1)	4(1)	4(1)	10(1)
O(2)	24(1)	25(1)	37(1)	-1(1)	7(1)	1(1)
O(3)	43(1)	38(1)	50(2)	10(1)	1(1)	6(1)
O(4)	28(1)	38(1)	70(2)	9(1)	23(1)	5(1)
O(5)	50(2)	52(1)	42(1)	4(1)	22(1)	-12(1)
N(1)	22(1)	25(1)	32(1)	-5(1)	7(1)	0(1)
N(2)	20(1)	36(1)	32(2)	-1(1)	4(1)	9(1)
N(3)	26(1)	25(1)	32(1)	-6(1)	6(1)	2(1)
N(4)	22(1)	21(1)	33(1)	-2(1)	8(1)	1(1)
N(5)	35(2)	20(1)	45(2)	2(1)	17(1)	6(1)
C(1)	30(2)	26(2)	37(2)	6(1)	13(1)	3(1)
C(2)	29(2)	22(2)	37(2)	4(1)	4(1)	3(1)
C(3)	19(1)	22(1)	27(2)	-6(1)	2(1)	-1(1)
C(4)	25(1)	24(1)	26(1)	0(1)	6(1)	-1(1)
C(5)	22(2)	21(1)	33(2)	2(1)	3(1)	4(1)
C(6)	20(1)	19(1)	34(2)	-2(1)	3(1)	1(1)
C(7)	20(2)	21(1)	47(2)	2(1)	14(1)	-1(1)
C(8)	27(2)	28(2)	52(2)	3(1)	11(2)	1(1)
C(9)	26(2)	36(2)	88(3)	10(2)	20(2)	6(2)
C(10)	44(2)	47(2)	97(4)	-2(2)	46(2)	8(2)
C(11)	59(3)	53(2)	54(3)	-3(2)	34(2)	-1(2)
C(12)	34(2)	34(2)	45(2)	0(1)	16(2)	3(1)
C(13)	30(2)	19(1)	32(2)	-2(1)	1(1)	2(1)
C(14)	29(2)	22(1)	26(2)	-2(1)	6(1)	3(1)
C(15)	24(2)	20(1)	26(2)	-7(1)	2(1)	-1(1)
C(16)	32(2)	23(1)	29(2)	-2(1)	6(1)	3(1)
C(17)	37(2)	25(2)	31(2)	2(1)	13(1)	2(1)
C(18)	25(2)	23(2)	24(2)	-1(1)	2(1)	4(1)
C(19)	29(2)	23(1)	22(2)	0(1)	4(1)	7(1)
C(20)	26(2)	31(2)	38(2)	-6(1)	2(1)	2(1)

C(21)	25(2)	38(2)	46(2)	-1(1)	9(2)	8(1)
C(22)	42(2)	30(2)	34(2)	2(1)	11(2)	15(1)
C(23)	45(2)	21(1)	28(2)	2(1)	11(1)	7(1)
C(24)	32(2)	24(1)	28(2)	5(1)	9(1)	4(1)

Table S12. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1b.

	x	y	z	U(eq)
H(1)	7390(20)	7290(30)	4184(14)	29(8)
H(2)	5910(20)	8470(30)	4436(13)	22(7)
H(2N)	5069(17)	7410(40)	6182(13)	45(11)
H(4)	5850(20)	5220(30)	5804(15)	27(8)
H(4N)	12138(13)	-1200(30)	3585(12)	15(7)
H(5)	7280(20)	4180(30)	5437(13)	18(7)
H(8)	2640(20)	8690(40)	5452(15)	34(9)
H(9)	1360(30)	9760(40)	6012(17)	52(11)
H(10)	1650(30)	9840(50)	7100(20)	70(12)
H(11)	3190(30)	8800(40)	7631(17)	40(10)
H(12)	4480(20)	7830(30)	7103(14)	33(9)
H(13)	10230(20)	4520(30)	3454(14)	25(7)
H(14)	11640(20)	3310(30)	3071(13)	23(7)
H(16)	11760(30)	250(40)	4545(16)	46(9)
H(17)	10380(20)	1650(30)	4859(14)	26(8)
H(20)	14730(30)	-500(40)	3349(17)	49(10)
H(21)	15840(30)	-2380(40)	2992(16)	47(10)
H(22)	15190(20)	-4920(40)	2708(14)	33(8)
H(23)	13460(20)	-5600(30)	2817(14)	29(8)
H(24)	12340(20)	-3630(30)	3173(13)	29(8)

Table S13. Torsion angles [°] for 1b.

N(3)-Ag(1)-O(4)-N(5)	-39.1(2)
N(1)-Ag(1)-O(4)-N(5)	147.4(2)
Ag(1)#1-Ag(1)-O(4)-N(5)	34.1(2)
N(3)-Ag(1)-N(1)-C(5)	101.0(8)
O(4)-Ag(1)-N(1)-C(5)	-162.5(2)
Ag(1)#1-Ag(1)-N(1)-C(5)	-81.2(2)
N(3)-Ag(1)-N(1)-C(1)	-80.6(8)
O(4)-Ag(1)-N(1)-C(1)	15.9(2)
Ag(1)#1-Ag(1)-N(1)-C(1)	97.2(2)
N(1)-Ag(1)-N(3)-C(13)	74.0(8)
O(4)-Ag(1)-N(3)-C(13)	-22.3(2)
Ag(1)#1-Ag(1)-N(3)-C(13)	-103.8(2)
N(1)-Ag(1)-N(3)-C(17)	-105.6(8)
O(4)-Ag(1)-N(3)-C(17)	158.0(2)
Ag(1)#1-Ag(1)-N(3)-C(17)	76.6(2)
Ag(1)-O(4)-N(5)-O(5)	135.2(2)
Ag(1)-O(4)-N(5)-O(3)	-44.0(3)
C(5)-N(1)-C(1)-C(2)	-1.1(4)
Ag(1)-N(1)-C(1)-C(2)	-179.5(2)
N(1)-C(1)-C(2)-C(3)	1.2(5)
C(1)-C(2)-C(3)-C(4)	-1.1(4)
C(1)-C(2)-C(3)-C(6)	-177.6(3)
C(2)-C(3)-C(4)-C(5)	0.8(4)
C(6)-C(3)-C(4)-C(5)	177.2(3)
C(1)-N(1)-C(5)-C(4)	0.9(4)
Ag(1)-N(1)-C(5)-C(4)	179.3(2)
C(3)-C(4)-C(5)-N(1)	-0.8(4)
C(7)-N(2)-C(6)-O(1)	-3.3(5)
C(7)-N(2)-C(6)-C(3)	178.3(2)
C(2)-C(3)-C(6)-O(1)	27.0(4)
C(4)-C(3)-C(6)-O(1)	-149.3(3)
C(2)-C(3)-C(6)-N(2)	-154.5(3)
C(4)-C(3)-C(6)-N(2)	29.2(4)
C(6)-N(2)-C(7)-C(12)	-162.1(3)

