Chemistry–A European Journal

Supporting Information

Altering Charges on Heterobimetallic Transition-Metal Carbonyl Clusters

Wiebke Unkrig, Konstantin Kloiber, Burkhard Butschke, Daniel Kratzert, and Ingo Krossing*[a]

This PDF file includes:

Figs. S1 to S23 and Tables S1 to S19

Abbreviations

4FB = 1,2,3,4-tetrafluorobenzene, $F_4C_6H_2$

$[Al(OR^F)_4]^- = [Al\{OC(CF_3)_3\}_4]^-$

Compounds

1 $[NEt_4]^+[Ag\{M(CO)_6\}_2]^-$; **1**$^-$ $[Ag\{M(CO)_6\}_2]^-$; M = Nb (**1a**), Ta (**1b**)

2 $[NEt_4]^+[Ag_2\{M(CO)_6\}_3]^-$; **2**$^-$ $[Ag_2\{M(CO)_6\}_3]^-$; M = Nb (**2a**), Ta (**2b**)

3 $[Ag_6\{M(CO)_6\}_5]^+[Al(OR^F)_4]^-$; **3**$^+$ $[Ag_6\{M(CO)_6\}_5]^+$; M = Nb (**3a**)

4 $[Ag_6\{M(CO)_6\}_4]^{2+}[Al(OR^F)_4]^-_2$; **4**$^{2+}$ $[Ag_6\{M(CO)_6\}_4]^{2+}$; M = Nb (**4a**), Ta (**4b**)

Material and Methods

The methods and techniques established in our group were used [1]. Due to minor deviations, however, these were described again in detail here.

Techniques and Instruments

All reactions were carried out in an inert atmosphere using standard vacuum and Schlenk techniques and a glovebox filled with Ar or N_2. Special double-Schlenk flasks [2] separated by a G3 or G4 frit and sealed with grease-free teflon or glass valves were used for most of the manipulations. Pentane was dried using a conventional MBraun Grubbs apparatus, while 1,2,3,4-tetrafluorobenzene ($F_4C_6H_2$, 4FB, Fluorochem) was dried over CaH_2 and distilled afterwards. Besides the general practice, 4FB was stirred for 24h with $Ag[Al(OR^F)_4]$ at room temperature to remove traces of benzene and other fluorobenzenes and condensed subsequently. Consequently, the solvent was contaminated with $HOC(CF_3)_3$, but as the alcohol is formed in low quantity (<<1 %) in each reaction anyway, it had no influence to the reaction. All solvents were degassed before used and stored over molecular sieves (4 Å). $[NEt_4]^+[M(CO)_6]^-$ (M = Nb, Ta) and $Ag[Al(OR^F)_4]$ (commercially available at www.iolitec.de) were synthesized according to literature [3].

Vibrational Spectroscopy

IR spectra (range: 4000-550 cm^{-1}, resolution: 2 cm^{-1}, 64 scans) were recorded in the glovebox on a Bruker ALPHA FT-IR spectrometer equipped with an Eco-ZnSe-ATR module. The ATR attachment of FT-IR spectrometer was precooled prior to the measurements. The Bruker OPUS 7.5.18 software was used to collect, evaluate and edit the vibrational spectra. Unless otherwise noted, the spectra were baseline corrected (default parameters, 1 iteration). All IR spectra were normalized to 1 and intensities are given as follows: vw = very weak (< 0.2), w = weak (< 0.4), m = medium (< 0.6), s = strong (< 0.8), vs = very strong (≥ 0.8), sh = shoulder, br = broad. Graphical representations were visualized with OPUS or OriginPro (version 9.2). Only bands that can be assigned to the desired products, the co-product or solvents were detected. Bands caused by the co-product $[NEt_4]^+[Al(OR^F)_4]^-$ or solvents are given below.

$[NEt_4]^+[Al(OR^F)_4]^-$:

FTIR (ZnSe): ν [cm^{-1}] = 3018 (vw), 3012 (vw), 3000 (vw), 1487 (vw), 1458 (vw), 1444 (vw), 1399 (vw), 1352 (w), 1297 (w), 1272 (s), 1249 (m), 1240 (s), 1209 (vs), 1161 (s), 1068 (vw), 1052 (vw), 998 (vw), 969 (vs), 832 (w), 782 (vw), 756 (vw), 726 (vs), 636 (vw), 571 (vw), 561 (w).

1,2,3,4-$F_4C_6H_2$:

FTIR (ZnSe): ν [cm^{-1}] = 3097 (vw), 2310 (vw), 1845 (vw), 1792 (vw), 1728 (vw), 1633 (vw), 1609 (vw), 1507 (vs), 1438 (vw), 1398 (vw), 1327 (w), 1313 (vw), 1266 (vw), 1236 (m), 1160 (w), 1093 (vw), 1045 (s), 982 (vs), 962 (w), 861 (vw), 800 (m), 745 (m), 729 (vw), 681 (m), 604 (vw), 593 (w).

$[NEt_4][Nb(CO)_6]$:

FTIR (ZnSe): ν [cm^{-1}] = 3865 (vw), 3845 (vw), 3731 (vw), 3696 (vw), 3015 (vw), 2998 (vw), 2984 (vw), 2954 (vw), 1805 (vs), 1520 (vw), 1514 (vw), 1481 (w), 1470 (w), 1450 (w), 1431 (w), 1387 (vw), 1374 (vw), 1363 (vw), 1330 (vw), 1285 (vw), 1278 (vw), 1272 (vw), 1184 (vw), 1169 (w), 1113 (vw), 1092 (vw), 1067 (vw), 1050 (vw), 1016 (vw), 992 (w), 930 (vw), 903 (w), 888 (vw), 850 (vw), 823 (w), 779 (m), 751 (w), 722 (vw), 701 (vw), 690 (vw), 665 (vw), 638 (vw), 632 (vw), 620 (vw).

$[NEt_4][Ta(CO)_6]$:

FTIR (individual baseline correction, ZnSe): ν [cm^{-1}] = 3860 (vw), 3845 (vw), 3779 (vw), 3714 (vw), 3685 (vw), 3015 (vw), 2996 (vw), 2983 (vw), 2954 (vw), 2254 (vw), 2024 (vw), 2017 (vw), 1801 (vs), 1643 (m), 1481 (w), 1469 (w), 1450 (w), 1430 (w), 1386 (w), 1374 (vw), 1363 (w), 1330 (vw), 1268 (vw), 1184 (vw), 1169 (w), 1112 (vw), 1092 (vw), 1066 (vw), 1050 (vw), 992 (m), 949 (vw), 912 (w), 888 (vw), 851 (w), 779 (m), 653 (vw), 639 (vw), 601 (vw), 593 (vw).

Single Crystal X-ray Diffraction

Crystals were grown by layering 1,2,3,4-Tetrafluorobenzene solutions with pentane. The data for all compounds were collected from a shock-cooled single crystal at 100(2) K (compounds **1a**, **b**, **2b**, **3a**, **4a**, **b**) or 200(2) K (compound **2a**) on a Bruker D8 VENTURE dual wavelength Mo/Cu three-circle diffractometer with a microfocus sealed X-ray tube using mirror optics as monochromator and a Bruker PHOTON III detector. The diffractometer was equipped with an Oxford Cryostream 800 low temperature device and used MoK_α radiation (λ = 0.71073 Å). All crystals were selected under perfluoropolyalkylether oil (AB128330, ABCR GmbH & Co. KG) at about –30 °C in a cold nitrogen gas stream using a custom-built low temperature mounting device and mounted on 0.1, 0.2 or 0.3 mm micromounts (M1-L19-100/200/300). All data were integrated with SAINT and a multi-scan absorption correction using SADABS-2016/2 [4] was applied. The structures were solved by direct methods using SHELXT 2018/2 (Sheldrick, 2018) [5,6], and refined by full-matrix least-squares methods against F^2 by SHELXL-2018/3 (Sheldrick, 2018).[6] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their U_{iso} values constrained

to 1.5 times the U_{eq} of their pivot atoms for terminal sp^3 carbon atoms and 1.2 times for all other carbon atoms. Disordered fragments were modeled with the DSR-tool.[7] All graphics of crystal structures were plotted with OLEX2 (version 1.2.10).[8] Crystallographic data (including structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre. (CCDC 1998854 (**1a**), CCDC 1998851 (**2a**), CCDC 1998852 (**2b**), CCDC 1998853 (**3a**), CCDC 1909279 (**4a**), CCDC 1998922 (**4b**) contain the supplementary crystallographic data for this paper. Copies of the data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.

Computational Details

Quantum chemical calculations were performed with the TURBOMOLE [9] (version 7.2) program package. The investigated molecular structures were optimized at the density functional theory (DFT) level and were run in redundant internal coordinates using the BP86 [10] functional with the resolution-of-identity (RI) approximation [11] together with the basis set def2-TZVPP [12] and with dispersion correction (DFT-D3(BJ))[13]. A fine integration grid (m4) and the default SCF convergence criteria (10^{-6} a. u.) were used. All optimized structures were checked for minima and imaginary frequencies with the implemented module AOFORCE [14] and for proper spin occupancies using the implemented module EIGER. Entropic contributions to enthalpy and Gibbs free energy with inclusion of zero point energies (ZPE) were calculated at the BP86-D3(BJ)/def2-TZVPP level for standard conditions with the FREEH module. IR spectra were calculated at the BP86-D3(BJ)/def2-TZVPP level of theory and simulated with an FWHM of 10 cm^{-1}. The AIM [15] analysis was done using the program Multiwfn 3.6 [16], based on a wfn file generated with TURBOMOLE.

Detailed Synthesis of Compounds 1 – 4

The syntheses of compounds **1** to **4** only differ in stoichiometry. Thus, the procedure is exclusively described for **1** in detail. All used quantities for syntheses of compounds **1** to **4** are listed in Table S1.

*Synthesis of **1***: $[NEt_4]^+[Nb(CO)_6]^-$ (0.05 g, 0.128 mmol, 2 eq) and $Ag[Al(OR^F)_4]$ (0.07 g, 0.0649 mmol, 1 eq) were weighed in the glovebox each in one side of a small double-Schlenk flask and dissolved in 4FB (each ca. 1.5 ml). The solution of $Ag[Al(OR^F)_4]$ was transferred to the other side through the frit at –40 °C. The dark red solution was stirred for 30 minutes at –40 °C to –30 °C, layered with cold pentane and crystallized at –30 °C. After 3 days $[NEt_4]^+[Ag\{Nb(CO)_6\}_2]^-$ was obtained as red crystals and the co-product $[NEt_4]^+[Al(OR^F)_4]^-$ as colorless crystals. Due to the sensitivity of the material, no yield can be given.

Table S1. Used quantities of the reactions of **1** – **4**.

	$[NEt_4][M(CO)_6]$			**$Ag[Al(OR^F)_4]$**		
	g	mmol	eq	g	mmol	eq
1a	0.05	0.128	2	0.07	0.0649	1
1b	0.06	0.125	2	0.07	0.0626	1
2a	0.05	0.128	3	0.09	0.0852	2
2b	0.06	0.125	3	0.09	0.0835	2
3a	0.05	0.128	5	0.165	0.153	6
4a	0.06	0.128	4	0.206	0.192	6
4b	0.05	0.125	4	0.168	0.157	6

FTIR (precipitated at 243 K, individual baseline correction, ZnSe):

1a: ν [cm^{-1}] = 3014 (vw), 2986 (vw), 2954 (vw), 2050 (vw), 2024 (m), 1943 (w), 1847 (vs), 1823 (vs), 1521 (vw), 1482 (w), 1452 (vw), 1438 (vw), 1417 (vw), 1392 (vw), 1363 (vw), 1353 (vw), 1297 (vw), 1272 (w), 1249 (w), 1240 (w), 1212 (w), 1170 (w), 1162 (w), 1093 (vw), 1067 (vw), 1051 (vw), 996 (vw), 970 (m), 889 (vw), 889 (vw), 831 (vw), 805 (vw), 781 (w), 756 (vw), 727 (w).

1b: ν [cm^{-1}] = 3014 (vw), 2982 (vw), 2964 (vw), 2953 (vw), 2939 (vw), 2912 (vw), 2890 (vw), 2067 (vw), 2051 (vw), 2024 (s), 1980 (vw), 1954 (w), 1936 (w), 1855 (vs), 1822 (vs), 1520 (vw), 1513 (vw), 1482 (vw), 1452 (vw), 1438 (vw), 1416 (vw), 1398 (vw), 1391 (vw), 1352 (vw), 1297 (vw), 1272 (w), 1250 (w), 1240 (w), 1213 (m), 1161 (w), 1092 (vw), 1067 (vw), 1051 (vw), 996 (vw), 971 (s), 910 (vw), 899 (vw), 851 (vw), 831 (vw), 802 (vw), 781 (w), 756 (vw), 727 (m), 682 (vw).

2a: ν [cm^{-1}] = 3018 (vw), 2992 (vw), 2955 (vw), 2067 (vw), 2049 (vw), 2025 (s), 1947 (w), 1858 (vs), 1520 (vw), 1512 (vw), 1483 (vw), 1457 (vw), 1439 (vw), 1418 (vw), 1398 (vw), 1392 (vw), 1352 (vw), 1297 (w), 1272 (m), 1251 (w), 1239 (m), 1212 (vs), 1161 (m), 1067 (vw), 1046 (vw), 997 (vw), 970 (vs), 888 (vw), 831 (vw), 804 (vw), 781 (vw), 756 (vw), 745 (vw), 727 (s), 682 (vw).

2b: ν [cm^{-1}] = 2983 (vw), 2965 (vw), 2920 (vw), 2851 (vw), 2066 (w), 2032 (s), 1947 (w), 1873 (vs), 1842 (vs), 1520 (vw), 1511 (vw), 1483 (w), 1455 (vw), 1441 (vw), 1417 (vw), 1392 (vw), 1352 (vw), 1298 (w), 1272 (m), 1255 (m), 1240 (m), 1214 (vs), 1171 (w), 1162 (m), 1067 (vw), 1046 (vw), 998 (vw), 971 (vs), 904 (vw), 892 (vw), 831 (vw), 802 (vw), 781 (vw), 756 (vw), 745 (vw), 727 (vs), 682 (vw), 636 (vw), 571 (vw), 561 (vw).

3a: ν [cm^{-1}] = 3097 (vw), 3017 (vw), 2168 (vw), 2090 (vw), 2064 (vw), 2046 (vw), 2003 (vw), 1945 (vw), 1633 (vw), 1486 (vw), 1458 (vw), 1444 (vw), 1398 (vw), 1352 (vw), 1327 (vw), 1297 (w), 1271 (m), 1265 (m), 1238 (m), 1206 (vs), 1172 (m), 1159 (m), 1068 (vw), 1046 (vw), 998 (vw), 967 (vs), 864 (vw), 831 (vw), 803 (vw), 781 (vw), 756 (vw), 745 (vw), 725 (vs), 682 (vw), 645 (vw), 603 (vw), 593 (vw), 571 (vw), 560 (vw).

