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Investigations on template CrO₄²⁻/Cr₂O₇²⁻ influence in forming series of silver-chalcogenide clusters

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Preparation of ligand 2-(methylthio)naphthalene (HSCH₂C₁₀H₇)

A mixture of 2-methylnaphthalene (2.84 g, 0.0200 mol), N-Bromosuccinimide (NBS) (3.92 g, 0.0220 mol) and tetrachloromethane (100.0 mL) in a 250-ml three-necked, round-bottom flask was heated to 80 °C under stirring. Then 0.125 g (0.000761 mol) of azodiisobutyronitrile (AIBN) was added as initiator. The reaction mixture was refluxed for 12 h, afterwards the resultant solution was filtered and extracted by deionized water, and dried over anhydrous magnesium sulfate. The product 2-bromomethyl-naphthalene was got by rotationally evaporation. ¹HNMR (CDCl₃): δ 4.70 (s, 2H), 7.50–7.57 (m, 3H), 7.82–7.93 (m, 4H). IR data (KBr, cm⁻¹): 3060 w, 897 w, 823 s, 752 s.

20.0 mL of acetone solution containing 2-bromomethyl-naphthalene (0.77 g, 0.0035 mol) and thiourea (0.40 g, 0.0051 mol) was stirring for 2 h when refluxing. The mother solution was cooled to room temperature, and the precipitates were collected by filtration and dried overnight in vacuum. The precipitates were dissolved in aqueous NaOH solution (2 mol/L). The aqueous solution was refluxed for 2 h, and then cooled to room temperature and adjusted to pH≈2.0 using hydrochloric acid (2 mol/L). The solution was extracted by dichloromethane and dried over anhydrous magnesium sulfate. The product of 2-(methylthio)naphthalene was got by successively suction filtrating and rotationally evaporating, and dried in vacuum. ¹HNMR (CDCl₃): δ 1.84 (t, 1H), 3.94 (d, 2H), 7.46–7.52 (m, 3H), 7.76–7.85 (m, 4H). Anal. Calcd for C₁₁H₁₀S: C 75.82, H 5.78, S 18.40 %. Found: C 75.44, H 6.08, S 18.48 %. IR data (KBr, cm⁻¹): 3050 w, 866 m, 823 m, 742 s.

X-Ray Crystallography

Single-crystal X-ray diffraction measurement of complexes **1** - **3** were performed on a Rigaku XtaLAB Pro diffractometer. Data collection and reduction were performed using the program CrysAlisPro.^[S1] Data collection and reduction were performed using the program SADABS.^[S2] All the structures were solved with direct methods (*SHELXS*)^[S3] and refined by full-matrix least squares on F^2 using *OLEX2*,^[S4] which utilizes the *SHELXL*-2015 module.^[S5] All the atoms were refined anisotropically. Hydrogen atoms were placed in calculated positions refined using idealized geometries and assigned fixed isotropic displacement parameters. Structure refinement was handled with different strategies according to the electron density distribution and the complexity of the disorder.

The detailed information of the crystal data, data collection and refinement results for all compounds are summarized in Table S1.



Figure S1. Representative TEM image of cluster [Ag₁₄(SCH₂C₁₀H₇)₆(CF₃CO₂)₈(DMAc)₆] (**1**) in ethonal.



Figure S2. Representative TEM image of cluster $[Ag_{30}(SCH_2C_{10}H_7)_{18}(CrO_4)_2(DMAc)_2(CF_3CO_2)_8]$ (2) in ethonal.



Figure S3. The PXRD pattern of compound **1** at room temperature.



Figure S4. UV-vis spectrum for 1 in solid state.



Figure S5. The PXRD pattern of compound **2** at room temperature.



Figure S6. UV-vis spectrum for 2 in solid state.



Figure S7. IR absorption spectrum for **1**.