C(6)-N(2)-C(7)-C(8)	17.7(4)
C(12)-C(7)-C(8)-C(9)	2.4(4)
N(2)-C(7)-C(8)-C(9)	-177.4(3)
C(7)-C(8)-C(9)-C(10)	-1.3(5)
C(8)-C(9)-C(10)-C(11)	-1.0(5)
C(9)-C(10)-C(11)-C(12)	2.1(6)
C(10)-C(11)-C(12)-C(7)	-1.0(5)
C(8)-C(7)-C(12)-C(11)	-1.3(4)
N(2)-C(7)-C(12)-C(11)	178.5(3)
C(17)-N(3)-C(13)-C(14)	-1.4(4)
Ag(1)-N(3)-C(13)-C(14)	179.0(2)
N(3)-C(13)-C(14)-C(15)	2.7(4)
C(13)-C(14)-C(15)-C(16)	-1.7(4)
C(13)-C(14)-C(15)-C(18)	180.0(2)
C(14)-C(15)-C(16)-C(17)	-0.4(4)
C(18)-C(15)-C(16)-C(17)	177.9(3)
C(13)-N(3)-C(17)-C(16)	-0.8(4)
Ag(1)-N(3)-C(17)-C(16)	178.8(2)
C(15)-C(16)-C(17)-N(3)	1.7(4)
C(19)-N(4)-C(18)-O(2)	-0.4(5)
C(19)-N(4)-C(18)-C(15)	179.2(2)
C(16)-C(15)-C(18)-O(2)	-136.2(3)
C(14)-C(15)-C(18)-O(2)	42.0(4)
C(16)-C(15)-C(18)-N(4)	44.2(4)
C(14)-C(15)-C(18)-N(4)	-137.5(3)
C(18)-N(4)-C(19)-C(20)	22.6(4)
C(18)-N(4)-C(19)-C(24)	-158.2(3)
C(24)-C(19)-C(20)-C(21)	0.6(4)
N(4)-C(19)-C(20)-C(21)	179.8(3)
C(19)-C(20)-C(21)-C(22)	-1.4(5)
C(20)-C(21)-C(22)-C(23)	1.1(5)
C(21)-C(22)-C(23)-C(24)	-0.1(5)
C(22)-C(23)-C(24)-C(19)	-0.6(4)
C(20)-C(19)-C(24)-C(23)	0.4(4)
N(4)-C(19)-C(24)-C(23)	-178.8(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1

Table S14. Hydrogen bonds for 1b [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
N(2)-H(2N)...O(2)#1	0.814(10)	2.20(2)	2.906(3)	145(3)
N(4)-H(4N)...O(5)#2	0.817(10)	2.186(15)	2.944(3)	154(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z+1 #2 x,y-1,z

Table S15. Crystal data and structure refinement for **1c**.

Identification code	1c		
Empirical formula	C <sub>24</sub> H <sub>20</sub> AgN <sub>5</sub> O <sub>5</sub>		
Formula weight	566.32		
Temperature	150(1) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	<i>P</i> 2 <sub>1</sub> /c		
Unit cell dimensions	a = 8.87310(10) Å	α= 90°.	
	b = 36.1311(5) Å	β= 93.3705(5)°.	
	c = 13.9696(2) Å	γ= 90°.	
Volume	4470.83(10) Å <sup>3</sup>		
Z	8		
Density (calculated)	1.683 Mg/m <sup>3</sup>		
Absorption coefficient	0.950 mm <sup>-1</sup>		
F(000)	2288		
Crystal size	0.25 x 0.10 x 0.10 mm <sup>3</sup>		
Theta range for data collection	3.13 to 28.14°.		
Index ranges	-11≤h≤11, -47≤k≤43, -18≤l≤18		
Reflections collected	19602		
Independent reflections	10777 [R(int) = 0.0479]		
Completeness to theta = 28.14°	98.4 %		
Absorption correction	Multi-scan		

Max. and min. transmission	0.9110 and 0.7971
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	10777 / 0 / 791
Goodness-of-fit on F <sup>2</sup>	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0747
R indices (all data)	R1 = 0.0774, wR2 = 0.0843
Largest diff. peak and hole	0.843 and -0.711 e.Å <sup>-3</sup>

Table S16. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for 1c. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
Ag(1)	7082(1)	1309(1)	1624(1)	26(1)
Ag(2)	8075(1)	1043(1)	3913(1)	24(1)
O(1)	10058(2)	-486(1)	995(2)	30(1)
O(1A)	12231(2)	-641(1)	4321(2)	28(1)
O(2)	2826(2)	2952(1)	901(2)	32(1)
O(2A)	5058(2)	2865(1)	4156(2)	30(1)
O(3)	10612(2)	1463(1)	3356(2)	40(1)
O(3A)	5643(2)	604(1)	3445(2)	34(1)
O(4)	9514(2)	1723(1)	2099(2)	34(1)
O(4A)	4579(3)	893(1)	2224(2)	39(1)
O(5)	10698(2)	2058(1)	3182(1)	25(1)
O(5A)	4398(2)	297(1)	2333(2)	27(1)
N(1)	8419(2)	816(1)	1487(2)	22(1)
N(1A)	9688(2)	588(1)	3898(2)	20(1)
N(2)	12337(3)	-210(1)	1346(2)	22(1)
N(2A)	14141(3)	-286(1)	3788(2)	22(1)
N(3)	5530(2)	1767(1)	1565(2)	20(1)
N(3A)	6752(2)	1549(1)	3999(2)	20(1)
N(4)	1070(3)	2642(1)	1729(2)	19(1)
N(4A)	2789(3)	2568(1)	4032(2)	20(1)
N(5)	10275(2)	1744(1)	2883(2)	21(1)
N(5A)	4876(2)	602(1)	2666(2)	20(1)