4a: ν [cm^{-1}] = 2965 (vw), 2946 (vw), 2110 (w), 2091 (w), 2077 (w), 1962 (vw), 1931 (w), 1886 (vw), 1745 (vw), 1635 (vw), 1523 (vw), 1507 (vw), 1486 (vw), 1458 (vw), 1444 (vw), 1398 (vw), 1352 (vw), 1326 (vw), 1297 (w), 1273 (m), 1240 (s), 1212 (vs), 1161 (m), 1068 (vw), 1044 (vw), 998 (vw), 970 (vs), 831 (vw), 805 (vw), 782 (vw), 756 (vw), 743 (vw), 727 (vs), 682 (vw), 602 (vw), 592 (vw), 571 (vw), 560 (vw).

4b: ν [cm^{-1}] = 2972 (vw), 2965 (vw), 2880 (vw), 2106 (w), 2081 (w), 2081 (w), 2067 (w), 1928 (w), 1632 (vw), 1522 (vw), 1507 (vw), 1486 (vw), 1458 (vw), 1444 (vw), 1398 (vw), 1352 (vw), 1326 (vw), 1297 (w), 1273 (m), 1240 (s), 1213 (vs), 1161 (m), 1068 (vw), 1044 (vw), 998 (vw), 971 (vs), 831 (vw), 805 (vw), 781 (vw), 756 (vw), 743 (vw), 727 (vs), 682 (vw), 602 (vw), 591 (vw), 571 (vw), 560 (vw).

Vibrational Analysis

Full IR spectra of **1**, **2**, **3**, **4**, $[NEt_4][Nb(CO)_6]$ and $[NEt_4][Al(OR^F)_4]$

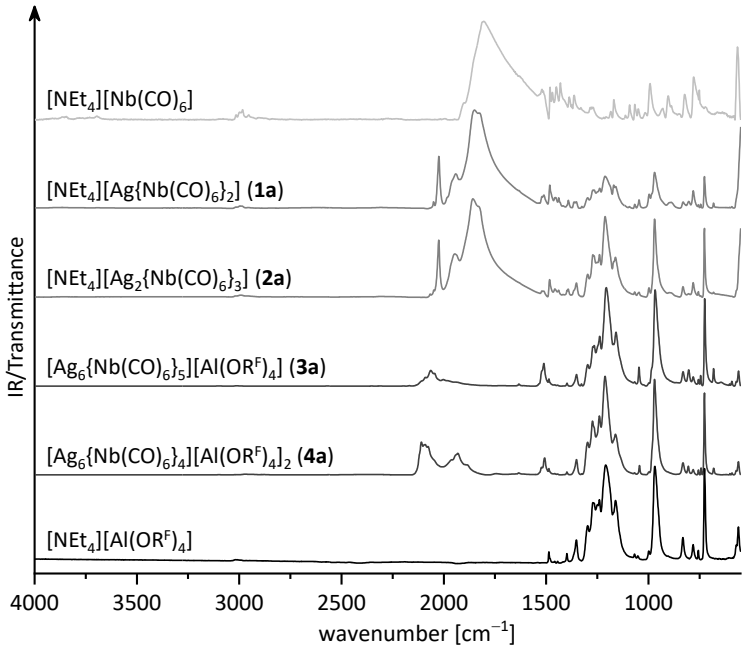


Fig. S1. Experimental IR spectra of the starting material $[NEt_4][Nb(CO)_6]$, **1a**, **2a**, **4a** and the co product $[NEt_4]^+[Al(OR^F)_4]^-$.

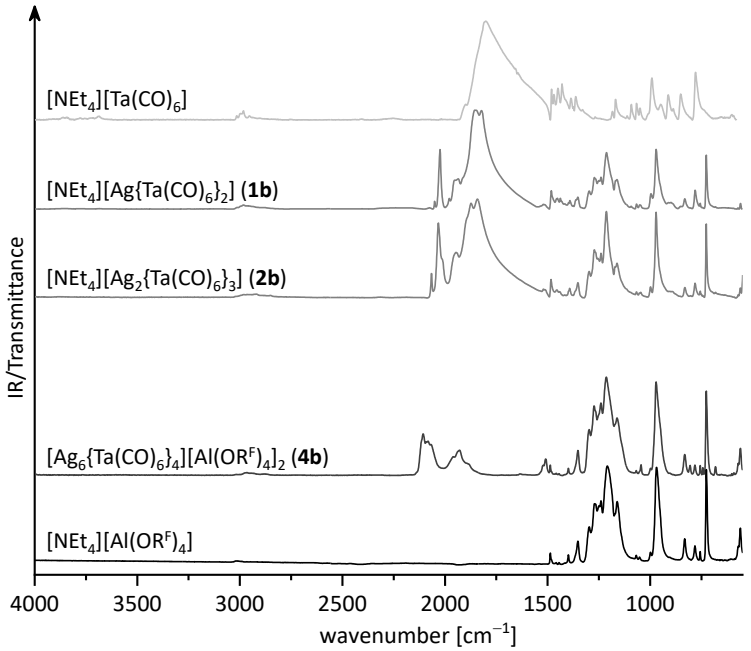


Fig. S2. Experimental IR spectra of the starting material $[NEt_4][Ta(CO)_6]$, **1b**, **2b**, **4b** and the co product $[NEt_4]^+[Al(OR^F)_4]^-$.

Table S2. Experimental IR data in the ν(CO) [cm^{-1}] range of **1ab**, **2ab**, **3a** and **4ab**. The relative intensities refer only to the CO vibration range. Thus, the most intensive CO band was set to 100%.

1a	**1b**	**2a**	**2b**	**3a**	**4a**	**4b**
				2168 (vw)	2110 (vs)	
						2106 (vs)
				2090 (m)	2091 (vs)	
					2077 (vs)	2081 (vs)
	2067 (vw)	2067 (vw)	2066 (w)	2064 (vs)		2067 (vs)
2050 (vw)	2051 (vw)	2049 (vw)		2046 (w)		
2024 (m)	2024 (s)	2025 (s)	2032 (s)			
				2003 (w)		
	1980 (vw)					
	1954 (w)				1962 (m)	
1943 (w)	1936 (w)	1947 (w)	1947 (w)	1945 (vw)	1931 (s)	1928 (s)
			1873 (vs)	1890 (vw)	1886 (w)	
1847 (vs)	1855 (vs)	1858 (vs)	1842 (vs)			
1823 (vs)	1822 (vs)					
					1745 (vw)	
				1633 (vw)	1635 (vw)	1632 (vw)

Table S3. Experimental and calculated (* BP86-D3(BJ)/def2-TZVPP) IR data in the ν(CO) [cm^{-1}] range of **1a** and **b**. The relative intensities refer only to the CO vibration range. Thus, the most intensive CO band was set to 100%. [a] An imaginary frequency of –3.12 cm^{-1} was obtained. [b] Imaginary frequencies of –15.07 cm^{-1} were obtained.

1a	**1a calc. (C_2) *[a]**	**1b**	**1b calc. (D_{3d})*[b]**
	2032 (a, 0%)		
	2008 (b, 58%)		2007 (a_{2u}, 62 %)
	1943 (b, 31%)	2067 (vw)	1935 (e_u, 44 %)
2050 (vw)	1943 (a, 10%)	2051 (vw)	
2024 (m)	1939 (a, 1%)	2024 (s)	
	1938 (b, 38%)	1980 (vw)	
	1928 (a, 100%)		
	1924 (b, 62%)	1954 (w)	1915 (e_u, 83 %)
1943 (w)	1901 (b, 35%)	1936 (w)	1901 (a_{2u}, 100 %)
1847 (vs)	1895 (a, 1%)	1855 (vs)	
1823 (vs)	1889 (b, 47%)	1822 (vs)	
	1880 (a, 8%)		

Table S4. Experimental and calculated (* BP86-D3(BJ)/def2-TZVPP) IR data in the ν(CO) [cm^{-1}] range of **2a** and **b**. The relative intensities refer only to the CO vibration range. Thus, the most intensive CO band was set to 100%.

2a	**2a calc. (C_2)***	**2b**	**2b calc. (C_2)***
2067 (vw)	2044 (a, 0%)	2066 (w)	2043 (a, 0%)
2049 (vw)	2023 (b, 40%)		2021 (b, 40%)
2025 (s)	2015 (a, 100%)	2032 (s)	2014 (a, 100%)
	1959 (b, 61%)		1955 (b, 62%)
	1958 (a, 4%)		1955 (a, 4%)
	1957 (b, 1%)		1954 (b, 0%)
	1957 (a, 25%)		1953 (a, 24%)
	1950 (b, 95%)		1947 (b, 80%)
1947 (w)	1949 (a, 2%)	1947 (w)	1946 (a, 3%)
	1948 (b, 17%)		1944 (b, 30%)
	1932 (b, 73%)		1928 (b, 71%)
	1927 (a, 12%)		1924 (a, 10%)
	1915 (b, 79%)		1911 (b, 81%)
	1912 (a, 46%)		1908 (a, 40%)
	1905 (a, 19%)		1902 (a, 29%)
	1902 (a, 7%)		1899 (a, 2%)
	1900 (b, 21%)	1873 (vs)	1897 (b, 17%)
1858 (vs)	1891 (b, 5%)	1842 (vs)	1887 (b, 6%)

Table S5. Experimental and calculated (* BP86-D3(BJ)/def2-TZVPP) IR data in the ν(CO) [cm^{-1}]range of **3a**. The relative intensities refer only to the CO vibration range. Thus, the most intensive CO band was set to 100%.

3a	**3a calc. (C_{3h})***
2168 (vw)	2075 (a'', 100%)
2090 (m)	2068 (e', 75%)
	2041 (e', 18%)
2064 (vs)	2033 (e', 5%)
2046 (s)	2010 (a'', 28%)
2003 (w)	1965 (e', 27%)
1945 (vw)	1951 (a'', 1%)
	1936 (a'', 26)
	1929 (e', 9%)
	1902 (e', 8%)
1890 (vw)	
1633 (vw)	

Table S6. Experimental and calculated (* BP86-D3(BJ)/def2-TZVPP) IR data in the ν(CO) [cm^{-1}] range of **4a** and **b**. The relative intensities refer only to the CO vibration range. Thus, the most intensive CO band was set to 100%.

4a	**4a calc. (*T*)***	**4b**	**4b calc. (*T*)***
2110 (vs)			
2091 (vs)	2096 (t, 100 %)	2106 (vs)	2093 (t, 100%)
2077 (vs)	2073 (t, 33 %)	2081 (vs)	2068 (t, 33%)
1962 (m)	2070 (t, 0 %)	2067 (vs)	2064 (t, 0%)
1931 (s)	1953 (t, 23 %)	1928 (s)	1949 (t, 21%)
1886 (w)	1935 (t, 13 %)		1931 (t, 13%)
1745 (vw)	1914 (t, 1 %)		1911 (t, 1%)
1635 (vw)		1632 (vw)	

Details of the AIM Analysis

Table S7. Calculated charges located at the niobium/tantalum atoms of complexes **1**, **2**, **3** and **4**.

	M:Ag	hapticity	Nb	Ta
$M(CO)_6^-$_O_h			1.53	1.69
AgM2_C_2/D_{3d}	2	μ_1	1.57	1.71
Ag2M3_C_2	1.5	μ_1	1.58	1.72
		μ_2	1.58	1.71
Ag6M5_C_{3h}	0.8	μ_2	1.59	-
		μ_3	1.59	-
Ag6M4_T	0.7	μ_3	1.58	1.72

Table S8. Calculated charges located at the silver atoms of complexes **1**, **2**, **3** and **4**.

	M:Ag	Nb	Ta
AgM2_C_2/D_{3d}	2	0.22	0.18
Ag2M3_C_2	1.5	0.17	0.15
Ag6M5_C_{3h}	0.8	0.11	-
Ag6M4_T	0.7	0.14	0.13

Table S9. Calculated charges located at the $[M(CO)_6]$ fragments of complexes **1**, **2**, **3** and **4**.

	M:Ag	hapticity	Nb	Ta
AgM2_C_2/D_{3d}	2	μ_1	-0.61	-0.59
Ag2M3_C_2	1.5	μ_1	-0.49	-0.49
		μ_2	-0.34	-0.33
Ag6M5_C_{3h}	0.8	μ_2	0.03	-
		μ_3	0.14	-
Ag6M4_T	0.7	μ_3	0.28	0.31

Table S10. Calculated averaged charges located at the CO ligands of complexes **1**, **2**, **3** and **4**.

	hapticity		Nb	Ta
M(CO)$_6^-$_*O*$_h$			-2.53	-2.69
AgM2_*C*$_2$/*D*$_{3d}$	μ_1	CO_{Ag}	-0.39	-0.20
		$CO_{terminal}$	-0.35	-0.18
Ag2M3_*C*$_2$	μ_1	CO_{Ag}	-0.38	-0.40
		$CO_{terminal}$	-0.31	-0.33
	μ_2	CO_{Ag}	-0.33	-0.35
		$CO_{terminal}$	-0.29	-0.31
Ag6M5_*C*$_{3h}$	μ_2	CO_{Ag}	-0.33	-
		$CO_{terminal}$	-0.20	-
	μ_3	CO_{Ag}	-0.33	-
		$CO_{terminal}$	-0.16	-
Ag6M4_*T*	μ_3	CO_{Ag}	-0.33	-0.35
		$CO_{terminal}$	-0.11	-0.12

Table S11. Overview of calculated averaged charges of the complexes **1** – **4**.

			δ_M		δ_{Ag}		$\delta_{M(CO)6}$		δ_{COAg}	δ_{COterm}	δ_{COAg}	δ_{COterm}
	M:Ag	**hapticity**	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**		**Ta**	
*			1.53	1.69					-2.53		-2.69	
1	2	μ_1	1.57	1.71	0.22	0.18	-0.61	-0.59	-0.39	-0.35	-0.20	-0.18
2	1.5	μ_1	1.58	1.72	0.17	0.15	-0.49	-0.49	-0.38	-0.31	-0.40	-0.33
		μ_2	1.58	1.71			-0.34	-0.33	-0.33	-0.29	-0.35	-0.31
3	0.8	μ_2	1.59	-	0.11	-	0.03	-	-0.33	-0.20	-	-
		μ_3	1.59	-			0.14	-	-0.33	-0.16	-	-
4	0.7	μ_3	1.58	1.72	0.14	0.13	0.28	0.31	-0.33	-0.11	-0.35	-0.12

* $[M(CO)_6]^-$.