Figure S8. IR absorption spectrum for 2



Figure S9. The temperature-dependent luminescence spectra of cluster **1** excited at 360 nm in the solid state



Figure S10. Coordination environments of Ag atoms of cluster 2.



Figure S11. The lingkage mode of CrO₄²⁻ anions of cluster **2**.

Table S1 Crystal data and structure refinement for **1**-3. 3 Cluster 1 2 CCDC number 1869847 1869848 1869846 Empirical formula $C_{106}H_{108}N_6O_{22}S_6F_{24}Ag_{14}$ $C_{230}H_{198}N_4O_{28}S_{18}F_{24}Cr_2Ag_{30}$ C₈₆ H₆₈ Ag₁₂ Cr₂ F₁₂ N₆ O₁₅ S₆ Formula weight 3976.52 7839.09 3244.26 Crystal size, mm³ $0.20 \times 0.18 \times 0.16$ $0.20 \times 0.21 \times 0.25$ $0.18 \times 0.18 \times 0.16$ Crystal system Orthorhombic Triclinic triclinic $P\bar{1}$ $P\bar{1}$ Space group Pbca *a*, Å 17.109(13) 17.8479(4) 10.5753(3)b, Å 26.729(9) 21.0072(4) 16.3742(8) *c*, Å 29.365(13) 21.9628(4) 17.2297(9) α , deg 90 62.618(2) 66.079(5) β , deg 90 83.842(2) 72.957(4) γ, deg 90 65.100(2) 82.717(3) Volume, Å³ 13429(12) 6594.1(3) 2607.4(2)Ζ 4 1 1 Temperature, K 293(2) 293(2) 102 Density (calcd.), g cm⁻³ 1.967 1.974 2.066 Absorption coeff., mm⁻¹ 2.180 2.465 2.597 *F*(000), e 7728 3792 1562 Theta range for data 3.02 to 25.00° 3.426 to 26.00° 2.89 to 25.00

collection Index ranges $-10 \le h \le 20, -29 \le k \le 31, -34 \le l \le 22$ -22≤h≤20, -20≤k≤25, -24≤l≤27 -12 ≤h≤12, -19≤k≤19, -20≤l≤18 Completeness to theta = 99.8% 99.7% 99.7% 25.00° Absorption correction Semi–empirical from equivalents Semi-empirical from equivalents Semi-empirical from equivalents Max. and min. transmission 0.7218 and 0.6696 1.000 and 0.899 0.660 and 0.633 Refinement method Full-matrix least-squares on F² Full-matrix least-squares on F² Full-matrix least-squares on F² 9178 /1420 /689 Data/restraints/parameters 11813/262/808 25823/57/1519 0.71073 Å 0.71073 Å 0.71073 Å Wavelength Reflections 32173[R(int) = 0.0421]61028[R(int) = 0.0459]17036 [R(int)=0.0477] collected/independent/*R*_{int} 0.0432 / 0.0913 0.0688 / 0.2005 0.0630/0.1096 Final $R1/wR2[I \ge 2\sigma(I)]$ Final R1/wR2 (all data) 0.1083 / 0.2278 0.0657 / 0.1032 0.1442/0.1313 Goodness of fit (GOF) 1.056 1.014 0.991 Final diff. peaks(max/min), 1.979/-0.780 1.743/-2.461 1.452/-0.883 e Å-3

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 $R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|. \ wR_2 = [\sum w (F_0^2 - F_c^2)^2 / \sum w (F_0^2)^2]^{1/2}$