C(1)	9927(3)	811(1)	1592(2)	23(1)
C(1A)	11170(3)	641(1)	4107(2)	23(1)
C(2)	10764(3)	493(1)	1518(2)	21(1)
C(2A)	12195(3)	353(1)	4162(2)	21(1)
C(3)	10043(3)	159(1)	1336(2)	19(1)
C(3A)	11704(3)	-8(1)	4000(2)	18(1)
C(4)	8474(3)	165(1)	1218(2)	21(1)
C(4A)	10166(3)	-62(1)	3801(2)	20(1)
C(5)	7717(3)	493(1)	1294(2)	23(1)
C(5A)	9208(3)	238(1)	3754(2)	21(1)
C(6)	10803(3)	-211(1)	1218(2)	20(1)
C(6A)	12715(3)	-346(1)	4058(2)	19(1)
C(7)	13308(3)	-504(1)	1097(2)	19(1)
C(7A)	15248(3)	-561(1)	3653(2)	19(1)
C(8)	12935(3)	-872(1)	1180(2)	27(1)
C(8A)	15280(3)	-898(1)	4119(2)	25(1)
C(9)	13906(3)	-1139(1)	863(3)	30(1)
C(9A)	16375(3)	-1155(1)	3919(2)	29(1)
C(10)	15245(4)	-1044(1)	485(2)	32(1)
C(10A)	17441(3)	-1076(1)	3258(2)	31(1)
C(11)	15650(3)	-676(1)	439(2)	28(1)
C(11A)	17430(3)	-735(1)	2812(2)	27(1)
C(12)	14694(3)	-406(1)	754(2)	24(1)
C(12A)	16346(3)	-477(1)	3010(2)	24(1)
C(13)	5993(3)	2121(1)	1579(2)	21(1)
C(13A)	7438(3)	1876(1)	4152(2)	22(1)
C(14)	5007(3)	2416(1)	1516(2)	22(1)
C(14A)	6668(3)	2206(1)	4178(2)	21(1)
C(15)	3469(3)	2350(1)	1451(2)	17(1)
C(15A)	5098(3)	2207(1)	4051(2)	18(1)
C(16)	2978(3)	1987(1)	1435(2)	18(1)
C(16A)	4382(3)	1868(1)	3915(2)	18(1)
C(17)	4028(3)	1703(1)	1491(2)	19(1)
C(17A)	5230(3)	1549(1)	3886(2)	20(1)
C(18)	2422(3)	2680(1)	1336(2)	19(1)
C(18A)	4322(3)	2579(1)	4083(2)	20(1)

C(19)	-105(3)	2909(1)	1737(2)	19(1)
C(19A)	1793(3)	2867(1)	4170(2)	19(1)
C(20)	-148(3)	3231(1)	1188(2)	25(1)
C(20A)	2112(3)	3227(1)	3905(2)	23(1)
C(21)	-1315(3)	3480(1)	1286(2)	29(1)
C(21A)	1128(4)	3508(1)	4117(3)	31(1)
C(22)	-2440(4)	3412(1)	1902(2)	32(1)
C(22A)	-176(3)	3433(1)	4577(2)	29(1)
C(23)	-2408(3)	3092(1)	2430(2)	29(1)
C(23A)	-522(3)	3073(1)	4807(2)	26(1)
C(24)	-1254(3)	2837(1)	2352(2)	23(1)
C(24A)	457(3)	2788(1)	4601(2)	22(1)

Table S17. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 1c.

Ag(1)-N(3)	2.153(2)
Ag(1)-N(1)	2.154(2)
Ag(2)-N(3A)	2.179(2)
Ag(2)-N(1A)	2.183(2)
O(1)-C(6)	1.222(3)
O(1A)-C(6A)	1.216(3)
O(2)-C(18)	1.220(3)
O(2A)-C(18A)	1.225(3)
O(3)-N(5)	1.239(3)
O(3A)-N(5A)	1.249(3)
O(4)-N(5)	1.255(3)
O(4A)-N(5A)	1.239(3)
O(5)-N(5)	1.260(3)
O(5A)-N(5A)	1.262(3)
N(1)-C(1)	1.338(3)
N(1)-C(5)	1.343(4)
N(1A)-C(5A)	1.343(4)
N(1A)-C(1A)	1.344(4)
N(2)-C(6)	1.363(3)
N(2)-C(7)	1.422(4)

N(2)-H(2N)	0.82(3)
N(2A)-C(6A)	1.358(3)
N(2A)-C(7A)	1.417(4)
N(2A)-H(2NA)	0.83(3)
N(3)-C(13)	1.341(4)
N(3)-C(17)	1.350(3)
N(3A)-C(13A)	1.340(4)
N(3A)-C(17A)	1.351(3)
N(4)-C(18)	1.355(3)
N(4)-C(19)	1.420(4)
N(4)-H(4N)	0.79(3)
N(4A)-C(18A)	1.358(3)
N(4A)-C(19A)	1.416(4)
N(4A)-H(4NA)	0.77(3)
C(1)-C(2)	1.375(4)
C(1)-H(1)	0.94(3)
C(1A)-C(2A)	1.383(4)
C(1A)-H(1A)	0.88(3)
C(2)-C(3)	1.382(4)
C(2)-H(2)	0.89(3)
C(2A)-C(3A)	1.387(4)
C(2A)-H(2A)	0.86(3)
C(3)-C(4)	1.393(4)
C(3)-C(6)	1.512(4)
C(3A)-C(4A)	1.391(4)
C(3A)-C(6A)	1.516(4)
C(4)-C(5)	1.370(4)
C(4)-H(4)	0.89(3)
C(4A)-C(5A)	1.378(4)
C(4A)-H(4A)	0.90(3)
C(5)-H(5)	0.89(2)
C(5A)-H(5A)	0.95(3)
C(7)-C(8)	1.377(4)
C(7)-C(12)	1.391(4)
C(7A)-C(8A)	1.381(4)
C(7A)-C(12A)	1.397(4)