Examples for the calculation of the electron transfer from $[Nb(CO)_6]$ to Ag_6:

Calculation for $\mathbf{3}^{+}$:

$\delta_{CO}(\mathbf{3}^{+}) = \delta_{CO}(\mu_3) * 2 + \delta_{CO}(\mu_2) * 3 = -1.47 * 2 + (-1.59 * 3) = -7.71$

$\delta_{CO}(\mathbf{[Nb(CO)_6]}) = -2.53 * 5 = -12.65$

Transferred electrons: $\delta_{CO}(\mathbf{3}^{+}) - \delta_{CO}(\mathbf{[Nb(CO)_6]}) = -7.71 - (-12.65) = \mathbf{4.94}$

Calculation for $\mathbf{4a}^{2+}$:

$\delta_{CO}(\mathbf{4a}^{2+}) = \delta_{CO}(\mu_3) * 4 = -1.32 * 4 = -5.28$

$\delta_{CO}(\mathbf{[Nb(CO)_6]}) = -2.53 * 4 = -10.12$

Transferred electrons: $\delta_{CO}(\mathbf{4a}^{2+}) - \delta_{CO}(\mathbf{[Nb(CO)_6]}) = -5.28 - (-10.12) = \mathbf{4.84}$

Table S12. Average values of the electron density [eÅ^{-3}] at bond critical points of the complexes **1** – **4**.

	bcp	**Ag-Ag**		**Ag-M**		**Ag-C**		**M-C**		**C-O$_{Ag}$**		**C-O$_{terminal}$**	
	M =	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**	**Ta**	**Nb**	**Ta**
M(CO)$_6^-$_*O*$_h$		-	-	-	-	-	-	0.62	0.65	-	-	3.09	3.08
AgM2_*C*$_2$/*D*$_{3d}$	μ_1	-	-	0.26	0.28	0.34	0.26	0.63	0.64	3.11	3.11	3.15	3.16
Ag2M3_*C*$_2$	μ_1	0.25	0.26	0.29	0.30	0.26	0.26	0.62	0.65	3.12	3.11	3.16	3.16
	μ_2			*	*	0.42	0.41	0.63	0.65	3.12	3.11	3.16	3.16
Ag6M5_*C*$_{3h}$	μ_2	0.24	-	0.25	-	0.31	-	0.61	-	3.17	-	3.26	-
	μ_3		-	0.22	-	0.26	-	0.63	-	3.16	-	3.27	-
Ag6M4_*T*	μ_3	0.21	0.21	*	*	0.35	0.34	0.60	0.64	3.16	3.15	3.31	3.30

* No bond critical point was found on this interaction line.

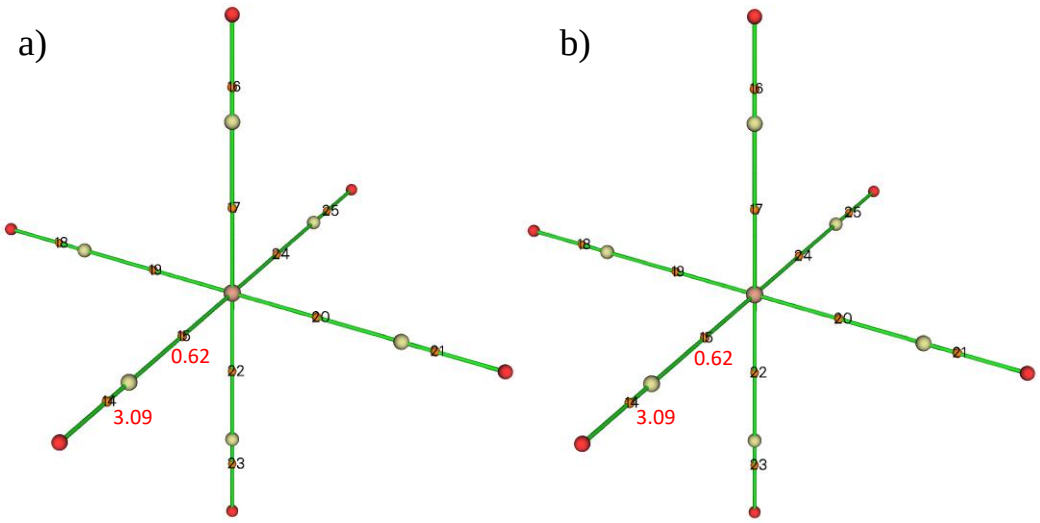


Fig. S3. Electron density [eÅ^{-3}] at bond critical points of the starting materials $[M(CO)_6]^-$ (M = Nb (a), Ta (b)).

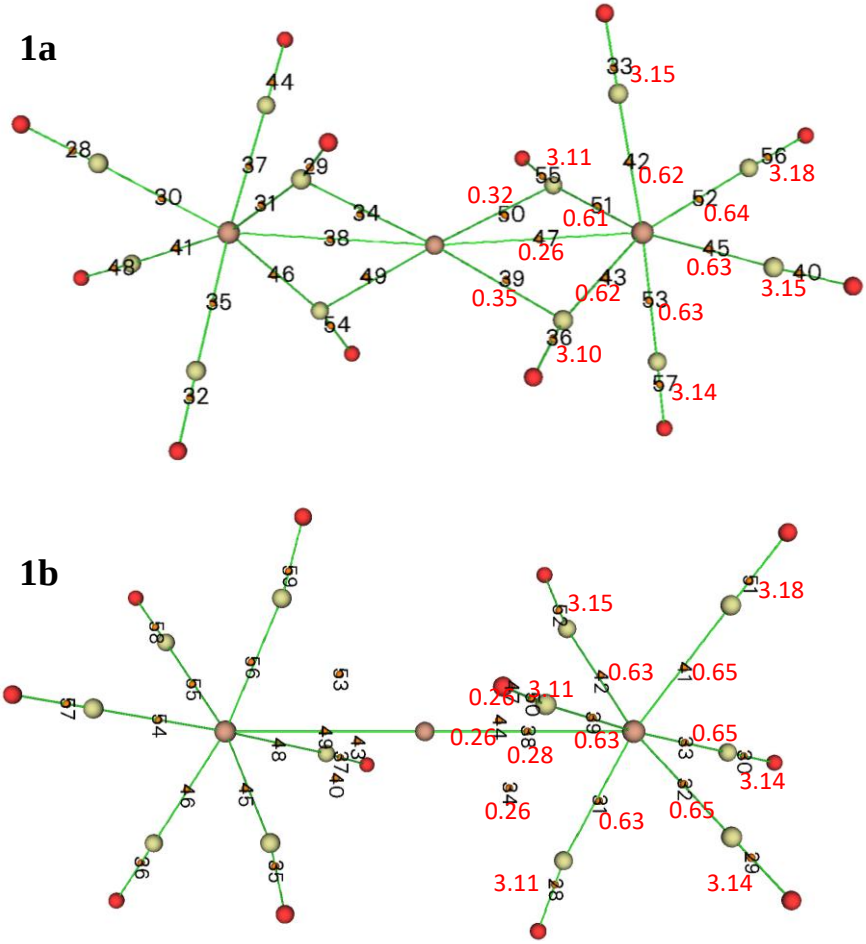


Fig. S4. Electron density [eÅ^{-3}] at bond critical points of **1a** and **b**.

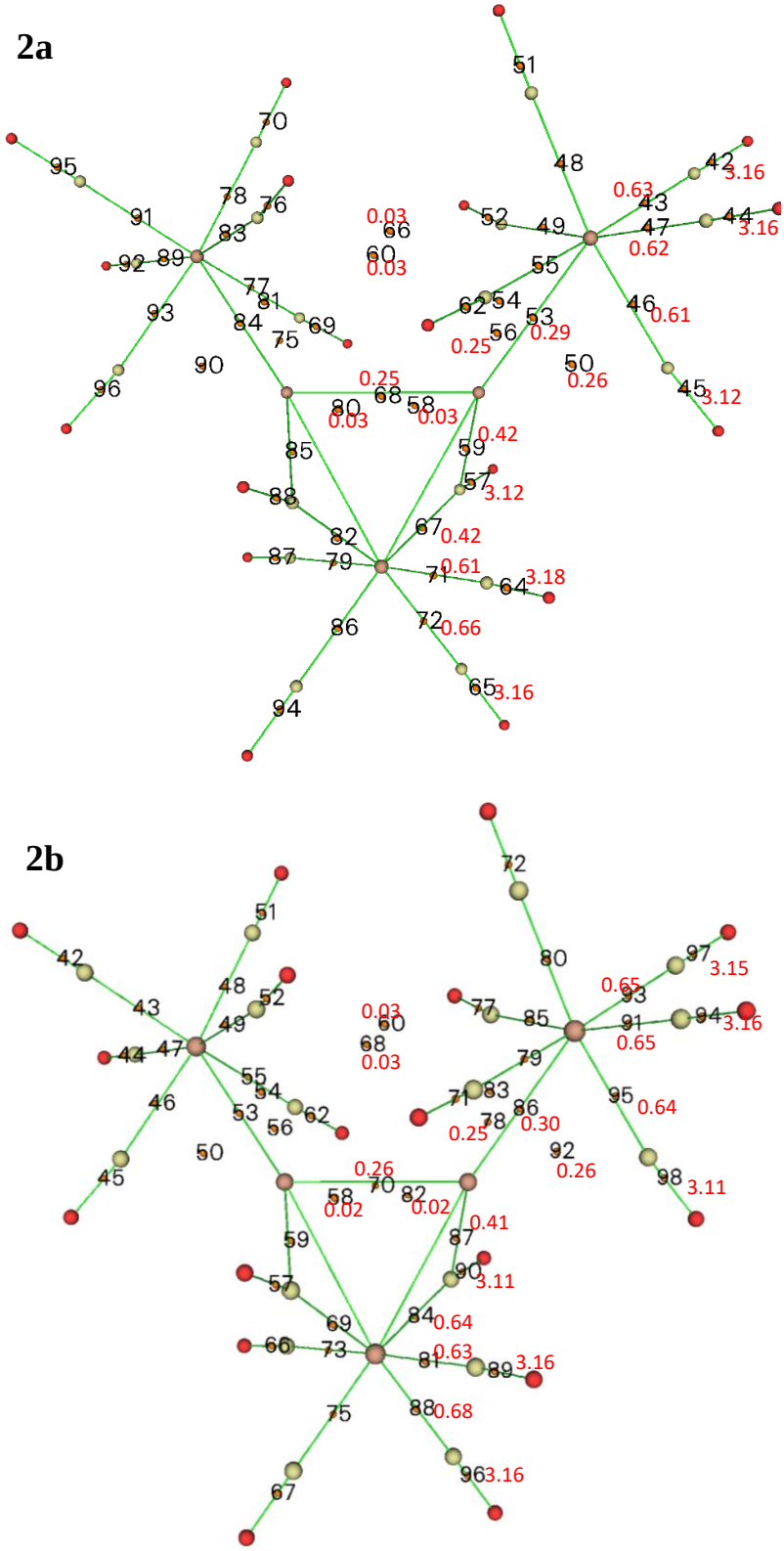


Fig. S5. Electron density [eÅ^{-3}] at bond critical points of **2a** and **b**.

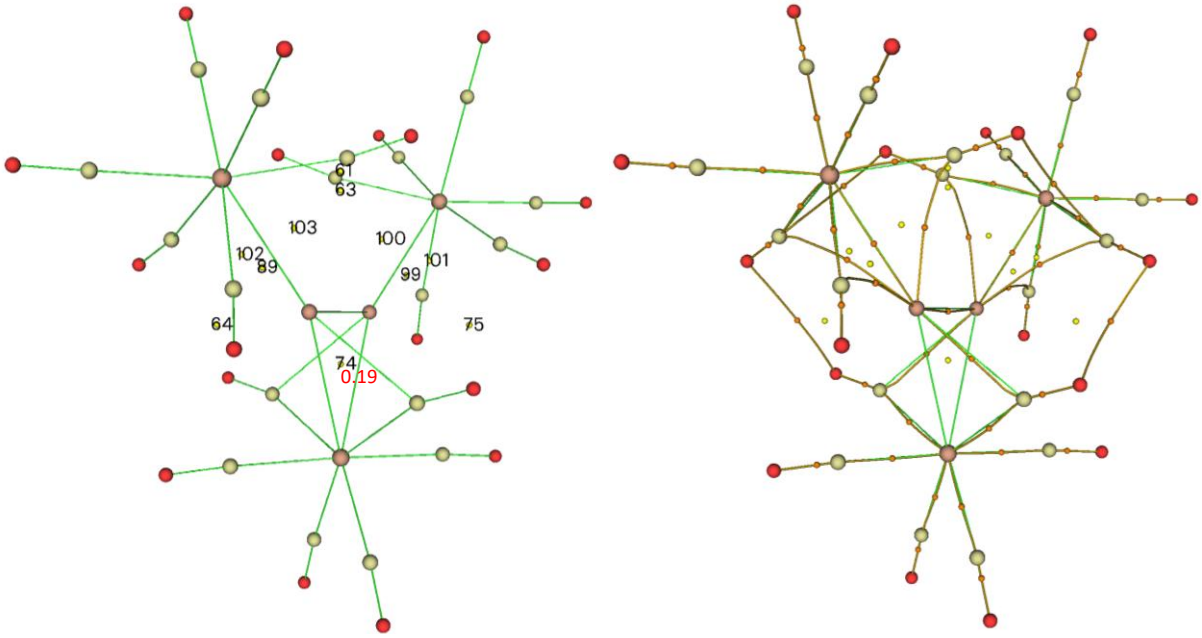
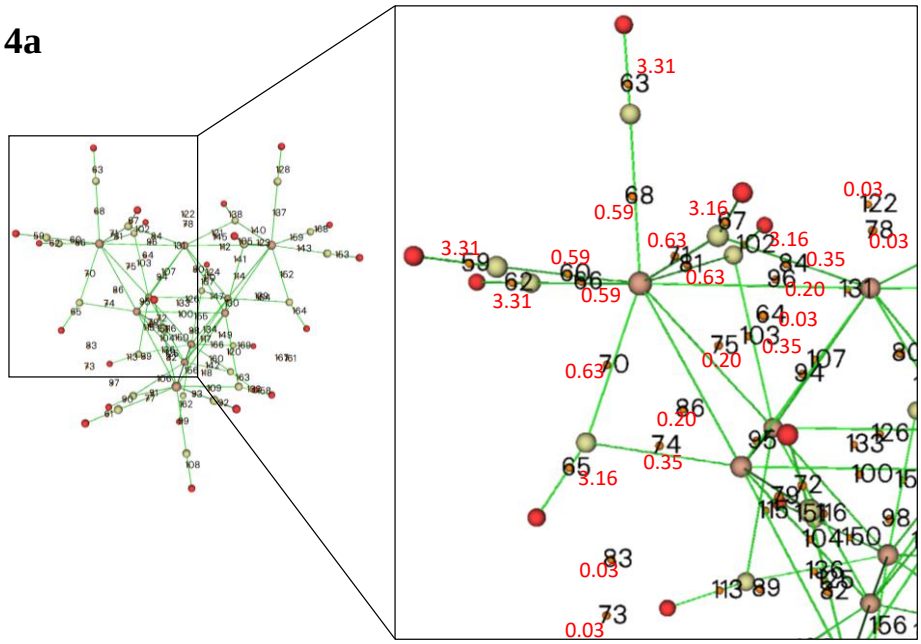


Fig. S6. Electron density [eÅ^{-3}] at ring critical point and connecting path of bond critical points of **2a**.