| | 1 | | |
|----------------|------------|---------------|------------|
| | Bond ler | ngths (Å) | |
| Ag1-01 | 2.249(9) | Ag6-05 | 397(11) |
| Ag1-09 | 2.436(9) | Ag6-S2 | 2.474(3) |
| Ag1-Ag2 | 2.948(2) | Ag6-Ag7 | 3.138(2) |
| Ag1-Ag7#1 | 3.0957(17) | Ag7-06 | 2.262(11) |
| Ag2-03 | 2.340(9) | Ag7-08#1 | 2.385(11) |
| Ag2-02 | 2.414(8) | Ag7-S1#1 | 2.554(3) |
| Ag2-Ag3 | 3.0084(15) | Ag7-Ag1#1 | 3.0957(17) |
| Ag2-Ag6 | 3.103(2) | Ag4-S1 | 2.888(3) |
| Ag3-04 | 2.421(8) | Ag4-Ag7#1 | 2.9539(16) |
| Ag3-Ag6 | 2.9152(17) | Ag5-S3 | 2.636(3) |
| Ag3-Ag4 | 3.077(2) | Ag4-S2#1 | 2.496(3) |
| Ag3-Ag5 | 3.3057(18) | Ag4-010 | 2.544(8) |
| S2-Ag5#1 | 2.510(3) | 09-Ag7#1 | 2.581(9) |
| S3-Ag1#1 | 2.535(3) | | |
| | Bond A | ngles (°) | |
| 01-Ag1-09 | 104.6(4) | 09-Ag1-S3#1 | 113.5(2) |
| 01-Ag1-S3#1 | 125.2(3) | 01-Ag1-S1 | 125.3(2) |
| S1-Ag1-Ag2 | 54.13(6) | S1-Ag1-Ag7#1 | 51.36(6) |
| 01-Ag1-Ag7#1 | 153.7(3) | Ag2-Ag1-Ag7#1 | 104.52(5) |
| 09-Ag1-Ag7#1 | 54.1(2) | 02-Ag2-S1 | 118.7(3) |
| 03-Ag2-Ag3 | 85.5(3) | S1-Ag2-Ag1 | 59.16(7) |
| 02-Ag2-Ag3 | 162.2(3) | 02-Ag2-Ag6 | 136.0(3) |
| S2-Ag2-Ag3 | 104.83(7) | S2-Ag2-Ag6 | 50.67(7) |
| 04-Ag3-S3 | 92.1(3) | 04-Ag3-S1 | 104.1(3) |
| S3-Ag3-010 | 98.7(2) | 010-Ag3-Ag6 | 151.4(2) |
| S3-Ag3-Ag2 | 116.60(7) | S1-Ag3-Ag4 | 61.22(7) |
| 010-Ag3-Ag2 | 142.99(19) | S3-Ag3-Ag4 | 115.46(8) |
| S2#1-Ag4-Ag6#1 | 52.69(6) | 010-Ag4-Ag3 | 53.25(18) |

 Table S2 Selected bond lengths [Å] and angles [°] for 1 - 3.