C(8)-C(9)	1.384(4)
C(8)-H(8)	0.88(3)
C(8A)-C(9A)	1.383(4)
C(8A)-H(8A)	0.91(3)
C(9)-C(10)	1.372(5)
C(9)-H(9)	0.84(3)
C(9A)-C(10A)	1.390(5)
C(9A)-H(9A)	0.90(3)
C(10)-C(11)	1.381(5)
C(10)-H(10)	0.92(3)
C(10A)-C(11A)	1.379(5)
C(10A)-H(10A)	0.90(3)
C(11)-C(12)	1.382(4)
C(11)-H(11)	0.96(3)
C(11A)-C(12A)	1.379(4)
C(11A)-H(11A)	0.98(3)
C(12)-H(12)	0.81(3)
C(12A)-H(12A)	0.86(3)
C(13)-C(14)	1.381(4)
C(13)-H(13)	0.97(3)
C(13A)-C(14A)	1.374(4)
C(13A)-H(13A)	0.90(2)
C(14)-C(15)	1.383(4)
C(14)-H(14)	0.94(3)
C(14A)-C(15A)	1.394(4)
C(14A)-H(14A)	0.88(3)
C(15)-C(16)	1.382(4)
C(15)-C(18)	1.515(4)
C(15A)-C(16A)	1.387(4)
C(15A)-C(18A)	1.511(4)
C(16)-C(17)	1.384(4)
C(16)-H(16)	0.89(2)
C(16A)-C(17A)	1.380(4)
C(16A)-H(16A)	0.92(3)
C(17)-H(17)	0.93(3)
C(17A)-H(17A)	0.91(3)

C(19)-C(24)	1.395(4)
C(19)-C(20)	1.395(4)
C(19A)-C(20A)	1.385(4)
C(19A)-C(24A)	1.390(4)
C(20)-C(21)	1.384(4)
C(20)-H(20)	0.90(3)
C(20A)-C(21A)	1.383(4)
C(20A)-H(20A)	0.92(3)
C(21)-C(22)	1.378(5)
C(21)-H(21)	0.91(3)
C(21A)-C(22A)	1.383(4)
C(21A)-H(21A)	0.86(3)
C(22)-C(23)	1.372(5)
C(22)-H(22)	0.87(3)
C(22A)-C(23A)	1.378(5)
C(22A)-H(22A)	0.92(3)
C(23)-C(24)	1.385(4)
C(23)-H(23)	0.90(3)
C(23A)-C(24A)	1.387(4)
C(23A)-H(23A)	0.98(3)
C(24)-H(24)	0.91(3)
C(24A)-H(24A)	0.90(3)
N(3)-Ag(1)-N(1)	170.72(9)
N(3A)-Ag(2)-N(1A)	171.46(9)
C(1)-N(1)-C(5)	117.3(3)
C(1)-N(1)-Ag(1)	123.7(2)
C(5)-N(1)-Ag(1)	119.01(18)
C(5A)-N(1A)-C(1A)	117.7(3)
C(5A)-N(1A)-Ag(2)	120.55(18)
C(1A)-N(1A)-Ag(2)	121.5(2)
C(6)-N(2)-C(7)	125.5(3)
C(6)-N(2)-H(2N)	118.4(19)
C(7)-N(2)-H(2N)	115.3(19)
C(6A)-N(2A)-C(7A)	126.1(3)
C(6A)-N(2A)-H(2NA)	118(2)

C(7A)-N(2A)-H(2NA)	114(2)
C(13)-N(3)-C(17)	117.7(3)
C(13)-N(3)-Ag(1)	122.46(18)
C(17)-N(3)-Ag(1)	119.9(2)
C(13A)-N(3A)-C(17A)	117.5(3)
C(13A)-N(3A)-Ag(2)	120.46(18)
C(17A)-N(3A)-Ag(2)	122.0(2)
C(18)-N(4)-C(19)	127.0(3)
C(18)-N(4)-H(4N)	117(2)
C(19)-N(4)-H(4N)	115(2)
C(18A)-N(4A)-C(19A)	127.0(3)
C(18A)-N(4A)-H(4NA)	118(2)
C(19A)-N(4A)-H(4NA)	113(2)
O(3)-N(5)-O(4)	121.1(3)
O(3)-N(5)-O(5)	120.3(3)
O(4)-N(5)-O(5)	118.6(3)
O(4A)-N(5A)-O(3A)	121.3(3)
O(4A)-N(5A)-O(5A)	120.0(3)
O(3A)-N(5A)-O(5A)	118.6(3)
N(1)-C(1)-C(2)	123.0(3)
N(1)-C(1)-H(1)	116.4(17)
C(2)-C(1)-H(1)	120.6(17)
N(1A)-C(1A)-C(2A)	122.3(3)
N(1A)-C(1A)-H(1A)	116.0(18)
C(2A)-C(1A)-H(1A)	121.7(18)
C(1)-C(2)-C(3)	119.8(3)
C(1)-C(2)-H(2)	120(2)
C(3)-C(2)-H(2)	120(2)
C(1A)-C(2A)-C(3A)	120.0(3)
C(1A)-C(2A)-H(2A)	119(2)
C(3A)-C(2A)-H(2A)	121(2)
C(2)-C(3)-C(4)	117.3(3)
C(2)-C(3)-C(6)	126.0(2)
C(4)-C(3)-C(6)	116.7(3)
C(2A)-C(3A)-C(4A)	117.5(3)
C(2A)-C(3A)-C(6A)	124.7(2)