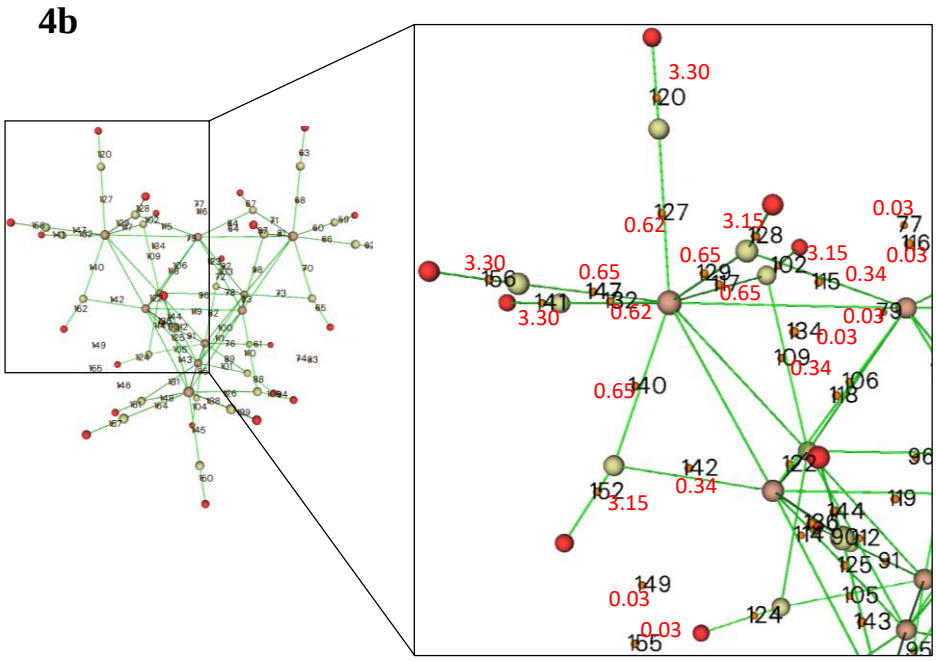
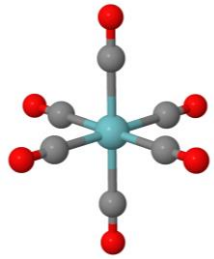


Fig. S7. Electron density [eÅ^{-3}] at bond critical points of **4a** and **b**.

Computational Details to the Structure Determination

All structures were optimized at the (RI-)BP86-D3BJ/def-TZVPP level of theory.

Calculated Structure of $Nb(CO)_6$ (O_h)



Symmetry: oh
Method: (RI-)b-p/def2-TZVPP

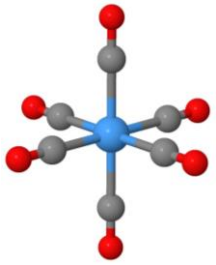
Nb	0.00000	0.00000	0.00000
C	-2.12125	-0.00000	0.00000
C	2.12125	0.00000	-0.00000
C	-0.00000	-0.00000	-2.12125
C	0.00000	-2.12125	0.00000
C	0.00000	0.00000	2.12125
C	-0.00000	2.12125	0.00000
O	-0.00000	0.00000	3.28863
O	-0.00000	3.28863	0.00000
O	3.28863	0.00000	-0.00000
O	0.00000	-0.00000	-3.28863
O	0.00000	-3.28863	0.00000
O	-3.28863	-0.00000	0.00000

SCF energy GEOOPT = -737.6545788163 H
ZPE = 118.5 kJ/mol
FREEH energy = 158.85 kJ/mol
FREEH entropy = 0.52945 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	t2u	36.72	0.00000	NO	NO
8	t2u	36.72	0.00000	NO	NO
9	t2u	36.72	0.00000	NO	NO
10	t1u	59.30	0.58573	YES	NO
11	t1u	59.30	0.58573	YES	NO
12	t1u	59.30	0.58573	YES	NO
13	t2g	64.87	0.00000	NO	YES
14	t2g	64.87	0.00000	NO	YES
15	t2g	64.87	0.00000	NO	YES
16	t1g	333.41	0.00000	NO	NO
17	t1g	333.41	0.00000	NO	NO
18	t1g	333.41	0.00000	NO	NO
19	eg	382.52	0.00000	NO	YES
20	eg	382.52	0.00000	NO	YES
21	a1g	391.16	0.00000	NO	YES
22	t1u	392.76	17.87460	YES	NO
23	t1u	392.76	17.87460	YES	NO
24	t1u	392.76	17.87460	YES	NO
25	t2g	445.96	0.00000	NO	YES
26	t2g	445.96	0.00000	NO	YES
27	t2g	445.96	0.00000	NO	YES
28	t2u	493.84	0.00000	NO	NO
29	t2u	493.84	0.00000	NO	NO
30	t2u	493.84	0.00000	NO	NO
31	t1u	579.03	63.86825	YES	NO
32	t1u	579.03	63.86825	YES	NO
33	t1u	579.03	63.86825	YES	NO
34	t1u	1881.16	2516.98749	YES	NO
35	t1u	1881.16	2516.98749	YES	NO
36	t1u	1881.16	2516.98749	YES	NO
37	eg	1897.73	0.00000	NO	YES
38	eg	1897.73	0.00000	NO	YES
39	a1g	2007.05	0.00000	NO	YES

Calculated Structure of $Ta(CO)_6$ (O_h)



Symmetry: oh
Method: (RI-)b-p/def2-TZVPP

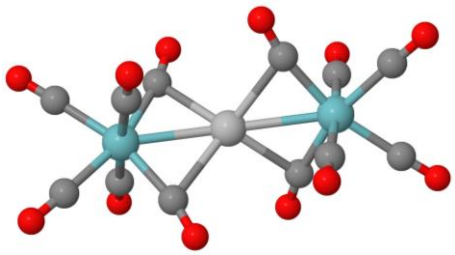
Ta	0.00000	0.00000	-0.00000
C	-2.12436	-0.00000	-0.00000
C	2.12436	0.00000	0.00000
C	-0.00000	-0.00000	-2.12436
C	0.00000	-2.12436	-0.00000
C	0.00000	0.00000	2.12436
C	-0.00000	2.12436	0.00000
O	-0.00000	0.00000	3.29283
O	-0.00000	3.29283	-0.00000
O	3.29283	0.00000	0.00000
O	0.00000	-0.00000	-3.29283
O	0.00000	-3.29283	0.00000
O	-3.29283	-0.00000	-0.00000

SCF energy GEOOPT = -737.7018863041 H
ZPE = 118.1 kJ/mol
FREEH energy = 158.48 kJ/mol
FREEH entropy = 0.53370 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	t2u	36.38	0.00000	NO	NO
8	t2u	36.38	0.00000	NO	NO
9	t2u	36.38	0.00000	NO	NO
10	t1u	57.46	0.95349	YES	NO
11	t1u	57.46	0.95349	YES	NO
12	t1u	57.46	0.95349	YES	NO
13	t2g	66.94	0.00000	NO	YES
14	t2g	66.94	0.00000	NO	YES
15	t2g	66.94	0.00000	NO	YES
16	t1g	343.57	0.00000	NO	NO
17	t1g	343.57	0.00000	NO	NO
18	t1g	343.57	0.00000	NO	NO
19	t1u	378.08	17.19927	YES	NO
20	t1u	378.08	17.19927	YES	NO
21	t1u	378.08	17.19927	YES	NO
22	eg	394.74	0.00000	NO	YES
23	eg	394.74	0.00000	NO	YES
24	a1g	403.83	0.00000	NO	YES
25	t2g	437.70	0.00000	NO	YES
26	t2g	437.70	0.00000	NO	YES
27	t2g	437.70	0.00000	NO	YES
28	t2u	496.47	0.00000	NO	NO
29	t2u	496.47	0.00000	NO	NO
30	t2u	496.47	0.00000	NO	NO
31	t1u	554.73	40.72341	YES	NO
32	t1u	554.73	40.72341	YES	NO
33	t1u	554.73	40.72341	YES	NO
34	t1u	1879.19	2523.16473	YES	NO
35	t1u	1879.19	2523.16473	YES	NO
36	t1u	1879.19	2523.16473	YES	NO
37	eg	1895.87	0.00000	NO	YES
38	eg	1895.87	0.00000	NO	YES
39	a1g	2006.60	0.00000	NO	YES

Calculated Structure of $[Ag\{Nb(CO)_6\}_2]^-$ (C_2)



Symmetry: c2
Method: (RI-)b-p/def2-TZVPP

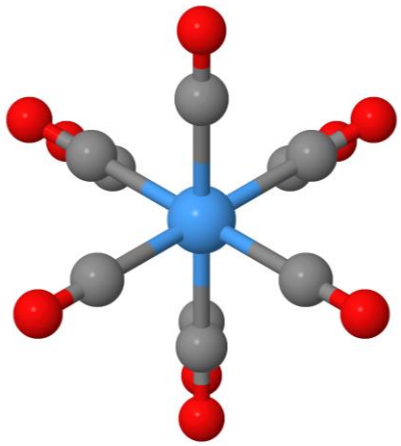
Ag	0.00000	-0.00000	-0.16825
O	0.84474	2.76511	1.11659
C	1.41627	1.84392	0.68760
Nb	2.80218	0.36410	0.00318
Nb	-2.80218	-0.36410	0.00318
O	5.00447	2.35592	1.40135
C	4.20932	1.66504	0.91719
O	5.54076	-1.31517	-0.66800
C	4.56134	-0.73649	-0.44385
C	2.93632	1.44577	-1.81927
O	3.00061	2.03588	-2.81702
C	1.89268	-1.20937	-1.12444
O	1.62164	-2.12380	-1.79750
O	2.43816	-1.31429	2.80969
C	2.56275	-0.72387	1.81860
O	-1.62164	2.12380	-1.79750
C	-1.89268	1.20937	-1.12444
O	-2.43816	1.31429	2.80969
C	-2.56275	0.72387	1.81860
C	-4.56134	0.73649	-0.44385
O	-5.54076	1.31517	-0.66800
C	-4.20932	-1.66504	0.91719
O	-5.00447	-2.35592	1.40135
C	-2.93632	-1.44577	-1.81927
O	-3.00061	-2.03588	-2.81702
C	-1.41627	-1.84392	0.68760
O	-0.84474	-2.76511	1.11659

SCF energy GEOOPT = -1622.440919816 H
ZPE = 241.8 kJ/mol
FREEH energy = 331.53 kJ/mol
FREEH entropy = 0.98944 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-3.12	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	b	9.44	0.00736	YES	YES
9	a	9.60	0.00021	YES	YES
10	b	17.50	0.02759	YES	YES
11	a	20.65	0.01415	YES	YES
12	b	22.85	0.03641	YES	YES
13	a	28.49	0.22164	YES	YES
14	a	35.55	0.00472	YES	YES
15	b	39.02	0.08162	YES	YES
16	a	50.50	0.02987	YES	YES
17	b	54.12	0.23035	YES	YES
18	a	60.82	0.05690	YES	YES
19	a	61.16	0.47398	YES	YES
20	b	61.95	1.16599	YES	YES
21	a	64.92	0.79411	YES	YES
22	b	64.94	0.37208	YES	YES
23	b	66.79	0.02486	YES	YES
24	a	67.29	0.00174	YES	YES
25	b	68.93	0.37696	YES	YES
26	a	71.13	0.02341	YES	YES
27	b	72.02	0.80901	YES	YES
28	a	93.12	0.25800	YES	YES
29	a	97.95	0.01945	YES	YES
30	b	106.41	0.42804	YES	YES
31	b	115.86	0.50598	YES	YES
32	a	122.55	0.00157	YES	YES
33	b	167.57	5.78259	YES	YES
34	a	332.28	0.11050	YES	YES
35	b	334.07	0.22343	YES	YES
36	a	336.09	0.02317	YES	YES
37	b	336.27	0.08779	YES	YES
38	a	337.16	0.01037	YES	YES
39	b	337.18	0.08623	YES	YES
40	a	353.97	0.05354	YES	YES
41	b	356.20	1.35673	YES	YES
42	a	372.92	2.62179	YES	YES
43	b	372.95	4.70693	YES	YES
44	b	381.53	3.47949	YES	YES
45	a	381.60	4.99167	YES	YES
46	b	386.40	7.35871	YES	YES
47	a	386.62	19.96736	YES	YES
48	b	398.09	46.86708	YES	YES
49	a	399.62	0.15308	YES	YES
50	a	407.40	6.50188	YES	YES
51	b	408.44	15.02753	YES	YES
52	b	443.59	0.09197	YES	YES
53	a	443.66	0.01912	YES	YES
54	a	444.69	0.04585	YES	YES
55	b	444.91	0.13343	YES	YES
56	b	457.09	3.93669	YES	YES
57	a	459.69	0.00631	YES	YES
58	b	460.42	1.35243	YES	YES
59	a	463.81	0.10683	YES	YES
60	b	478.98	33.14539	YES	YES
61	a	479.80	0.17870	YES	YES
62	a	484.99	0.01909	YES	YES
63	b	485.31	0.17724	YES	YES
64	b	557.55	311.36664	YES	YES
65	a	563.22	9.03205	YES	YES
66	a	563.61	11.34863	YES	YES
67	b	564.50	59.44273	YES	YES
68	b	565.48	37.36421	YES	YES
69	a	566.44	74.25832	YES	YES
70	a	1880.18	256.20372	YES	YES
71	b	1888.85	1504.07520	YES	YES
72	a	1894.72	20.58223	YES	YES
73	b	1900.80	1105.05238	YES	YES
74	b	1924.35	1989.13412	YES	YES
75	a	1928.04	3198.11844	YES	YES
76	b	1938.40	1230.15007	YES	YES
77	a	1938.98	18.15382	YES	YES
78	a	1943.26	311.00963	YES	YES
79	b	1943.40	1004.43986	YES	YES
80	b	2008.05	1867.00542	YES	YES
81	a	2032.49	6.18270	YES	YES

Calculated Structure of $[Ag\{Ta(CO)_6\}_2]^-$ (D_{3d})



Symmetry: d3d
Method: (RI-)b-p/def2-TZVPP

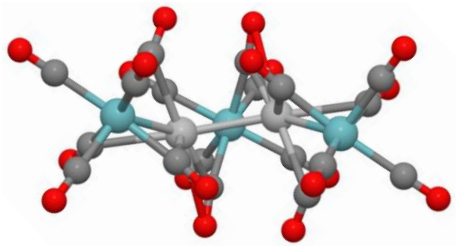
Ag	0.00000	0.00000	0.00000
O	2.59700	1.49938	1.44039
C	1.64631	0.95050	1.83011
Ta	-0.00000	0.00000	2.81777
Ta	-0.00000	-0.00000	-2.81777
O	-0.00000	2.65083	4.76387
C	0.00000	1.71810	4.07245
O	-2.29568	-1.32541	4.76387
C	-1.48792	-0.85905	4.07245
C	1.48792	-0.85905	4.07245
O	2.29568	-1.32541	4.76387
C	0.00000	-1.90100	1.83011
O	0.00000	-2.99876	1.44039
O	-2.59700	1.49938	1.44039
C	-1.64631	0.95050	1.83011
O	2.59700	-1.49938	-1.44039
C	1.64631	-0.95050	-1.83011
O	0.00000	2.99876	-1.44039
C	0.00000	1.90100	-1.83011
C	1.48792	0.85905	-4.07245
O	2.29568	1.32541	-4.76387
C	-1.48792	0.85905	-4.07245
O	-2.29568	1.32541	-4.76387
C	0.00000	-1.71810	-4.07245
O	-0.00000	-2.65083	-4.76387
C	-1.64631	-0.95050	-1.83011
O	-2.59700	-1.49938	-1.44039