| 010-Ag4-Ag6#1 | 125.43(19) | S1-Ag4-Ag3 | 49.74(6) |
|-----------------|------------|----------------|------------|
| S1-Ag4-Ag6#1 | 72.28(5) | Ag7#1-Ag4-Ag3 | 98.78(5) |
| Ag7#1-Ag4-Ag6#1 | 63.74(4) | Ag6#1-Ag4-Ag3 | 76.24(3) |
| 07-Ag4-Ag3 | 125.2(4) | 011-Ag5-S2#1 | 133.7(3) |
| S2#1-Ag5-S3 | 99.44(9) | 011-Ag5-S3 | 126.6(3) |
| 011-Ag5-Ag3 | 128.7(3) | 05-Ag6-S2 | 94.3(3) |
| S2#1-Ag5-Ag3 | 76.94(6) | 05-Ag6-S3 | 104.9(3) |
| S3-Ag5-Ag3 | 48.80(7) | S2-Ag6-S3 | 160.36(10) |
| S2-Ag6-Ag4#1 | 53.38(7) | 05-Ag6-Ag3 | 123.8(3) |
| S3-Ag6-Ag4#1 | 128.03(7) | S2-Ag6-Ag3 | 110.13(8) |
| Ag3-Ag6-Ag2 | 59.89(4) | Ag3-S1-Ag7#1 | 129.21(11) |
| Ag4#1-Ag6-Ag7 | 57.59(3) | Ag1-S1-Ag4 | 128.47(9) |
| Ag2-Ag6-Ag7 | 162.07(4) | Ag2-S1-Ag1 | 66.71(7) |
| 06-Ag7-08#1 | 90.5(5) | Ag3-S1-Ag4 | 69.04(7) |
| 06-Ag7-S1#1 | 154.8(3) | Ag7#1-S1-Ag4 | 65.42(7) |
| 08#1-Ag7-S1#1 | 108.5(4) | S1#1-Ag7-09#1 | 95.3(2) |
| 06-Ag7-09#1 | 97.2(4) | 06-Ag7-Ag4#1 | 105.1(4) |
| 08#1-Ag7-09#1 | 101.0(4) | S1#1-Ag7-Ag4#1 | 62.74(7) |
| 08#1-Ag7-Ag4#1 | 82.6(3) | Ag6-S2-Ag4#1 | 73.94(9) |
| | 2 | | |
| | Bond leng | gths (Å) | |
| Ag1-Ag3 | 2.8754(6) | Ag1-Ag4 | 2.9396(6) |
| Ag1-Ag5 | 2.9577(7) | Ag1-Ag7 | 3.1215(7) |
| Ag1-S4 | 2.4355(16) | Ag1-01 | 2.193(4) |
| Ag1-02#1 | 2.555(5) | Ag2-Ag7 | 2.9821(7) |
| Ag2-Ag9 | 3.1999(6) | Ag2-Ag14 | 2.8706(7) |
| Ag2-S1 | 2.4304(16) | Ag2-S2 | 2.4132(15) |
| Ag3-Ag7 | 3.2067(7) | Ag3-Ag13 | 2.9747(7) |
| Ag3-S2 | 2.6511(17) | Ag3-S4 | 2.5333(16) |
| Ag3-S7 | 2.5577(14) | Ag3-011 | 2.413(4) |
| Ag4-Ag5 | 2.9843(7) | Ag4-Ag12 | 2.9391(7) |
| Ag4-S3 | 2.4267(17) | Ag4-S5 | 2.5595(15) |