C(4A)-C(3A)-C(6A)	117.8(3)
C(5)-C(4)-C(3)	119.7(3)
C(5)-C(4)-H(4)	121.9(17)
C(3)-C(4)-H(4)	118.2(17)
C(5A)-C(4A)-C(3A)	119.5(3)
C(5A)-C(4A)-H(4A)	121.5(19)
C(3A)-C(4A)-H(4A)	119.0(19)
N(1)-C(5)-C(4)	123.0(3)
N(1)-C(5)-H(5)	117.0(18)
C(4)-C(5)-H(5)	120.0(19)
N(1A)-C(5A)-C(4A)	123.0(3)
N(1A)-C(5A)-H(5A)	114(2)
C(4A)-C(5A)-H(5A)	123(2)
O(1)-C(6)-N(2)	123.8(3)
O(1)-C(6)-C(3)	120.6(2)
N(2)-C(6)-C(3)	115.6(3)
O(1A)-C(6A)-N(2A)	125.1(3)
O(1A)-C(6A)-C(3A)	120.4(2)
N(2A)-C(6A)-C(3A)	114.5(3)
C(8)-C(7)-C(12)	119.7(3)
C(8)-C(7)-N(2)	123.2(3)
C(12)-C(7)-N(2)	117.1(3)
C(8A)-C(7A)-C(12A)	119.8(3)
C(8A)-C(7A)-N(2A)	123.4(3)
C(12A)-C(7A)-N(2A)	116.7(3)
C(7)-C(8)-C(9)	119.3(3)
C(7)-C(8)-H(8)	116(2)
C(9)-C(8)-H(8)	124(2)
C(7A)-C(8A)-C(9A)	119.5(3)
C(7A)-C(8A)-H(8A)	119.8(18)
C(9A)-C(8A)-H(8A)	120.6(18)
C(10)-C(9)-C(8)	121.2(3)
C(10)-C(9)-H(9)	119(2)
C(8)-C(9)-H(9)	119(2)
C(8A)-C(9A)-C(10A)	120.7(3)
C(8A)-C(9A)-H(9A)	117.9(19)

C(10A)-C(9A)-H(9A)	121.3(19)
C(9)-C(10)-C(11)	119.5(3)
C(9)-C(10)-H(10)	121(2)
C(11)-C(10)-H(10)	119(2)
C(11A)-C(10A)-C(9A)	119.7(3)
C(11A)-C(10A)-H(10A)	118(2)
C(9A)-C(10A)-H(10A)	122(2)
C(10)-C(11)-C(12)	119.9(3)
C(10)-C(11)-H(11)	118.6(19)
C(12)-C(11)-H(11)	121.5(19)
C(10A)-C(11A)-C(12A)	120.0(3)
C(10A)-C(11A)-H(11A)	122(2)
C(12A)-C(11A)-H(11A)	118(2)
C(11)-C(12)-C(7)	120.2(3)
C(11)-C(12)-H(12)	122(2)
C(7)-C(12)-H(12)	118(2)
C(11A)-C(12A)-C(7A)	120.3(3)
C(11A)-C(12A)-H(12A)	124.8(19)
C(7A)-C(12A)-H(12A)	115.0(19)
N(3)-C(13)-C(14)	122.9(3)
N(3)-C(13)-H(13)	119.2(19)
C(14)-C(13)-H(13)	117.8(19)
N(3A)-C(13A)-C(14A)	123.1(3)
N(3A)-C(13A)-H(13A)	115.1(18)
C(14A)-C(13A)-H(13A)	121.8(18)
C(13)-C(14)-C(15)	119.3(3)
C(13)-C(14)-H(14)	122.1(17)
C(15)-C(14)-H(14)	118.6(17)
C(13A)-C(14A)-C(15A)	119.7(3)
C(13A)-C(14A)-H(14A)	118.0(19)
C(15A)-C(14A)-H(14A)	122.2(19)
C(16)-C(15)-C(14)	118.3(3)
C(16)-C(15)-C(18)	123.7(2)
C(14)-C(15)-C(18)	117.9(3)
C(16A)-C(15A)-C(14A)	117.4(3)
C(16A)-C(15A)-C(18A)	125.6(2)

C(14A)-C(15A)-C(18A)	117.0(3)
C(15)-C(16)-C(17)	119.4(3)
C(15)-C(16)-H(16)	122.1(18)
C(17)-C(16)-H(16)	118.2(18)
C(17A)-C(16A)-C(15A)	119.8(3)
C(17A)-C(16A)-H(16A)	113(2)
C(15A)-C(16A)-H(16A)	128(2)
N(3)-C(17)-C(16)	122.4(3)
N(3)-C(17)-H(17)	117.4(17)
C(16)-C(17)-H(17)	120.2(17)
N(3A)-C(17A)-C(16A)	122.6(3)
N(3A)-C(17A)-H(17A)	115.4(17)
C(16A)-C(17A)-H(17A)	121.9(17)
O(2)-C(18)-N(4)	125.2(3)
O(2)-C(18)-C(15)	119.3(2)
N(4)-C(18)-C(15)	115.4(3)
O(2A)-C(18A)-N(4A)	123.8(3)
O(2A)-C(18A)-C(15A)	120.8(2)
N(4A)-C(18A)-C(15A)	115.4(3)
C(24)-C(19)-C(20)	119.7(3)
C(24)-C(19)-N(4)	116.4(3)
C(20)-C(19)-N(4)	123.9(3)
C(20A)-C(19A)-C(24A)	120.1(3)
C(20A)-C(19A)-N(4A)	122.7(3)
C(24A)-C(19A)-N(4A)	117.2(3)
C(21)-C(20)-C(19)	119.0(3)
C(21)-C(20)-H(20)	122(2)
C(19)-C(20)-H(20)	119(2)
C(21A)-C(20A)-C(19A)	119.4(3)
C(21A)-C(20A)-H(20A)	121(2)
C(19A)-C(20A)-H(20A)	119(2)
C(22)-C(21)-C(20)	121.4(3)
C(22)-C(21)-H(21)	125.4(18)
C(20)-C(21)-H(21)	113.2(18)
C(22A)-C(21A)-C(20A)	120.7(3)
C(22A)-C(21A)-H(21A)	120.9(19)

C(20A)-C(21A)-H(21A)	118.2(19)
C(23)-C(22)-C(21)	119.4(3)
C(23)-C(22)-H(22)	118(2)
C(21)-C(22)-H(22)	122(2)
C(23A)-C(22A)-C(21A)	119.9(3)
C(23A)-C(22A)-H(22A)	121.4(19)
C(21A)-C(22A)-H(22A)	118.7(19)
C(22)-C(23)-C(24)	120.7(3)
C(22)-C(23)-H(23)	121(2)
C(24)-C(23)-H(23)	118(2)
C(22A)-C(23A)-C(24A)	120.0(3)
C(22A)-C(23A)-H(23A)	117(2)
C(24A)-C(23A)-H(23A)	123(2)
C(23)-C(24)-C(19)	119.8(3)
C(23)-C(24)-H(24)	122.4(18)
C(19)-C(24)-H(24)	117.8(18)
C(23A)-C(24A)-C(19A)	119.9(3)
C(23A)-C(24A)-H(24A)	120.4(17)
C(19A)-C(24A)-H(24A)	119.7(17)