SCF energy GEOOPT = -1622.533459927 H

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	eu	-15.07	0.00000	YES	NO
2	eu	-15.07	0.00000	YES	NO
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8		0.00	0.00000	-	-
9	eg	10.83	0.00000	NO	YES
10	eg	10.83	0.00000	NO	YES
11	a1u	11.82	0.00000	NO	NO
12	eu	14.34	0.03723	YES	NO
13	eu	14.34	0.03723	YES	NO
14	a2g	45.12	0.00000	NO	NO
15	a1u	45.92	0.00000	NO	NO
16	a1g	55.05	0.00000	NO	YES
17	eg	57.15	0.00000	NO	YES
18	eg	57.15	0.00000	NO	YES
19	eu	59.61	0.68971	YES	NO
20	eu	59.61	0.68971	YES	NO
21	eu	65.09	1.08091	YES	NO
22	eu	65.09	1.08091	YES	NO
23	eg	65.23	0.00000	NO	YES
24	eg	65.23	0.00000	NO	YES
25	a2u	66.79	2.04959	YES	NO
26	a1g	82.13	0.00000	NO	YES
27	eg	83.38	0.00000	NO	YES
28	eg	83.38	0.00000	NO	YES
29	eu	91.83	0.43605	YES	NO
30	eu	91.83	0.43605	YES	NO
31	a2u	102.94	2.16686	YES	NO
32	a1g	104.74	0.00000	NO	YES
33	a2u	162.91	5.18203	YES	NO
34	eg	336.63	0.00000	NO	YES
35	eg	336.63	0.00000	NO	YES
36	eu	338.30	1.22581	YES	NO
37	eu	338.30	1.22581	YES	NO
38	a2g	348.23	0.00000	NO	NO
39	a1u	348.58	0.00000	NO	NO
40	a1g	365.15	0.00000	NO	YES
41	a2u	366.93	24.23989	YES	NO
42	eg	374.61	0.00000	NO	YES
43	eg	374.61	0.00000	NO	YES
44	eu	375.13	35.85831	YES	NO
45	eu	375.13	35.85831	YES	NO
46	eu	385.85	0.43735	YES	NO
47	eu	385.85	0.43735	YES	NO
48	eg	386.14	0.00000	NO	YES
49	eg	386.14	0.00000	NO	YES
50	a2u	395.80	37.29611	YES	NO
51	a1g	397.08	0.00000	NO	YES
52	eg	435.40	0.00000	NO	YES
53	eg	435.40	0.00000	NO	YES
54	eu	436.76	0.98869	YES	NO
55	eu	436.76	0.98869	YES	NO
56	a2u	441.03	8.83567	YES	NO
57	a1g	444.57	0.00000	NO	YES
58	eg	476.20	0.00000	NO	YES
59	eg	476.20	0.00000	NO	YES
60	eu	476.75	3.51502	YES	NO
61	eu	476.75	3.51502	YES	NO
62	a2g	493.85	0.00000	NO	NO
63	a1u	494.24	0.00000	NO	NO
64	a2u	531.41	229.85225	YES	NO
65	a1g	537.10	0.00000	NO	YES
66	eu	542.45	54.26372	YES	NO
67	eu	542.45	54.26372	YES	NO
68	eg	543.16	0.00000	NO	YES
69	eg	543.16	0.00000	NO	YES
70	eg	1894.45	0.00000	NO	YES
71	eg	1894.45	0.00000	NO	YES
72	a2u	1901.01	3076.54607	YES	NO
73	a1g	1910.43	0.00000	NO	YES
74	eu	1915.30	2561.68709	YES	NO
75	eu	1915.30	2561.68709	YES	NO
76	eg	1934.85	0.00000	NO	YES
77	eg	1934.85	0.00000	NO	YES
78	eu	1935.09	1366.03698	YES	NO
79	eu	1935.09	1366.03698	YES	NO
80	a2u	2007.07	1900.42628	YES	NO
81	a1g	2031.13	0.00000	NO	YES

Calculated Structure of $[Ag_2\{Nb(CO)_6\}_3]^-$ (C_2)



Symmetry: c2
Method: (RI-)b-p/def2-TZVPP

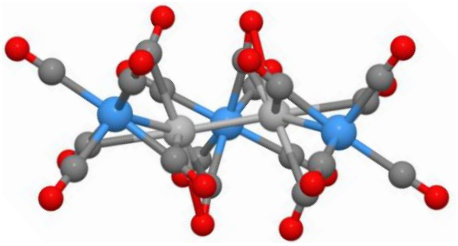
Ag	-0.73791	-1.18448	-0.53588
Nb	-0.00000	0.00000	-3.06686
O	-0.32866	2.06058	-5.58369
C	-0.25689	1.34323	-4.67893
C	-2.22078	-3.34131	-0.19409
O	-2.29099	-4.09517	-1.07865
C	-2.95152	-0.31137	0.68314
O	-3.44871	0.66116	0.28905
C	0.98617	-1.61986	-2.03689
O	1.71009	-2.49063	-1.76499
Nb	-2.27668	-2.13859	1.56951
O	-3.09181	-1.12755	-3.19382
C	-2.00078	-0.75099	-3.10928
O	-5.46333	-2.93592	1.64689
C	-4.34238	-2.64846	1.60949
C	-1.88327	-3.96081	2.59065
O	-1.67551	-4.96072	3.13784
C	-2.55968	-1.13549	3.43019
O	-2.72599	-0.59942	4.44107
C	-0.20757	-1.77010	1.95947
O	0.87894	-1.64581	2.35338
Ag	0.73791	1.18448	-0.53588
O	0.32866	-2.06058	-5.58369
C	0.25689	-1.34323	-4.67893
C	2.22078	3.34131	-0.19409
O	2.29099	4.09517	-1.07865
C	2.95152	0.31137	0.68314
O	3.44871	-0.66116	0.28905
C	-0.98617	1.61986	-2.03689
O	-1.71009	2.49063	-1.76499
Nb	2.27668	2.13859	1.56951
O	3.09181	1.12755	-3.19382
C	2.00078	0.75099	-3.10928
O	5.46333	2.93592	1.64689
C	4.34238	2.64846	1.60949
C	1.88327	3.96081	2.59065
O	1.67551	4.96072	3.13784
C	2.55968	1.13549	3.43019
O	2.72599	0.59942	4.44107
C	0.20757	1.77010	1.95947
O	-0.87894	1.64581	2.35338

SCF energy GEOOPT = -2507.224133926 H
ZPE = 367.0 kJ/mol
FREEH energy = 509.60 kJ/mol
FREEH entropy = 1.41442 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b	7.15	0.00118	YES	YES
8	b	14.00	0.00057	YES	YES
9	a	14.96	0.07428	YES	YES
10	a	18.03	0.00372	YES	YES
11	b	19.19	0.03012	YES	YES
12	b	24.07	0.17494	YES	YES
13	a	24.18	0.28989	YES	YES
14	a	27.11	0.02752	YES	YES
15	b	28.10	0.09621	YES	YES
16	a	30.77	0.17882	YES	YES
17	b	33.90	0.00456	YES	YES
18	a	36.25	0.00014	YES	YES
19	b	49.88	0.13535	YES	YES
20	a	52.33	0.00383	YES	YES
21	b	54.50	0.06272	YES	YES
22	a	55.86	0.12374	YES	YES
23	a	59.37	0.15900	YES	YES
24	b	59.48	0.38424	YES	YES
25	a	60.78	0.53224	YES	YES
26	b	61.95	0.05492	YES	YES
27	b	62.48	0.05819	YES	YES
28	a	63.00	0.02985	YES	YES
29	a	67.71	0.14595	YES	YES
30	b	68.74	1.36447	YES	YES
31	a	68.96	0.18672	YES	YES
32	b	71.99	0.49217	YES	YES
33	b	72.43	1.41403	YES	YES
34	a	73.54	0.15657	YES	YES
35	b	74.15	1.69969	YES	YES
36	a	74.51	0.02964	YES	YES
37	a	77.81	0.96377	YES	YES
38	a	81.02	0.09945	YES	YES
39	b	81.25	0.09409	YES	YES
40	b	88.43	0.30301	YES	YES
41	b	93.91	0.03005	YES	YES
42	a	97.80	0.05941	YES	YES
43	b	99.54	0.60375	YES	YES
44	a	104.07	0.01759	YES	YES
45	a	110.55	0.30467	YES	YES
46	b	114.52	0.35355	YES	YES
47	a	118.48	1.20695	YES	YES
48	b	131.93	2.63084	YES	YES
49	a	143.50	0.27700	YES	YES
50	b	166.87	1.91358	YES	YES
51	a	182.44	2.54328	YES	YES
52	b	328.76	1.02190	YES	YES
53	a	328.76	0.03682	YES	YES
54	b	329.29	0.59155	YES	YES
55	a	329.65	0.66028	YES	YES
56	a	334.27	0.25295	YES	YES
57	b	336.30	2.04496	YES	YES
58	b	338.89	0.02929	YES	YES
59	a	339.87	0.01201	YES	YES
60	b	347.65	0.34967	YES	YES
61	a	348.33	2.53223	YES	YES
62	b	365.24	4.75803	YES	YES
63	b	368.30	0.42586	YES	YES
64	a	368.41	4.50621	YES	YES
65	b	371.64	6.54638	YES	YES
66	a	371.90	0.63639	YES	YES
67	b	373.13	3.70510	YES	YES
68	a	373.14	0.07945	YES	YES
69	a	373.47	0.00860	YES	YES
70	b	387.18	15.80975	YES	YES
71	a	387.57	6.29169	YES	YES
72	b	389.82	19.97096	YES	YES
73	b	393.35	22.26771	YES	YES
74	a	393.90	0.07181	YES	YES
75	a	394.66	33.16627	YES	YES
76	b	395.61	28.37231	YES	YES
77	b	403.58	8.33454	YES	YES
78	a	406.60	12.31125	YES	YES
79	a	430.69	4.26405	YES	YES
80	b	440.78	7.56569	YES	YES
81	a	442.05	0.25397	YES	YES
82	b	442.33	4.79416	YES	YES
83	a	445.71	0.21695	YES	YES
84	b	446.20	2.27291	YES	YES
85	b	447.13	17.67921	YES	YES
86	a	447.79	0.30042	YES	YES
87	a	453.26	1.32520	YES	YES
88	a	466.53	23.70581	YES	YES
89	b	470.87	6.20104	YES	YES
90	a	471.43	2.90917	YES	YES
91	b	475.97	3.38372	YES	YES
92	a	476.37	0.41889	YES	YES
93	b	480.86	6.55454	YES	YES
94	a	485.92	0.07198	YES	YES
95	b	488.71	0.03030	YES	YES
96	a	489.63	0.01862	YES	YES
97	b	545.51	89.27153	YES	YES
98	a	548.09	227.33718	YES	YES
99	b	550.64	27.29041	YES	YES
100	b	556.23	123.68533	YES	YES
101	a	560.36	63.07573	YES	YES
102	b	561.67	76.31702	YES	YES
103	a	562.07	3.97008	YES	YES
104	b	562.89	80.50319	YES	YES
105	a	564.04	22.54474	YES	YES
106	b	1890.57	147.28517	YES	YES
107	b	1900.35	594.73196	YES	YES
108	a	1901.58	190.45673	YES	YES
109	a	1904.90	525.40232	YES	YES
110	a	1911.97	1312.81855	YES	YES
111	b	1914.81	2233.23393	YES	YES
112	a	1927.39	343.54813	YES	YES
113	b	1932.10	2080.84707	YES	YES
114	b	1948.16	471.67373	YES	YES
115	a	1949.29	43.01352	YES	YES
116	b	1950.17	2689.50294	YES	YES
117	a	1957.00	715.15009	YES	YES
118	b	1957.37	29.28081	YES	YES
119	a	1958.12	104.70841	YES	YES
120	b	1958.58	1741.39253	YES	YES
121	a	2015.01	2832.83969	YES	YES
122	b	2022.85	1120.79542	YES	YES
123	a	2044.29	4.04310	YES	YES

Calculated Structure of $[Ag_2\{Ta(CO)_6\}_3]^-$ (C_2)



Symmetry: c2
Method: (RI-)b-p/def2-TZVPP

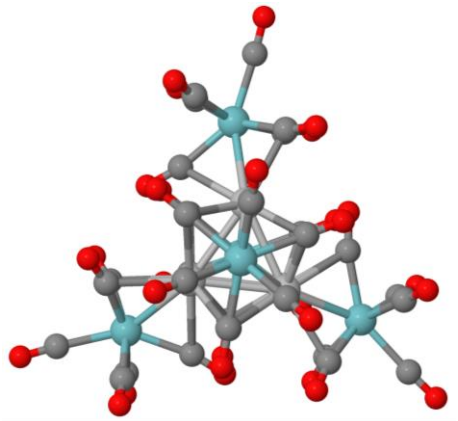
Ag	-0.74509	-1.17576	-0.53616
Ta	0.00000	0.00000	-3.08080
O	-0.28694	2.06264	-5.60835
C	-0.23104	1.34505	-4.70137
C	-2.19788	-3.35719	-0.18266
O	-2.24276	-4.11164	-1.07001
C	-2.95789	-0.31671	0.68815
O	-3.44680	0.65932	0.28875
C	0.99079	-1.61976	-2.05327
O	1.70608	-2.49192	-1.76071
Ta	-2.28684	-2.14657	1.57738
O	-3.09344	-1.13885	-3.18509
C	-2.00207	-0.75770	-3.11176
O	-5.47741	-2.95006	1.59517
C	-4.35520	-2.66103	1.58191
C	-1.90837	-3.96742	2.61479
O	-1.71137	-4.96464	3.17279
C	-2.59428	-1.14461	3.43816
O	-2.77108	-0.60927	4.44881
C	-0.21882	-1.76935	1.97995
O	0.87079	-1.63284	2.36391
Ag	0.74509	1.17576	-0.53616
O	0.28694	-2.06264	-5.60835
C	0.23104	-1.34505	-4.70137
C	2.19788	3.35719	-0.18266
O	2.24276	4.11164	-1.07001
C	2.95789	0.31671	0.68815
O	3.44680	-0.65932	0.28875
C	-0.99079	1.61976	-2.05327
O	-1.70608	2.49192	-1.76071
Ta	2.28684	2.14657	1.57738
O	3.09344	1.13885	-3.18509
C	2.00207	0.75770	-3.11176
O	5.47741	2.95006	1.59517
C	4.35520	2.66103	1.58191
C	1.90837	3.96742	2.61479
O	1.71137	4.96464	3.17279
C	2.59428	1.14461	3.43816
O	2.77108	0.60927	4.44881
C	0.21882	1.76935	1.97995
O	-0.87079	1.63284	2.36391