| Ag4-012 | 2.281(4) | Ag5-Ag15 | 3.0237(7) | |
|-----------------|------------|--------------|-------------|--|
| Ag5-S4 | 2.5363(15) | Ag5-S5 | 2.6355(16) | |
| Ag5-S9 | 2.5515(16) | Ag5-010 | 2.392(4) | |
| Ag6-Ag10 | 3.0019(7) | Ag6-Ag14 | 2.9295(6) | |
| Ag6-Ag15 #1 | 3.2283(7) | Ag6-S1 | 2.5861(15) | |
| Ag6-S8 | 2.5472(16) | Ag6-06 | 2.496(4) | |
| Ag6-09 | 2.364(5) | Ag7-S2 | 2.6254(15) | |
| Ag7-S3 | 2.4313(15) | Ag7-04 | 2.277(4) | |
| Ag8-Ag10 | 3.0187(7) | Ag8-Ag12 | 2.8686(7) | |
| Ag8-Ag13#1 | 2.9282(6) | Ag8-S6 | 2.6254(16) | |
| Ag8-S7#1 | 2.4454(15) | Ag8-05 | 2.301(4) | |
| Ag9-Ag12 | 3.3434(7) | Ag9-S1 | 2.6008(16) | |
| Ag9-S3 | 2.5324(16) | Ag9-S6 | 2.6457(16) | |
| Ag9-013 | 2.517(5) | Ag10-Ag13#1 | 3.0321(7) | |
| Ag10-S6 | 2.5600(16) | Ag10-S8 | 2.5348(15) | |
| Ag10-06 | 2.556(5) | Ag10-08 | 2.324(4) | |
| Ag11-S2 | 2.4388(15) | Ag11-S5#1 | 2.4611(15) | |
| Ag11-02 | 2.424(5) | Ag11-014#1 | 2.462(6) | |
| Ag12-S5 | 2.4199(17) | Ag12-S6 | 2.4146(17) | |
| Ag13-S7 | 2.4431(17) | Ag13-S8#1 | 2.4398(17) | |
| Ag14-Ag15#1 | 2.9342(7) | Ag14-S1 | 2.5472(15) | |
| Ag14-S9#1 | 2.4415(15) | Ag14-07 | 2.346(5) | |
| Ag15-S8#1 | 2.4577(15) | Ag15-S9 | 2.4534(15) | |
| Cr1-01 | 1.578(4) | Cr1-02 | 1.528(5) | |
| Cr1-03 | 1.537(5) | Cr1-014 | 1.542(5) | |
| Bond Angles (°) | | | | |
| 01-Ag1-Ag7 | 82.63(11) | 01-Ag1-S4 | 174.24(12) | |
| 01-Ag1-02#1 | 97.41(17) | 02#1-Ag1-Ag3 | 99.60(10) | |
| Ag14-Ag2-Ag7 | 169.92(2) | Ag14-Ag2-Ag9 | 104.972(19) | |
| S1-Ag2-Ag7 | 127.65(4) | S1-Ag2-Ag9 | 52.90(4) | |
| S2-Ag2-S1 | 171.67(6) | Ag1-Ag3- Ag7 | 61.472(15) | |
| Ag1-Ag3-Ag13 | 108.98(2) | Ag13-Ag3-Ag7 | 164.73(2) | |

| S2-Ag3-Ag1 | 77.36(3) | S2-Ag3-Ag7 | 52.21(3) |
|-----------------|-------------|-----------------|------------|
| S2-Ag3-Ag13 | 140.52(4) | S4-Ag3-Ag1 | 53.07(4) |
| 011-Ag3-S4 | 99.85(13) | 011-Ag3-S7 | 98.84(12) |
| Ag1-Ag4-Ag5 | 59.899(16) | Ag12-Ag4-Ag1 | 87.001(17) |
| 012-Ag4-Ag12 | 121.28(12) | 012-Ag4-S3 | 123.80(13) |
| 012-Ag4-S5 | 97.46(13) | Ag1-Ag5-Ag4 | 59.301(16) |
| Ag1-Ag5-Ag15 | 100.602(18) | Ag4-Ag5-Ag15 | 158.67(2) |
| S4-Ag5-Ag1 | 51.94(4) | S4-Ag5-Ag4 | 91.24(4) |
| 010-Ag5-Ag15 | 116.45(11) | 010-Ag5-S4 | 106.14(12) |
| 010-Ag5-S5 | 100.43(11) | 010-Ag5-S9 | 104.30(13) |
| Ag10-Ag6-Ag15#1 | 94.235(18) | Ag14-Ag6-Ag10 | 133.20(2) |
| Ag14-Ag6-Ag15#1 | 56.663(15) | S1-Ag6-Ag10 | 102.94(4) |
| S1-Ag6-Ag14 | 54.58(3) | S1-Ag6-Ag15#1 | 98.55(4) |
| 09-Ag6-S1 | 100.23(11) | 09-Ag6-S8 | 121.29(11) |
| 09-Ag6-06 | 103.98(15) | Ag1-Ag7-Ag3 | 54.029(14) |
| Ag2-Ag7-Ag1 | 80.199(17) | Ag2-Ag7-Ag3 | 97.965(18) |
| S2-Ag7-Ag1 | 73.42(4) | S2-Ag7-Ag2 | 50.49(3) |
| S2-Ag7-Ag3 | 52.94(4) | S3-Ag7-Ag1 | 71.97(4) |
| 04-Ag7-S2 | 92.57(11) | 04-Ag7-S3 | 139.29(11) |
| Ag12-Ag8-Ag10 | 97.57(2) | Ag12-Ag8-Ag13#1 | 99.742(19) |
| Ag13#1-Ag8-Ag10 | 61.287(16) | S6-Ag8-Ag10 | 53.40(4) |
| S6-Ag8-Ag12 | 51.91(4) | S6-Ag8-Ag13#1 | 97.37(4) |
| S1-Ag9-Ag2 | 48.19(3) | S1-Ag9-Ag12 | 123.88(4) |
| S1-Ag9-S6 | 104.67(5) | S3-Ag9-Ag2 | 78.91(4) |
| Ag6-Ag10-Ag8 | 139.27(2) | Ag6-Ag10-Ag13#1 | 96.656(18) |
| Ag8-Ag10-Ag13#1 | 57.886(15) | S6-Ag10-Ag6 | 102.91(4) |
| 08-Ag10-06 | 97.78(15) | S2-Ag11-S5#1 | 156.27(5) |
| S2-Ag11-014#1 | 105.95(13) | S5#1-Ag11-O14#1 | 87.41(13) |
| 02-Ag11-S2 | 108.50(12) | 02-Ag11-S5 | 90.85(12) |
| 02-Ag11-014#1 | 89.23(19) | Ag4-Ag12-Ag9 | 77.023(17) |
| Ag8-Ag12-Ag4 | 166.67(2) | Ag8-Ag12-Ag9 | 108.27(2) |
| S5-Ag12-Ag4 | 56.05(4) | S5-Ag12-Ag8 | 121.81(4) |