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Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1c. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
Ag(1)	20(1)	23(1)	35(1)	1(1)	3(1)	7(1)
Ag(2)	21(1)	21(1)	31(1)	0(1)	3(1)	7(1)
O(1)	21(1)	22(1)	47(1)	-7(1)	1(1)	-2(1)
O(1A)	26(1)	17(1)	41(1)	6(1)	9(1)	0(1)
O(2)	35(1)	18(1)	45(1)	10(1)	15(1)	5(1)
O(2A)	20(1)	22(1)	49(1)	0(1)	4(1)	-2(1)
O(3)	46(1)	21(1)	54(2)	12(1)	3(1)	4(1)
O(3A)	26(1)	44(2)	32(1)	-3(1)	-8(1)	-8(1)

O(4)	29(1)	42(2)	32(1)	-4(1)	-5(1)	-12(1)
O(4A)	54(1)	16(1)	48(2)	9(1)	4(1)	4(1)
O(5)	25(1)	16(1)	33(1)	-1(1)	2(1)	-5(1)
O(5A)	28(1)	16(1)	36(1)	-4(1)	-1(1)	-4(1)
N(1)	20(1)	22(2)	24(1)	0(1)	1(1)	3(1)
N(1A)	20(1)	20(2)	21(1)	2(1)	3(1)	2(1)
N(2)	18(1)	15(2)	31(2)	-7(1)	-1(1)	-2(1)
N(2A)	21(1)	14(2)	32(2)	5(1)	6(1)	1(1)
N(3)	19(1)	21(2)	21(1)	-1(1)	2(1)	4(1)
N(3A)	21(1)	20(2)	19(1)	2(1)	2(1)	3(1)
N(4)	20(1)	14(1)	24(1)	2(1)	1(1)	3(1)
N(4A)	16(1)	13(1)	31(2)	2(1)	2(1)	1(1)
N(5)	16(1)	19(2)	29(1)	2(1)	6(1)	-1(1)
N(5A)	16(1)	14(1)	31(2)	0(1)	8(1)	0(1)
C(1)	20(2)	21(2)	28(2)	1(2)	2(1)	-1(1)
C(1A)	23(2)	17(2)	29(2)	-1(1)	3(1)	-2(1)
C(2)	16(2)	22(2)	23(2)	-1(1)	0(1)	1(1)
C(2A)	16(1)	24(2)	24(2)	0(1)	0(1)	0(1)
C(3)	20(1)	20(2)	16(2)	-1(1)	2(1)	1(1)
C(3A)	20(1)	20(2)	15(1)	1(1)	6(1)	1(1)
C(4)	19(2)	21(2)	24(2)	-2(1)	3(1)	-4(1)
C(4A)	21(2)	18(2)	22(2)	-1(1)	3(1)	-3(1)
C(5)	14(1)	30(2)	25(2)	-1(1)	1(1)	2(1)
C(5A)	18(2)	27(2)	17(2)	0(1)	1(1)	-2(1)
C(6)	20(1)	21(2)	19(2)	1(1)	2(1)	1(1)
C(6A)	22(1)	16(2)	20(2)	-2(1)	1(1)	2(1)
C(7)	21(1)	18(2)	20(2)	-2(1)	-2(1)	4(1)
C(7A)	15(1)	16(2)	26(2)	-1(1)	-3(1)	3(1)
C(8)	22(2)	23(2)	36(2)	4(2)	3(1)	1(1)
C(8A)	22(2)	22(2)	30(2)	5(1)	1(1)	3(1)
C(9)	28(2)	16(2)	45(2)	-5(2)	-2(1)	3(1)
C(9A)	30(2)	19(2)	37(2)	2(2)	-4(1)	4(1)
C(10)	30(2)	33(2)	31(2)	-10(2)	-5(1)	13(2)
C(10A)	25(2)	29(2)	37(2)	-4(2)	0(1)	12(2)
C(11)	21(2)	33(2)	29(2)	-3(2)	4(1)	4(1)
C(11A)	20(2)	29(2)	31(2)	-3(2)	2(1)	3(1)

C(12)	25(2)	20(2)	26(2)	2(2)	1(1)	-2(1)
C(12A)	23(2)	22(2)	27(2)	1(2)	-1(1)	0(1)
C(13)	18(2)	25(2)	20(2)	-2(1)	3(1)	-1(1)
C(13A)	14(1)	26(2)	24(2)	-1(1)	2(1)	0(1)
C(14)	24(2)	16(2)	25(2)	-5(1)	4(1)	-4(1)
C(14A)	16(1)	21(2)	27(2)	-3(1)	3(1)	-3(1)
C(15)	20(1)	16(2)	15(1)	-1(1)	3(1)	1(1)
C(15A)	20(1)	21(2)	13(1)	-1(1)	2(1)	4(1)
C(16)	15(1)	18(2)	21(2)	0(1)	1(1)	-1(1)
C(16A)	15(1)	20(2)	20(2)	0(1)	1(1)	0(1)
C(17)	20(1)	15(2)	22(2)	2(1)	2(1)	1(1)
C(17A)	22(2)	17(2)	22(2)	0(1)	1(1)	-1(1)
C(18)	23(1)	14(2)	21(2)	-1(1)	0(1)	1(1)
C(18A)	19(1)	21(2)	19(2)	1(1)	3(1)	2(1)
C(19)	18(1)	16(2)	21(2)	-3(1)	-4(1)	2(1)
C(19A)	17(1)	19(2)	20(2)	-3(1)	-5(1)	4(1)
C(20)	29(2)	21(2)	25(2)	2(1)	0(1)	1(1)
C(20A)	19(2)	22(2)	29(2)	1(1)	2(1)	-1(1)
C(21)	35(2)	22(2)	29(2)	1(2)	-9(1)	9(2)
C(21A)	35(2)	16(2)	42(2)	4(2)	-4(2)	4(2)
C(22)	25(2)	32(2)	39(2)	-12(2)	-7(1)	13(2)
C(22A)	23(2)	31(2)	34(2)	-10(2)	-3(1)	11(2)
C(23)	20(2)	34(2)	35(2)	-10(2)	1(1)	3(1)
C(23A)	20(2)	33(2)	25(2)	-3(2)	1(1)	4(1)
C(24)	20(2)	19(2)	29(2)	-1(2)	-4(1)	-1(1)
C(24A)	18(1)	23(2)	23(2)	0(1)	-3(1)	-1(1)