SCF energy GEOOPT = -2507.364046323 H

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b	3.98	0.00025	YES	YES
8	b	12.92	0.00084	YES	YES
9	a	13.99	0.06498	YES	YES
10	a	16.43	0.00318	YES	YES
11	b	16.72	0.02674	YES	YES
12	a	22.74	0.26603	YES	YES
13	b	22.84	0.15824	YES	YES
14	a	26.30	0.00102	YES	YES
15	b	27.15	0.06328	YES	YES
16	a	29.39	0.23211	YES	YES
17	b	32.10	0.01603	YES	YES
18	a	33.77	0.00002	YES	YES
19	b	49.23	0.06793	YES	YES
20	a	52.24	0.00410	YES	YES
21	b	52.59	0.18757	YES	YES
22	a	56.42	0.28856	YES	YES
23	b	57.23	0.51039	YES	YES
24	a	57.31	0.00609	YES	YES
25	a	59.84	0.28410	YES	YES
26	b	61.26	0.26008	YES	YES
27	a	61.76	0.23237	YES	YES
28	b	61.91	0.13434	YES	YES
29	b	65.95	1.33216	YES	YES
30	a	67.59	0.13976	YES	YES
31	a	67.95	0.17271	YES	YES
32	b	70.53	0.18548	YES	YES
33	b	70.78	1.25600	YES	YES
34	b	72.03	1.08535	YES	YES
35	a	73.02	0.11460	YES	YES
36	a	75.81	0.05397	YES	YES
37	a	76.96	0.73476	YES	YES
38	b	79.82	0.56643	YES	YES
39	a	81.75	0.08283	YES	YES
40	b	82.74	0.11121	YES	YES
41	b	93.42	0.02647	YES	YES
42	a	93.74	0.18075	YES	YES
43	a	98.36	0.01988	YES	YES
44	b	99.34	0.51809	YES	YES
45	a	105.78	1.24480	YES	YES
46	b	108.90	0.61818	YES	YES
47	a	112.79	0.17788	YES	YES
48	b	125.68	2.41896	YES	YES
49	a	134.81	0.59005	YES	YES
50	b	159.60	1.80609	YES	YES
51	a	177.20	2.64752	YES	YES
52	a	336.73	0.03617	YES	YES
53	b	337.24	1.24392	YES	YES
54	a	337.59	0.83033	YES	YES
55	b	337.72	1.98408	YES	YES
56	a	338.92	0.19460	YES	YES
57	b	344.91	2.69246	YES	YES
58	b	347.73	0.04736	YES	YES
59	a	348.72	0.04982	YES	YES
60	b	352.96	0.39780	YES	YES
61	a	353.83	4.28732	YES	YES
62	b	362.94	12.09621	YES	YES
63	b	365.83	12.09735	YES	YES
64	a	366.11	16.21495	YES	YES
65	b	371.64	22.97079	YES	YES
66	a	371.96	4.64250	YES	YES
67	a	374.22	5.30844	YES	YES
68	b	374.35	28.15496	YES	YES
69	b	381.51	22.09519	YES	YES
70	a	383.64	0.83434	YES	YES
71	b	384.07	0.64785	YES	YES
72	a	384.42	0.27180	YES	YES
73	a	387.14	2.10792	YES	YES
74	b	387.51	0.45716	YES	YES
75	b	393.32	7.98154	YES	YES
76	b	393.77	19.20607	YES	YES
77	a	394.31	22.97423	YES	YES
78	a	400.80	17.81783	YES	YES
79	a	427.87	1.84716	YES	YES
80	b	433.89	6.85817	YES	YES
81	b	435.77	0.84290	YES	YES
82	a	435.99	0.08064	YES	YES
83	a	437.74	0.26490	YES	YES
84	b	438.37	15.67638	YES	YES
85	b	441.93	0.24635	YES	YES
86	a	442.86	0.05226	YES	YES
87	a	452.93	5.25135	YES	YES
88	a	463.28	25.96176	YES	YES
89	b	473.32	5.73487	YES	YES
90	a	473.72	1.80956	YES	YES
91	b	477.46	3.59571	YES	YES
92	a	478.13	0.48662	YES	YES
93	b	480.68	12.53342	YES	YES
94	a	487.09	0.01546	YES	YES
95	b	492.05	0.02952	YES	YES
96	a	492.99	0.02139	YES	YES
97	b	523.10	49.60776	YES	YES
98	a	524.90	129.88028	YES	YES
99	b	528.98	27.93625	YES	YES
100	b	531.47	78.96795	YES	YES
101	a	534.28	43.11692	YES	YES
102	b	540.38	39.65645	YES	YES
103	a	540.89	4.72286	YES	YES
104	b	541.19	50.52296	YES	YES
105	a	541.92	11.12140	YES	YES
106	b	1887.09	187.11427	YES	YES
107	b	1896.85	485.33057	YES	YES
108	a	1898.78	53.15319	YES	YES
109	a	1901.60	837.29063	YES	YES
110	a	1908.09	1168.08421	YES	YES
111	b	1910.95	2346.27763	YES	YES
112	a	1923.81	299.98369	YES	YES
113	b	1928.28	2047.58886	YES	YES
114	b	1944.18	858.19871	YES	YES
115	a	1946.25	82.16806	YES	YES
116	b	1947.07	2321.01458	YES	YES
117	a	1953.45	705.77208	YES	YES
118	b	1954.14	0.02300	YES	YES
119	a	1954.84	123.18406	YES	YES
120	b	1955.40	1803.01928	YES	YES
121	a	2013.52	2890.42727	YES	YES
122	b	2021.41	1163.93610	YES	YES
123	a	2043.02	5.05609	YES	YES

Calculated Structure of $[Ag_6\{Nb(CO)_6\}_5]^+$ (C_{3h})



Symmetry: c3h
Method: (RI-)b-p/def2-TZVPP

Ag	1.32679	-0.96544	-1.41503
Nb	0.00000	0.00000	-3.88394
C	-1.57395	1.31563	-3.24429
O	-2.82322	2.16373	0.00000
Ag	0.17270	1.63175	-1.41503
Nb	0.00000	0.00000	3.88394
C	2.63948	-3.08886	1.46377
O	2.24441	3.90202	2.20183
Nb	3.65304	-1.88338	0.00000
Ag	-1.49949	-0.66631	-1.41503
C	0.29731	1.67554	-5.20230
O	-1.95494	5.23737	2.53500
Nb	-0.19547	4.10531	0.00000
Ag	1.32679	-0.96544	1.41503
O	-1.95494	5.23737	-2.53500
Nb	-3.45757	-2.22194	0.00000
Ag	0.17270	1.63175	1.41503
O	2.24441	3.90202	-2.20183
O	-2.44098	-0.88581	5.91585
Ag	-1.49949	-0.66631	1.41503
O	0.45336	2.55686	5.91585
O	-2.46830	2.05155	3.18834
O	-4.50145	-0.00729	2.20183
C	-3.99477	-0.74143	1.46377
O	-0.46224	-3.52684	0.00000
O	-4.50145	-0.00729	-2.20183
C	-1.80798	2.73270	0.00000
O	1.98762	-1.67105	-5.91585
O	-0.54254	-3.16339	-3.18834
O	3.01085	1.11184	-3.18834
C	3.27058	0.19941	0.00000
O	5.51317	-0.92566	-2.53500
O	5.94139	-4.26426	0.00000
O	3.01085	1.11184	3.18834
O	3.28545	1.36311	0.00000
O	-3.55823	-4.31172	2.53500
O	-6.66365	-3.01327	0.00000
C	-1.46259	-2.93211	0.00000
O	2.25704	-3.89473	2.20183
C	1.35529	3.83029	-1.46377
C	1.30240	-1.09524	-5.20230
C	4.87535	-1.23619	1.63135
O	0.72226	7.27752	0.00000
O	1.98762	-1.67105	5.91585
C	-3.99477	-0.74143	-1.46377
C	-0.35240	-2.02089	3.24429
C	-1.36710	4.84027	-1.63135
C	-1.57395	1.31563	3.24429
O	-3.55823	-4.31172	-2.53500
O	-0.54254	-3.16339	3.18834
O	-2.46830	2.05155	-3.18834
C	-1.36710	4.84027	1.63135
O	5.51317	-0.92566	2.53500
O	-2.44098	-0.88581	-5.91585
O	0.45336	2.55686	-5.91585
C	1.35529	3.83029	1.46377
C	0.44651	6.16735	0.00000
C	1.92634	0.70526	3.24429
O	2.25704	-3.89473	-2.20183
C	-5.56434	-2.69699	0.00000
C	0.29731	1.67554	5.20230
C	-1.59971	-0.58029	-5.20230
C	-0.35240	-2.02089	-3.24429
C	-1.59971	-0.58029	5.20230
C	4.87535	-1.23619	-1.63135
C	1.92634	0.70526	-3.24429
C	-3.50825	-3.60408	-1.63135
C	-3.50825	-3.60408	1.63135
C	1.30240	-1.09524	5.20230
C	2.63948	-3.08886	-1.46377
C	5.11783	-3.47036	0.00000

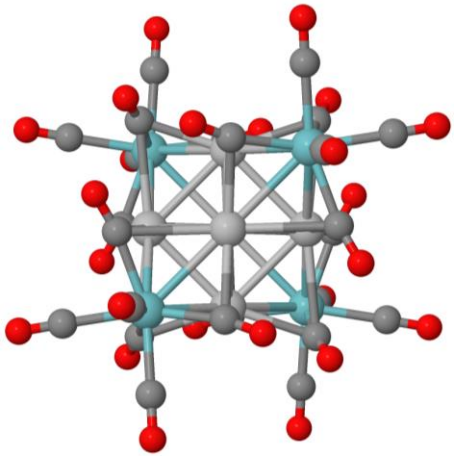
SCF energy GEOOPT = -4570.847347415 H
ZPE = 622.5 kJ/mol
FREEH energy = 878.66 kJ/mol
FREEH entropy = 2.27032 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e"	11.05	0.00000	NO	YES
8	e"	11.05	0.00000	NO	YES
9	a"	16.72	0.10491	YES	NO
10	e'	17.07	0.02566	YES	YES
11	e'	17.07	0.02566	YES	YES
12	e"	18.76	0.00000	NO	YES
13	e"	18.76	0.00000	NO	YES
14	a'	29.58	0.00000	NO	YES
15	e"	30.08	0.00000	NO	YES
16	e"	30.08	0.00000	NO	YES
17	e'	30.98	0.12385	YES	YES
18	e'	30.98	0.12385	YES	YES
19	a"	33.64	0.11633	YES	NO
20	e'	35.53	0.07121	YES	YES
21	e'	35.53	0.07121	YES	YES
22	a"	36.96	0.01081	YES	NO
23	a"	38.37	0.07167	YES	NO
24	a'	39.38	0.00000	NO	YES
25	e"	42.35	0.00000	NO	YES
26	e"	42.35	0.00000	NO	YES
27	a'	42.52	0.00000	NO	YES
28	a"	48.34	0.52263	YES	NO
29	a'	49.26	0.00000	NO	YES
30	e'	49.55	0.32656	YES	YES
31	e'	49.55	0.32656	YES	YES
32	e"	51.11	0.00000	NO	YES
33	e"	51.11	0.00000	NO	YES
34	e'	55.12	0.80013	YES	YES
35	e'	55.12	0.80013	YES	YES
36	a'	59.19	0.00000	NO	YES
37	e"	61.30	0.00000	NO	YES
38	e"	61.30	0.00000	NO	YES
39	a"	63.93	0.00012	YES	NO
40	e'	64.48	0.12359	YES	YES
41	e'	64.48	0.12359	YES	YES
42	a'	65.46	0.00000	NO	YES
43	e"	67.12	0.00000	NO	YES
44	e"	67.12	0.00000	NO	YES
45	a"	67.86	0.42884	YES	NO
46	e'	69.83	0.02829	YES	YES
47	e'	69.83	0.02829	YES	YES
48	a'	70.01	0.00000	NO	YES
49	e'	71.53	0.11159	YES	YES
50	e'	71.53	0.11159	YES	YES
51	a'	74.94	0.00000	NO	YES
52	e"	75.17	0.00000	NO	YES
53	e"	75.17	0.00000	NO	YES
54	a"	79.17	0.81177	YES	NO
55	e"	81.50	0.00000	NO	YES
56	e"	81.50	0.00000	NO	YES
57	e'	82.10	1.35641	YES	YES
58	e'	82.10	1.35641	YES	YES
59	a'	87.32	0.00000	NO	YES
60	a"	87.53	0.07446	YES	NO
61	e"	89.80	0.00000	NO	YES
62	e"	89.80	0.00000	NO	YES
63	e'	91.86	0.36582	YES	YES
64	e'	91.86	0.36582	YES	YES
65	a"	97.90	0.00311	YES	NO
66	e'	98.87	0.32959	YES	YES
67	e'	98.87	0.32959	YES	YES
68	a'	99.37	0.00000	NO	YES
69	a'	106.41	0.00000	NO	YES
70	e"	108.01	0.00000	NO	YES
71	e"	108.01	0.00000	NO	YES
72	a"	111.20	0.87493	YES	NO
73	e'	113.20	0.17610	YES	YES
74	e'	113.20	0.17610	YES	YES
75	a'	116.22	0.00000	NO	YES
76	e'	121.40	0.79666	YES	YES
77	e'	121.40	0.79666	YES	YES
78	e"	122.17	0.00000	NO	YES
79	e"	122.17	0.00000	NO	YES