| S6-Ag12-S5 | 173.46(5) | Ag3-Ag13-Ag10#1 | 159.14(2) |
|-----------------|------------|-------------------|------------|
| Ag8#1-Ag13-Ag3 | 104.09(2) | Ag8#1-Ag13-Ag10#1 | 60.828(16) |
| S7-Ag13-Ag3 | 55.29(4) | S7-Ag13-Ag8#1 | 53.24(4) |
| S7-Ag13-Ag10 | 113.69(4) | S8#1-Ag13-Ag3 | 137.37(4) |
| S8#1-Ag13-Ag8#1 | 114.65(4) | S8#1-Ag13-Ag10#1 | 53.88(4) |
| S1-Ag14-Ag15#1 | 107.50(4) | S9#1-Ag14-Ag2 | 109.50(4) |
| S9-Ag14-Ag6 | 118.70(4) | S9#1-Ag14-Ag15#1 | 53.36(4) |
| Ag14-Ag15-Ag6 | 56.526(15) | S8#1-Ag15-Ag5 | 146.11(4) |
| S8#1-Ag15-Ag6#1 | 51.06(4) | S8#1-Ag15-Ag14#1 | 107.16(4) |
| S9-Ag15-Ag5 | 54.33(4) | S9-Ag15-Ag6#1 | 108.29(4) |
| S9-Ag15-Ag14#1 | 52.98(4) | S9-Ag15-S8#1 | 159.14(6) |
| 02-Cr1-01 | 109.9(2) | 02-Cr1-03 | 110.9(3) |
| 02-Cr1-014 | 110.7(3) | 03-Cr1-01 | 109.1(3) |
| 03-Cr1-014 | 108.2(3) | 014-Cr1-01 | 108.0(3) |
| | 3 | | |
| | Bond ler | ngths (Å) | |
| Ag1-04 | 2.325(8) | Ag2-06 | 2.371(7) |
| Ag1-S8 | 2.486(2) | Ag2-S10 | 2.479(3) |
| Ag2-Ag6#1 | 3.1568(12) | Ag4-N1 | 2.304(10) |
| Ag3-N3 | 2.255(11) | Ag4-05 | 2.370(7) |
| Ag5-Ag6 | 2.9876(11) | Ag5-S9 | 2.421(2) |
| Ag6-N2 | 2.229(9) | Ag5-S8 | 2.426(2) |
| Ag6-S10#1 | 2.435(2) | Cr1-01 | 1.589(6) |
| Ag6-S8 | 2.590(3) | Cr1-03 | 1.599(7) |
| Cr1-02 | 1.575(6) | Cr1-08#1 | 1.789(14) |
| Cr1-08 | 1.783(14) | | |
| Bond Angles (°) | | | |
| 04-Ag1-S8 | 127.3(2) | 04-Ag1-03 | 82.4(3) |
| S8-Ag1-03 | 93.89(10) | 04-Ag1-S10 | 97.1(2) |