Table S19. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ )  
 for 1c.

	x	y	z	U(eq)
H(1)	10400(30)	1039(9)	1700(20)	19(8)
H(1A)	11460(30)	872(8)	4180(20)	14(7)
H(2)	11770(40)	500(10)	1620(20)	36(9)
H(2A)	13140(30)	400(9)	4300(20)	31(9)
H(2N)	12760(30)	-16(8)	1498(19)	11(8)
H(2NA)	14320(30)	-86(9)	3530(20)	21(9)
H(4)	7990(30)	-50(8)	1153(19)	11(7)
H(4A)	9810(30)	-296(9)	3740(20)	28(9)
H(4N)	940(30)	2460(10)	2030(20)	36(11)
H(5)	6710(30)	498(8)	1220(18)	11(7)
H(4NA)	2400(30)	2378(9)	4040(20)	16(9)
H(5A)	8140(30)	217(9)	3640(20)	27(8)
H(8)	12100(30)	-920(10)	1470(20)	32(9)
H(8A)	14550(30)	-955(8)	4528(19)	17(8)
H(9)	13660(30)	-1362(9)	880(20)	26(9)
H(9A)	16340(30)	-1378(9)	4200(20)	30(9)
H(10)	15860(40)	-1220(10)	240(20)	42(10)
H(10A)	18170(30)	-1237(9)	3130(20)	31(9)
H(11)	16590(30)	-614(9)	170(20)	26(8)
H(11A)	18130(30)	-676(9)	2320(20)	34(9)
H(12)	14910(30)	-188(9)	730(20)	19(9)
H(12A)	16280(30)	-259(9)	2770(20)	22(9)
H(13)	7060(30)	2173(9)	1585(19)	21(8)
H(13A)	8460(30)	1866(8)	4226(17)	9(7)
H(14)	5350(30)	2663(9)	1520(20)	23(8)
H(14A)	7200(30)	2411(9)	4240(20)	21(8)
H(16)	2010(30)	1928(7)	1333(17)	4(6)
H(16A)	3360(30)	1824(9)	3824(19)	23(8)
H(17)	3710(30)	1457(9)	1460(20)	18(8)
H(17A)	4800(30)	1324(8)	3762(19)	14(7)

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H(20)	580(30)	3273(9)	780(20)	30(9)
H(20A)	2970(30)	3274(10)	3580(20)	42(10)
H(21)	-1220(30)	3689(9)	930(20)	20(8)
H(21A)	1310(30)	3728(9)	3910(20)	17(8)
H(22)	-3150(40)	3573(11)	1990(20)	46(11)
H(22A)	-810(30)	3625(9)	4710(20)	24(8)
H(23)	-3120(30)	3043(9)	2850(20)	28(9)
H(23A)	-1430(30)	3033(9)	5170(20)	39(9)
H(24)	-1200(30)	2623(9)	2700(20)	22(8)
H(24A)	220(30)	2553(8)	4730(19)	11(7)

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Table S20. Torsion angles [°] for 1c.

N(3)-Ag(1)-N(1)-C(1)	139.1(5)
N(3)-Ag(1)-N(1)-C(5)	-41.5(6)
N(3A)-Ag(2)-N(1A)-C(5A)	172.2(5)
N(3A)-Ag(2)-N(1A)-C(1A)	-2.3(7)
N(1)-Ag(1)-N(3)-C(13)	-130.3(5)
N(1)-Ag(1)-N(3)-C(17)	48.3(6)
N(1A)-Ag(2)-N(3A)-C(13A)	8.4(7)
N(1A)-Ag(2)-N(3A)-C(17A)	-172.7(5)
C(5)-N(1)-C(1)-C(2)	-0.5(4)
Ag(1)-N(1)-C(1)-C(2)	178.9(2)
C(5A)-N(1A)-C(1A)-C(2A)	1.0(4)
Ag(2)-N(1A)-C(1A)-C(2A)	175.7(2)
N(1)-C(1)-C(2)-C(3)	-0.7(5)
N(1A)-C(1A)-C(2A)-C(3A)	-0.1(5)
C(1)-C(2)-C(3)-C(4)	1.2(4)
C(1)-C(2)-C(3)-C(6)	178.9(3)
C(1A)-C(2A)-C(3A)-C(4A)	-1.1(4)
C(1A)-C(2A)-C(3A)-C(6A)	-178.8(3)
C(2)-C(3)-C(4)-C(5)	-0.7(4)
C(6)-C(3)-C(4)-C(5)	-178.6(3)
C(2A)-C(3A)-C(4A)-C(5A)	1.3(4)
C(6A)-C(3A)-C(4A)-C(5A)	179.2(2)
C(1)-N(1)-C(5)-C(4)	1.0(4)
Ag(1)-N(1)-C(5)-C(4)	-178.4(2)
C(3)-C(4)-C(5)-N(1)	-0.4(5)
C(1A)-N(1A)-C(5A)-C(4A)	-0.8(4)
Ag(2)-N(1A)-C(5A)-C(4A)	-175.5(2)
C(3A)-C(4A)-C(5A)-N(1A)	-0.3(4)
C(7)-N(2)-C(6)-O(1)	10.7(5)
C(7)-N(2)-C(6)-C(3)	-167.3(3)
C(2)-C(3)-C(6)-O(1)	-175.1(3)
C(4)-C(3)-C(6)-O(1)	2.6(4)
C(2)-C(3)-C(6)-N(2)	2.9(4)
C(4)-C(3)-C(6)-N(2)	-179.4(2)