80	a"	126.45	0.03101	YES	NO
81	a'	130.29	0.00000	NO	YES
82	e"	130.40	0.00000	NO	YES
83	e"	130.40	0.00000	NO	YES
84	e'	133.10	0.05059	YES	YES
85	e'	133.10	0.05059	YES	YES
86	e"	134.64	0.00000	NO	YES
87	e"	134.64	0.00000	NO	YES
88	a"	137.94	0.00103	YES	NO
89	a'	137.97	0.00000	NO	YES
90	e'	160.55	1.18480	YES	YES
91	e'	160.55	1.18480	YES	YES
92	a"	168.25	1.44516	YES	NO
93	a'	181.77	0.00000	NO	YES
94	e"	319.82	0.00000	NO	YES
95	e"	319.82	0.00000	NO	YES
96	e'	319.97	0.61192	YES	YES
97	e'	319.97	0.61192	YES	YES
98	a'	327.22	0.00000	NO	YES
99	e'	327.81	1.38025	YES	YES
100	e'	327.81	1.38025	YES	YES
101	a"	330.37	0.05434	YES	NO
102	e"	330.49	0.00000	NO	YES
103	e"	330.49	0.00000	NO	YES
104	a"	332.91	0.35322	YES	NO
105	e"	333.31	0.00000	NO	YES
106	e"	333.31	0.00000	NO	YES
107	a'	334.80	0.00000	NO	YES
108	a"	334.92	0.83732	YES	NO
109	e'	342.60	7.18766	YES	YES
110	e'	342.60	7.18766	YES	YES
111	a'	342.83	0.00000	NO	YES
112	a"	343.26	0.50004	YES	NO
113	a'	344.07	0.00000	NO	YES
114	e"	345.40	0.00000	NO	YES
115	e"	345.40	0.00000	NO	YES
116	e'	345.94	17.74225	YES	YES
117	e'	345.94	17.74225	YES	YES
118	e'	347.86	13.27856	YES	YES
119	e'	347.86	13.27856	YES	YES
120	a'	347.88	0.00000	NO	YES
121	e"	359.56	0.00000	NO	YES
122	e"	359.56	0.00000	NO	YES
123	a"	359.75	0.77018	YES	NO
124	a'	378.49	0.00000	NO	YES
125	a"	379.67	56.00795	YES	NO
126	e"	380.17	0.00000	NO	YES
127	e"	380.17	0.00000	NO	YES
128	a"	381.15	69.54198	YES	NO
129	e'	381.71	43.13813	YES	YES
130	e'	381.71	43.13813	YES	YES
131	a'	384.22	0.00000	NO	YES
132	e'	384.39	24.50381	YES	YES
133	e'	384.39	24.50381	YES	YES
134	e"	384.48	0.00000	NO	YES
135	e"	384.48	0.00000	NO	YES
136	e'	408.73	2.37949	YES	YES
137	e'	408.73	2.37949	YES	YES
138	a'	409.15	0.00000	NO	YES
139	a'	420.91	0.00000	NO	YES
140	e'	422.02	2.94422	YES	YES
141	e'	422.02	2.94422	YES	YES
142	e'	438.87	1.61483	YES	YES
143	e'	438.87	1.61483	YES	YES
144	a'	439.17	0.00000	NO	YES
145	e"	440.02	0.00000	NO	YES
146	e"	440.02	0.00000	NO	YES
147	e'	441.36	9.07092	YES	YES
148	e'	441.36	9.07092	YES	YES
149	e"	445.38	0.00000	NO	YES
150	e"	445.38	0.00000	NO	YES
151	a"	445.71	1.66204	YES	NO
152	a'	446.95	0.00000	NO	YES
153	a"	449.00	8.01291	YES	NO
154	e'	453.52	14.36297	YES	YES
155	e'	453.52	14.36297	YES	YES
156	e"	453.99	0.00000	NO	YES
157	e"	453.99	0.00000	NO	YES
158	e"	466.00	0.00000	NO	YES
159	e"	466.00	0.00000	NO	YES
160	a"	466.17	22.25298	YES	NO
161	e'	471.21	1.55417	YES	YES
162	e'	471.21	1.55417	YES	YES
163	a'	471.32	0.00000	NO	YES
164	a"	471.85	10.82692	YES	NO
165	a'	472.41	0.00000	NO	YES
166	a"	478.06	0.00296	YES	NO
167	e"	478.14	0.00000	NO	YES
168	e"	478.14	0.00000	NO	YES
169	a'	523.86	0.00000	NO	YES
170	a"	524.04	379.80397	YES	NO
171	a'	533.63	0.00000	NO	YES
172	e"	534.16	0.00000	NO	YES
173	e"	534.16	0.00000	NO	YES
174	e'	534.23	0.99728	YES	YES
175	e'	534.23	0.99728	YES	YES
176	e'	536.07	91.30455	YES	YES
177	e'	536.07	91.30455	YES	YES
178	e'	539.54	243.84618	YES	YES
179	e'	539.54	243.84618	YES	YES
180	e"	540.61	0.00000	NO	YES
181	e"	540.61	0.00000	NO	YES
182	a"	541.34	93.42558	YES	NO
183	a'	543.75	0.00000	NO	YES
184	a'	1896.94	0.00000	NO	YES
185	e'	1901.53	380.73626	YES	YES
186	e'	1901.53	380.73626	YES	YES
187	e"	1919.59	0.00000	NO	YES
188	e"	1919.59	0.00000	NO	YES
189	e'	1928.66	434.34032	YES	YES
190	e'	1928.66	434.34032	YES	YES
191	a"	1936.11	1204.90722	YES	NO
192	a'	1942.15	0.00000	NO	YES
193	e"	1947.57	0.00000	NO	YES
194	e"	1947.57	0.00000	NO	YES
195	a"	1951.36	26.39492	YES	NO
196	a'	1957.44	0.00000	NO	YES
197	e'	1965.37	1253.52491	YES	YES
198	e'	1965.37	1253.52491	YES	YES
199	e"	2008.76	0.00000	NO	YES
200	e"	2008.76	0.00000	NO	YES
201	a"	2009.98	1297.61489	YES	NO
202	a'	2032.42	0.00000	NO	YES
203	e'	2032.93	252.72285	YES	YES
204	e'	2032.93	252.72285	YES	YES
205	e"	2040.00	0.00000	NO	YES
206	e"	2040.00	0.00000	NO	YES
207	e'	2040.67	841.91751	YES	YES
208	e'	2040.67	841.91751	YES	YES
209	a'	2061.24	0.00000	NO	YES
210	e'	2067.83	3480.66610	YES	YES
211	e'	2067.83	3480.66610	YES	YES
212	a"	2075.07	4637.16055	YES	NO
213	a'	2095.70	0.00000	NO	YES

Calculated Structure of $[Ag_6\{Nb(CO)_6\}_4]^{2+}$ (*T*)



Symmetry: t
Method: (RI-)b-p/def2-TZVPP

Ag	-0.00000	0.00000	2.05523
Ag	2.05523	-0.00000	-0.00000
Ag	-2.05523	0.00000	0.00000
Ag	-0.00000	-2.05523	0.00000
Ag	0.00000	2.05523	-0.00000
Ag	0.00000	-0.00000	-2.05523
Nb	-2.08876	-2.08876	2.08876
Nb	-2.08876	2.08876	-2.08876
Nb	2.08876	2.08876	2.08876
O	3.37570	0.88298	-2.64146
Nb	2.08876	-2.08876	-2.08876
O	2.62186	-1.90566	-5.34750
O	2.64146	-3.37570	0.88298
O	-0.88298	-2.64146	-3.37570
O	-1.90566	5.34750	-2.62186
O	0.88298	2.64146	-3.37570
O	-3.37570	0.88298	2.64146
O	-2.64146	-3.37570	-0.88298
O	-5.34750	-2.62186	1.90566
O	0.88298	-2.64146	3.37570
O	-1.90566	-5.34750	2.62186
O	-3.37570	-0.88298	-2.64146
O	1.90566	-5.34750	-2.62186
O	-2.64146	3.37570	0.88298
O	2.62186	1.90566	5.34750
O	-5.34750	2.62186	-1.90566
O	5.34750	-2.62186	-1.90566
O	5.34750	2.62186	1.90566
O	3.37570	-0.88298	2.64146
O	-2.62186	1.90566	-5.34750
O	-0.88298	2.64146	3.37570
O	2.64146	3.37570	-0.88298
O	1.90566	5.34750	2.62186
O	-2.62186	-1.90566	5.34750
C	-2.81547	-0.07595	2.30554
C	4.22469	-2.42931	-1.96128
C	-1.96128	-4.22469	2.42931
C	-1.96128	4.22469	-2.42931
C	-2.30554	2.81547	-0.07595
C	-0.07595	-2.30554	2.81547
C	-2.81547	0.07595	-2.30554
C	-2.30554	-2.81547	0.07595
C	2.30554	-2.81547	-0.07595
C	-4.22469	-2.42931	1.96128
C	1.96128	-4.22469	-2.42931
C	2.81547	-0.07595	-2.30554
C	2.42931	1.96128	4.22469
C	2.30554	2.81547	0.07595
C	-0.07595	2.30554	-2.81547
C	0.07595	-2.30554	-2.81547
C	-4.22469	2.42931	-1.96128
C	2.81547	0.07595	2.30554
C	-2.42931	-1.96128	4.22469
C	-2.42931	1.96128	-4.22469
C	0.07595	2.30554	2.81547
C	4.22469	2.42931	1.96128
C	1.96128	4.22469	2.42931
C	2.42931	-1.96128	-4.22469

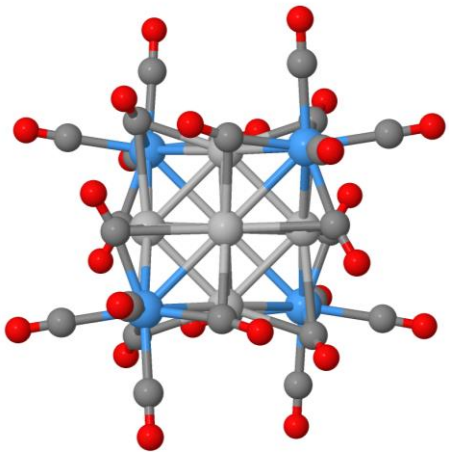
SCF energy GEOOPT = -3832.916269829 H
ZPE = 501.3 kJ/mol
FREEH energy = 711.80 kJ/mol
FREEH entropy = 1.86279 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e	22.98	0.00000	NO	YES
8	e	22.98	0.00000	NO	YES
9	t	26.48	0.11237	YES	YES
10	t	26.48	0.11234	YES	YES
11	t	26.48	0.11234	YES	YES
12	e	28.36	0.00000	NO	YES
13	t	32.85	0.00491	YES	YES
14	t	32.85	0.00491	YES	YES
15	t	32.85	0.00488	YES	YES
16	t	35.50	0.05331	YES	YES
17	t	35.50	0.05332	YES	YES
18	t	35.51	0.05328	YES	YES
19	t	46.89	0.04547	YES	YES
20	t	46.89	0.04545	YES	YES
21	t	46.89	0.04546	YES	YES
22	e	49.47	0.00000	NO	YES
23	e	49.47	0.00000	NO	YES
24	t	52.31	0.33554	YES	YES
25	t	52.31	0.33555	YES	YES
26	t	52.31	0.33554	YES	YES
27	e	55.46	0.00000	NO	YES
28	e	55.46	0.00000	NO	YES
29	t	61.03	0.33948	YES	YES
30	t	61.03	0.33942	YES	YES
31	t	61.03	0.33939	YES	YES
32	e	66.61	0.00000	NO	YES
33	t	71.10	0.08085	YES	YES
34	t	71.10	0.08089	YES	YES
35	t	71.10	0.08087	YES	YES
36	e	72.70	0.00000	NO	YES
37	t	73.78	0.00108	YES	YES
38	t	73.78	0.00108	YES	YES
39	t	73.78	0.00109	YES	YES
40	e	73.97	0.00000	NO	YES
41	e	73.98	0.00000	NO	YES
42	t	77.07	0.01200	YES	YES
43	t	77.07	0.01196	YES	YES
44	t	77.07	0.01198	YES	YES
45	t	83.97	1.06137	YES	YES
46	t	83.97	1.06158	YES	YES
47	t	83.97	1.06138	YES	YES
48	t	90.30	1.39644	YES	YES
49	t	90.30	1.39636	YES	YES
50	t	90.30	1.39658	YES	YES
51	e	91.34	0.00000	NO	YES
52	e	91.34	0.00000	NO	YES
53	t	97.45	0.00315	YES	YES
54	t	97.45	0.00312	YES	YES
55	t	97.45	0.00315	YES	YES
56	t	98.23	0.14648	YES	YES
57	t	98.23	0.14653	YES	YES
58	t	98.23	0.14645	YES	YES
59	e	113.76	0.00000	NO	YES
60	t	114.83	0.06968	YES	YES
61	t	114.83	0.06968	YES	YES
62	t	114.83	0.06968	YES	YES
63	e	125.96	0.00000	NO	YES
64	e	126.80	0.00000	NO	YES
65	e	126.81	0.00000	NO	YES
66	t	129.11	0.19908	YES	YES
67	t	129.11	0.19914	YES	YES
68	t	129.11	0.19912	YES	YES
69	t	136.52	0.30399	YES	YES
70	t	136.52	0.30401	YES	YES
71	t	136.52	0.30404	YES	YES
72	t	145.49	0.00125	YES	YES
73	t	145.49	0.00125	YES	YES
74	t	145.49	0.00125	YES	YES
75	e	147.96	0.00000	NO	YES
76	t	164.78	0.23844	YES	YES
77	t	164.78	0.23844	YES	YES
78	t	164.78	0.23844	YES	YES
79	e	319.16	0.00000	NO	YES
80	e	319.16	0.00000	NO	YES
81	t	319.61	0.05238	YES	YES
82	t	319.62	0.05219	YES	YES
83	t	319.62	0.05241	YES	YES
84	t	321.09	1.98866	YES	YES
85	t	321.09	1.98907	YES	YES
86	t	321.09	1.98901	YES	YES
87	t	334.10	0.05778	YES	YES
88	t	334.10	0.05756	YES	YES
89	t	334.10	0.05765	YES	YES
90	t	336.17	14.46488	YES	YES
91	t	336.17	14.48537	YES	YES
92	t	336.17	14.48324	YES	YES
93	e	336.33	0.00000	NO	YES
94	e	336.33	0.00000	NO	YES

95	t	336.37	10.16940	YES	YES
96	t	336.38	10.16717	YES	YES
97	t	336.38	10.18898	YES	YES
98	e	337.04	0.00000	NO	YES
99	e	338.09	0.00000	NO	YES
100	t	338.31	10.07548	YES	YES
101	t	338.31	10.07622	YES	YES
102	t	338.31	10.07672	YES	YES
103	t	371.62	71.26247	YES	YES
104	t	371.62	71.26314	YES	YES
105	t	371.62	71.26299	YES	YES
106	e	376.20	0.00000	NO	YES
107	e	381.47	0.00000	NO	YES
108	e	381.47	0.00000	NO	YES
109	t	382.57	3.84334	YES	YES
110	t	382.57	3.84608	YES	YES
111	t	382.57	3.84388	YES	YES
112	t	387.92	12.97405	YES	YES
113	t	387.92	12.97236	YES	YES
114	t	387.92	12.97564	YES	YES
115	t	432.79	0.43275	YES	YES
116	t	432.79	0.43317	YES	YES
117	t	432.79	0.43296	YES	YES
118	t	434.28	7.44390	YES	YES
119	t	434.28	7.44374	YES	YES
120	t	434.28	7.44431	YES	YES
121	e	434.88	0.00000	NO	YES
122	e	434.88	0.00000	NO	YES
123	t	442.90	7.47188	YES	YES
124	t	442.90	7.47152	YES	YES
125	t	442.90	7.47179	YES	YES
126	e	445.95	0.00000	NO	YES
127	t	456.77	0.02584	YES	YES
128	t	456.77	0.02571	YES	YES
129	t	456.77	0.02596	YES	YES
130	e	461.14	0.00000	NO	YES
131	e	461.14	0.00000	NO	YES
132	t	461.71	7.54792	YES	YES
133	t	461.71	7.55549	YES	YES
134	t	461.71	7.55216	YES	YES
135	e	462.00	0.00000	NO	YES
136	t	462.94	11.30788	YES	YES
137	t	462.94	11.30930	YES	YES
138	t	462.94	11.31412	YES	YES
139	t	523.17	263.36322	YES	YES
140	t	523.17	263.38672	YES	YES
141	t	523.17	263.39234	YES	YES
142	t	528.40	1.97854	YES	YES
143	t	528.40	1.97726	YES	YES
144	t	528.40	1.97818	YES	YES
145	e	529.71	0.00000	NO	YES
146	e	529.71	0.00000	NO	YES
147	t	531.32	94.15525	YES	YES
148	t	531.32	94.13395	YES	YES
149	t	531.32	94.12793	YES	YES
150	e	533.44	0.00000	NO	YES
151	t	1914.30	28.71881	YES	YES
152	t	1914.30	28.71925	YES	YES
153	t	1914.30	28.71887	YES	YES
154	e	1914.59	0.00000	NO	YES
155	e	1914.59	0.00000	NO	YES
156	t	1934.58	392.56880	YES	YES
157	t	1934.58	392.56411	YES	YES
158	t	1934.58	392.56262	YES	YES
159	t	1952.60	685.26579	YES	YES
160	t	1952.60	685.26392	YES	YES
161	t	1952.60	685.25926	YES	YES
162	a	1958.06	0.00000	NO	YES
163	t	2069.50	6.01825	YES	YES
164	t	2069.50	6.01828	YES	YES
165	t	2069.50	6.01826	YES	YES
166	t	2073.29	986.76978	YES	YES
167	t	2073.29	986.76950	YES	YES
168	t	2073.29	986.76954	YES	YES
169	e	2073.55	0.00000	NO	YES
170	e	2073.55	0.00000	NO	YES
171	t	2095.62	2997.45788	YES	YES
172	t	2095.62	2997.45770	YES	YES
173	t	2095.62	2997.45843	YES	YES
174	a	2118.00	0.00000	NO	YES