| S8-Ag1-S10 | 133.07(8) | 03-Ag1-S10 | 107.73(17) |
|----------------|------------|-----------------|------------|
| 04-Ag1-Ag4 | 82.8(2) | S8-Ag1-Ag4 | 111.46(5) |
| 03-Ag1-Ag4 | 154.63(16) | S10-Ag1-Ag4 | 54.02(6) |
| 04-Ag1-Ag5 | 162.7(2) | S8-Ag1-Ag5 | 49.98(6) |
| 03-Ag1-Ag5 | 80.85(16) | S10-Ag1-Ag5 | 92.17(7) |
| Ag4-Ag1-Ag5 | 114.35(3) | 06-Ag2-S10 | 106.7(2) |
| 06-Ag2-S9 | 111.4(2) | S10-Ag2-S9 | 138.60(8) |
| 06-Ag2-01 | 80.3(3) | S10-Ag2-O1 | 106.0(2) |
| S9-Ag2-01 | 95.8(2) | 06-Ag2-Ag5 | 152.9(2) |
| S10-Ag2-Ag5 | 97.08(6) | S9-Ag2-Ag5 | 51.72(6) |
| 01-Ag2-Ag5 | 80.83(18) | 06-Ag2-Ag3#1 | 77.79(19) |
| S10-Ag2-Ag3#1 | 118.76(6) | S9-Ag2-Ag3#1 | 56.99(5) |
| 01-Ag2-Ag3#1 | 134.1(2) | Ag5-Ag2-Ag3#1 | 102.16(3) |
| 06-Ag2-Ag6#1 | 92.6 (2) | S10-Ag2-Ag61 | 49.41(5) |
| S9-Ag2-Ag6#1 | 112.40(5) | 01-Ag2-Ag6#1 | 151.4(2) |
| Ag5-Ag2-Ag6#1 | 112.96(3) | Ag3#1-Ag2-Ag6#1 | 69.59(3) |
| N3-Ag3-07#1 | 110.8(4) | N3-Ag3-S8 | 110.2 (2) |
| 07#1-Ag3-S8 | 122.1(2) | N3-Ag3-S9#1 | 99.1(3) |
| 07#1-Ag3 -S9#1 | 117.45(18) | S8-Ag3-S9#1 | 94.11(7) |
| N3-Ag3 -Ag2#1 | 147.9(2) | 07#1-Ag3-Ag2#1 | 79.77(19) |
| S8-Ag3-Ag2#1 | 86.44(5) | S9#1-Ag3-Ag2#1 | 51.13(5) |
| N1-Ag4-05 | 93.3(3) | N1-Ag4-S9#1 | 107.3(2) |
| 05-Ag4-S9#1 | 122.6(2) | N1-Ag4-S10 | 119.0(3) |
| 05-Ag4-S10 | 98.3 (2) | S9#1-Ag4-S10 | 115.17(8) |
| N1-Ag4-Ag1 | 164.7 (2) | 05-Ag4-Ag1 | 76.3(2) |
| S9#1-Ag4-Ag1 | 87.85(5) | S10-Ag4-Ag1 | 53.20(5) |
| N1-Ag4-Ag5#1 | 100.4(3) | 05-Ag4-Ag5#1 | 165.2(2) |
| S9#1-Ag4-Ag5#1 | 47.69(5) | S10-Ag4-Ag5#1 | 79.99(6) |
| Ag1-Ag4-Ag5#1 | 91.31(3) | S9-Ag5-S8 | 166.70(7) |
| S9-Ag5-Ag2 | 54.58(6) | S8-Ag5-Ag6 | 56.00(6) |
| S8-Ag5-Ag2 | 122.36(6) | Ag2-Ag5-Ag6 | 154.70(3) |
| S9-Ag5-Ag6 | 120.15(6) | S9-Ag5-Ag1 | 125.37(6) |