C(7A)-N(2A)-C(6A)-O(1A)	8.2(5)
C(7A)-N(2A)-C(6A)-C(3A)	-171.2(3)
C(2A)-C(3A)-C(6A)-O(1A)	147.8(3)
C(4A)-C(3A)-C(6A)-O(1A)	-30.0(4)
C(2A)-C(3A)-C(6A)-N(2A)	-32.9(4)
C(4A)-C(3A)-C(6A)-N(2A)	149.4(3)
C(6)-N(2)-C(7)-C(8)	-35.8(4)
C(6)-N(2)-C(7)-C(12)	144.1(3)
C(6A)-N(2A)-C(7A)-C(8A)	-26.7(5)
C(6A)-N(2A)-C(7A)-C(12A)	153.2(3)
C(12)-C(7)-C(8)-C(9)	-4.1(5)
N(2)-C(7)-C(8)-C(9)	175.8(3)
C(12A)-C(7A)-C(8A)-C(9A)	-2.0(5)
N(2A)-C(7A)-C(8A)-C(9A)	177.9(3)
C(7)-C(8)-C(9)-C(10)	1.3(5)
C(7A)-C(8A)-C(9A)-C(10A)	0.1(5)
C(8)-C(9)-C(10)-C(11)	1.5(5)
C(8A)-C(9A)-C(10A)-C(11A)	1.5(5)
C(9)-C(10)-C(11)-C(12)	-1.4(5)
C(9A)-C(10A)-C(11A)-C(12A)	-1.3(5)
C(10)-C(11)-C(12)-C(7)	-1.5(5)
C(8)-C(7)-C(12)-C(11)	4.3(5)
N(2)-C(7)-C(12)-C(11)	-175.7(3)
C(10A)-C(11A)-C(12A)-C(7A)	-0.6(5)
C(8A)-C(7A)-C(12A)-C(11A)	2.3(4)
N(2A)-C(7A)-C(12A)-C(11A)	-177.6(3)
C(17)-N(3)-C(13)-C(14)	-0.4(4)
Ag(1)-N(3)-C(13)-C(14)	178.3(2)
C(17A)-N(3A)-C(13A)-C(14A)	-1.4(4)
Ag(2)-N(3A)-C(13A)-C(14A)	177.6(2)
N(3)-C(13)-C(14)-C(15)	1.1(4)
N(3A)-C(13A)-C(14A)-C(15A)	0.7(5)
C(13)-C(14)-C(15)-C(16)	-1.0(4)
C(13)-C(14)-C(15)-C(18)	-177.2(3)
C(13A)-C(14A)-C(15A)-C(16A)	0.9(4)
C(13A)-C(14A)-C(15A)-C(18A)	-179.7(3)

C(14)-C(15)-C(16)-C(17)	0.4(4)
C(18)-C(15)-C(16)-C(17)	176.4(3)
C(14A)-C(15A)-C(16A)-C(17A)	-1.6(4)
C(18A)-C(15A)-C(16A)-C(17A)	179.0(3)
C(13)-N(3)-C(17)-C(16)	-0.3(4)
Ag(1)-N(3)-C(17)-C(16)	-179.0(2)
C(15)-C(16)-C(17)-N(3)	0.2(4)
C(13A)-N(3A)-C(17A)-C(16A)	0.6(4)
Ag(2)-N(3A)-C(17A)-C(16A)	-178.4(2)
C(15A)-C(16A)-C(17A)-N(3A)	1.0(4)
C(19)-N(4)-C(18)-O(2)	-2.0(5)
C(19)-N(4)-C(18)-C(15)	179.0(3)
C(16)-C(15)-C(18)-O(2)	-143.9(3)
C(14)-C(15)-C(18)-O(2)	32.1(4)
C(16)-C(15)-C(18)-N(4)	35.1(4)
C(14)-C(15)-C(18)-N(4)	-148.9(3)
C(19A)-N(4A)-C(18A)-O(2A)	-8.4(5)
C(19A)-N(4A)-C(18A)-C(15A)	171.2(3)
C(16A)-C(15A)-C(18A)-O(2A)	-176.1(3)
C(14A)-C(15A)-C(18A)-O(2A)	4.5(4)
C(16A)-C(15A)-C(18A)-N(4A)	4.3(4)
C(14A)-C(15A)-C(18A)-N(4A)	-175.1(2)
C(18)-N(4)-C(19)-C(24)	-167.0(3)
C(18)-N(4)-C(19)-C(20)	12.0(5)
C(18A)-N(4A)-C(19A)-C(20A)	33.9(4)
C(18A)-N(4A)-C(19A)-C(24A)	-145.4(3)
C(24)-C(19)-C(20)-C(21)	1.9(4)
N(4)-C(19)-C(20)-C(21)	-177.1(3)
C(24A)-C(19A)-C(20A)-C(21A)	3.3(4)
N(4A)-C(19A)-C(20A)-C(21A)	-176.0(3)
C(19)-C(20)-C(21)-C(22)	-1.0(5)
C(19A)-C(20A)-C(21A)-C(22A)	-0.9(5)
C(20)-C(21)-C(22)-C(23)	-0.1(5)
C(20A)-C(21A)-C(22A)-C(23A)	-1.6(5)
C(21)-C(22)-C(23)-C(24)	0.3(5)
C(21A)-C(22A)-C(23A)-C(24A)	1.7(5)

C(22)-C(23)-C(24)-C(19)	0.6(5)
C(20)-C(19)-C(24)-C(23)	-1.7(4)
N(4)-C(19)-C(24)-C(23)	177.4(3)
C(22A)-C(23A)-C(24A)-C(19A)	0.6(5)
C(20A)-C(19A)-C(24A)-C(23A)	-3.1(4)
N(4A)-C(19A)-C(24A)-C(23A)	176.1(3)

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Symmetry transformations used to generate equivalent atoms:

Table S21. Hydrogen bonds for 1c [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	∠(DHA)
N(2)-H(2N)...O(5A)#1	0.82(3)	2.13(3)	2.883(3)	152(3)
N(2A)-H(2NA)...O(5A)#1	0.83(3)	2.17(3)	2.946(3)	155(3)
N(4)-H(4N)...O(5)#2	0.79(3)	2.18(3)	2.958(3)	165(3)
N(4A)-H(4NA)...O(5)#2	0.77(3)	2.20(3)	2.826(3)	139(3)

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Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z