| S8-Ag5-Ag1 | 51.70(6) | S8-Ag5-Ag4#1 | 124.92(6) |
|---------------|------------|-----------------|------------|
| Ag2-Ag5-Ag1 | 71.25(3) | Ag2-Ag5-Ag4#1 | 102.10(3) |
| Ag6-Ag5-Ag1 | 105.26(4) | Ag6-Ag5-Ag4#1 | 69.77 (3) |
| S9-Ag5-Ag4#1 | 50.61(6) | Ag1-Ag5-Ag4#1 | 154.22(3) |
| N2-Ag6-S10#1 | 136.4(3) | S10#1-Ag6-Ag5 | 87.51(6) |
| N2-Ag6-S8 | 103.3(3) | S8-Ag6-Ag5 | 50.97(5) |
| S10#1-Ag6-S8 | 119.32(8) | N2-Ag6-Ag2#1 | 151.0(3) |
| N2-Ag6-Ag5 | 115.1(3) | S10#1-Ag6-Ag2#1 | 50.64(6) |
| Ag5-Ag6-Ag2#1 | 91.60(3) | S8-Ag6-Ag2#1 | 84.26(5) |
| 02-Cr1-01 | 108.7(4) | 01-Cr1-08#2 | 121.7(6) |
| 02-Cr1-03 | 110.8(4) | 03-Cr1-08#2 | 110.1(6) |
| 01-Cr1-O3 | 112.3(4) | 08-Cr1-08#2 | 35.5(6) |
| 02-Cr1-08 | 124.6(5) | Ag5-S8-Ag1 | 78.32(7) |
| 01-Cr1-08 | 96.0(5) | Ag5-S8-Ag3 | 136.31(8) |
| 03-Cr1-08 | 103.6(6) | Ag1-S8-Ag3 | 100.49(9) |
| 02-Cr1-08#2 | 91.1(5) | Ag2-S9-Ag4#1 | 146.13(10) |
| Ag5-S8-Ag6 | 73.03(7) | Ag5-S9-Ag3#1 | 132.26(10) |
| Ag1-S8-Ag6 | 144.95(9) | Ag2-S9-Ag3#1 | 71.88(6) |
| Ag3-S8-Ag6 | 87.02(7) | Ag4#1-S9-Ag3#1 | 111.19(7) |
| Ag5-S9-Ag2 | 73.70(7) | Ag6#1-S10-Ag2 | 79.95(8) |
| Ag5-S9-Ag4#1 | 81.70(7) | Ag6#1-S10-Ag1 | 139.41(6) |
| Ag2-S10-Ag1 | 89.32(8) | Cr1-01-Ag2 | 129.9(4) |
| Ag6#1-S10-Ag4 | 90.77(4) | Cr1-03-Ag1 | 126.2(3) |
| Ag2-S10-Ag4 | 140.05(10) | 08#2-08-Cr1 | 72.5(14) |
| Ag1-S10-Ag4 | 72.78(7) | 08#2-08-Cr1#2 | 71.9(14) |
| Cr1-08-Cr1#2 | 144.5(6) | | |

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z for **1**; #1 1-x,2-y,-z for **2**; #1 1-x,1-y,-z; #2 -x,1-y,-z for **3**.

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