Calculated Structure of $[Ag_6\{Ta(CO)_6\}_4]^{2+}$ (*T*)



Symmetry: t
Method: (RI-)b-p/def2-TZVPP

Ag	-0.00000	0.00000	2.05308
Ag	2.05308	-0.00000	-0.00000
Ag	-2.05308	0.00000	0.00000
Ag	-0.00000	-2.05308	0.00000
Ag	0.00000	2.05308	-0.00000
Ag	0.00000	-0.00000	-2.05308
Ta	-2.09761	-2.09761	2.09761
Ta	-2.09761	2.09761	-2.09761
Ta	2.09761	2.09761	2.09761
O	3.37902	0.88619	-2.64222
Ta	2.09761	-2.09761	-2.09761
O	2.62843	-1.92400	-5.35983
O	2.64222	-3.37902	0.88619
O	-0.88619	-2.64222	-3.37902
O	-1.92400	5.35983	-2.62843
O	0.88619	2.64222	-3.37902
O	-3.37902	0.88619	2.64222
O	-2.64222	-3.37902	-0.88619
O	-5.35983	-2.62843	1.92400
O	0.88619	-2.64222	3.37902
O	-1.92400	-5.35983	2.62843
O	-3.37902	-0.88619	-2.64222
O	1.92400	-5.35983	-2.62843
O	-2.64222	3.37902	0.88619
O	2.62843	1.92400	5.35983
O	-5.35983	2.62843	-1.92400
O	5.35983	-2.62843	-1.92400
O	5.35983	2.62843	1.92400
O	3.37902	-0.88619	2.64222
O	-2.62843	1.92400	-5.35983
O	-0.88619	2.64222	3.37902
O	2.64222	3.37902	-0.88619
O	1.92400	5.35983	2.62843
O	-2.62843	-1.92400	5.35983
C	-2.82657	-0.08267	2.31923
C	4.23591	-2.43628	-1.97602
C	-1.97602	-4.23591	2.43628
C	-1.97602	4.23591	-2.43628
C	-2.31923	2.82657	-0.08267
C	-0.08267	-2.31923	2.82657
C	-2.82657	0.08267	-2.31923
C	-2.31923	-2.82657	0.08267
C	2.31923	-2.82657	-0.08267
C	-4.23591	-2.43628	1.97602
C	1.97602	-4.23591	-2.43628
C	2.82657	-0.08267	-2.31923
C	2.43628	1.97602	4.23591
C	2.31923	2.82657	0.08267
C	-0.08267	2.31923	-2.82657
C	0.08267	-2.31923	-2.82657
C	-4.23591	2.43628	-1.97602
C	2.82657	0.08267	2.31923
C	-2.43628	-1.97602	4.23591

C	-2.43628	1.97602	-4.23591
C	0.08267	2.31923	2.82657
C	4.23591	2.43628	1.97602
C	1.97602	4.23591	2.43628
C	2.43628	-1.97602	-4.23591

SCF energy GEOOPT = -3833.102315706 H
ZPE = 498.1 kJ/mol
FREEH energy = 710.05 kJ/mol
FREEH entropy = 1.88934 kJ/mol

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e	21.70	0.00000	NO	YES
8	e	21.70	0.00000	NO	YES
9	t	25.41	0.10055	YES	YES
10	t	25.41	0.10054	YES	YES
11	t	25.41	0.10053	YES	YES
12	e	27.92	0.00000	NO	YES
13	t	32.35	0.01201	YES	YES
14	t	32.35	0.01201	YES	YES
15	t	32.35	0.01199	YES	YES
16	t	34.53	0.04800	YES	YES
17	t	34.53	0.04801	YES	YES
18	t	34.53	0.04799	YES	YES
19	e	45.90	0.00000	NO	YES
20	e	45.90	0.00000	NO	YES
21	t	46.44	0.03328	YES	YES
22	t	46.44	0.03327	YES	YES
23	t	46.44	0.03328	YES	YES
24	t	50.80	0.18303	YES	YES
25	t	50.80	0.18304	YES	YES
26	t	50.80	0.18304	YES	YES
27	e	54.53	0.00000	NO	YES
28	e	54.53	0.00000	NO	YES
29	t	57.83	0.41431	YES	YES
30	t	57.83	0.41427	YES	YES
31	t	57.83	0.41426	YES	YES
32	e	66.29	0.00000	NO	YES
33	t	68.99	0.06422	YES	YES
34	t	68.99	0.06421	YES	YES
35	t	68.99	0.06421	YES	YES
36	e	70.60	0.00000	NO	YES
37	e	70.60	0.00000	NO	YES
38	e	72.78	0.00000	NO	YES
39	t	73.05	0.00011	YES	YES
40	t	73.05	0.00011	YES	YES
41	t	73.05	0.00011	YES	YES
42	t	75.95	0.00002	YES	YES
43	t	75.95	0.00002	YES	YES
44	t	75.95	0.00002	YES	YES
45	t	80.09	0.27427	YES	YES
46	t	80.09	0.27425	YES	YES
47	t	80.09	0.27431	YES	YES
48	t	87.46	1.09851	YES	YES
49	t	87.46	1.09849	YES	YES
50	t	87.46	1.09847	YES	YES
51	e	87.79	0.00000	NO	YES
52	e	87.79	0.00000	NO	YES
53	t	92.68	0.02452	YES	YES
54	t	92.68	0.02454	YES	YES
55	t	92.68	0.02451	YES	YES
56	t	96.03	0.15542	YES	YES
57	t	96.03	0.15543	YES	YES
58	t	96.03	0.15542	YES	YES
59	e	96.47	0.00000	NO	YES
60	t	111.67	0.02599	YES	YES
61	t	111.67	0.02598	YES	YES
62	t	111.67	0.02598	YES	YES
63	e	123.59	0.00000	NO	YES
64	e	123.59	0.00000	NO	YES
65	t	125.45	1.06214	YES	YES
66	t	125.45	1.06235	YES	YES
67	t	125.45	1.06234	YES	YES
68	e	126.94	0.00000	NO	YES
69	t	129.66	0.63934	YES	YES
70	t	129.66	0.63912	YES	YES
71	t	129.66	0.63915	YES	YES
72	e	140.14	0.00000	NO	YES
73	t	141.50	0.00320	YES	YES
74	t	141.50	0.00320	YES	YES
75	t	141.50	0.00320	YES	YES
76	t	155.86	0.85683	YES	YES
77	t	155.86	0.85682	YES	YES
78	t	155.86	0.85682	YES	YES
79	e	324.68	0.00000	NO	YES
80	e	324.68	0.00000	NO	YES
81	t	324.97	0.19928	YES	YES
82	t	324.97	0.19891	YES	YES
83	t	324.97	0.19925	YES	YES
84	t	326.47	9.26305	YES	YES
85	t	326.47	9.26324	YES	YES
86	t	326.47	9.26301	YES	YES
87	t	335.98	11.97834	YES	YES
88	t	335.98	11.97613	YES	YES
89	t	335.98	11.97807	YES	YES
90	e	337.01	0.00000	NO	YES
91	t	340.71	0.12353	YES	YES
92	t	340.71	0.12349	YES	YES
93	t	340.71	0.12354	YES	YES
94	t	342.45	33.44259	YES	YES
95	t	342.45	33.44026	YES	YES
96	t	342.45	33.44044	YES	YES
97	e	342.72	0.00000	NO	YES
98	e	342.72	0.00000	NO	YES
99	e	346.36	0.00000	NO	YES
100	t	346.43	11.83653	YES	YES
101	t	346.43	11.83652	YES	YES
102	t	346.43	11.83667	YES	YES
103	t	367.57	81.76590	YES	YES
104	t	367.57	81.76620	YES	YES
105	t	367.57	81.76711	YES	YES
106	e	370.90	0.00000	NO	YES
107	e	370.90	0.00000	NO	YES
108	t	372.10	2.41796	YES	YES
109	t	372.10	2.41827	YES	YES
110	t	372.10	2.41716	YES	YES
111	e	373.13	0.00000	NO	YES
112	t	377.37	15.76121	YES	YES
113	t	377.37	15.75960	YES	YES
114	t	377.37	15.76112	YES	YES
115	t	433.66	0.29812	YES	YES
116	t	433.66	0.29804	YES	YES
117	t	433.66	0.29811	YES	YES
118	t	435.36	3.27790	YES	YES
119	t	435.36	3.27820	YES	YES
120	t	435.36	3.27799	YES	YES
121	e	436.02	0.00000	NO	YES
122	e	436.02	0.00000	NO	YES
123	t	445.84	9.29743	YES	YES
124	t	445.84	9.29818	YES	YES
125	t	445.84	9.30013	YES	YES
126	t	446.74	1.22091	YES	YES
127	t	446.74	1.22041	YES	YES
128	t	446.74	1.21844	YES	YES
129	e	448.52	0.00000	NO	YES
130	e	451.00	0.00000	NO	YES
131	e	451.00	0.00000	NO	YES
132	t	451.61	21.76903	YES	YES
133	t	451.61	21.76804	YES	YES
134	t	451.61	21.76827	YES	YES
135	e	467.16	0.00000	NO	YES
136	t	467.37	0.52078	YES	YES
137	t	467.37	0.52080	YES	YES
138	t	467.37	0.52090	YES	YES
139	t	500.57	169.51734	YES	YES
140	t	500.57	169.52306	YES	YES
141	t	500.57	169.52242	YES	YES
142	e	509.14	0.00000	NO	YES
143	t	514.19	0.63774	YES	YES
144	t	514.19	0.63618	YES	YES
145	t	514.19	0.63730	YES	YES
146	e	514.59	0.00000	NO	YES
147	e	514.59	0.00000	NO	YES
148	t	516.06	47.58534	YES	YES
149	t	516.06	47.58185	YES	YES
150	t	516.06	47.58002	YES	YES
151	t	1910.80	28.69899	YES	YES
152	t	1910.80	28.69876	YES	YES
153	t	1910.80	28.69881	YES	YES
154	e	1911.25	0.00000	NO	YES
155	e	1911.25	0.00000	NO	YES
156	t	1931.09	418.54599	YES	YES
157	t	1931.09	418.54286	YES	YES
158	t	1931.09	418.54315	YES	YES
159	t	1949.45	655.18646	YES	YES
160	t	1949.45	655.18689	YES	YES
161	t	1949.45	655.18356	YES	YES
162	a	1954.67	0.00000	NO	YES
163	t	2064.02	6.38174	YES	YES
164	t	2064.02	6.38178	YES	YES
165	t	2064.02	6.38175	YES	YES
166	t	2068.08	1050.29014	YES	YES
167	t	2068.08	1050.28986	YES	YES
168	t	2068.08	1050.28991	YES	YES
169	e	2068.37	0.00000	NO	YES
170	e	2068.37	0.00000	NO	YES
171	t	2092.65	3143.09610	YES	YES
172	t	2092.65	3143.09595	YES	YES
173	t	2092.65	3143.09645	YES	YES
174	a	2115.85	0.00000	NO	YES

Structural Discussions of Compounds 1 – 4

Table S13. Experimental bond lengths *d* [Å] and angles [°] of the metallic core of all discussed compounds. Mean values are given for **3a**, **4a** and **4b**.

			$d_{Ag\text{-}Ag}$ [Å]	$d_{Ag\text{-}M1}$ [Å]	$d_{Ag\text{-}M2}$ [Å]	M-Ag-M [°]
1	**a**	$Ag\{M(CO)_6\}_2^-$	-	2.8359(5)	2.8467(5)	174.027(14)
	b		-	-	-	-
2	**a**	$Ag_2\{M(CO)_6\}_3^-$	2.8891(11)	2.8081(8)	2.8672(8)	167.49(3)
	b		2.8818(12)	2.8166(6)	2.8710(7)	167.40(3)
3	**a**	$Ag_6\{M(CO)_6\}_5^+$	2.851		2.957	150.84
4	**a**	$Ag_6\{M(CO)_6\}_4^{2+}$	2.9011		2.9858	177.27
	b		2.8995		2.9835	177.30

Table S14. Experimental bond lengths *d* [Å] of **1a**$^-$, **2a**$^-$, **2b**$^-$, **3a**$^+$, **4a**$^{2+}$ and **4b**$^{2+}$ sorted due to the hapticity.

		1a$^-$	**2a**$^-$	**2b**$^-$	**3a**$^+$	**4a**$^{2+}$	**4b**$^{2+}$
$d_{Ag\text{-}M}$	μ_1	2.836 – 2.847	2.808	2.817	-	-	-
	μ_2	-	2.867	2.871	2.891 – 2.952	-	-
	μ_3	-	-	-	2.941 – 3.067	2.966 – 3.015	2.966 – 3.016
$d_{Ag\text{-}C}$	μ_1	2.544 – 2.669	2.505 – 2.629	2.524 – 2.597	-	-	-
	μ_2	-	2.551	2.568	2.57 – 2.70	-	-
	μ_3	-	-	-	2.57 – 2.69	2.592 – 2.701	2.582 – 2.706
$d_{M\text{-}C}$	μ_1	2.111 – 2.150	2.107 – 2.149	2.091 – 2.128	-	-	-
	μ_2	-	2.124 – 2.164	2.110 – 2.141	2.07 – 2.21	-	-
	μ_3	-	-	-	2.07 – 2.23	2.110 – 2.219	2.102 – 2.173
$d_{CAg\text{-}O}$	μ_1	1.146 – 1.157	1.157 – 1.160	1.139 – 1.157	-	-	-
	μ_2	-	1.152	1.152	1.15 – 1.20	-	-
	μ_3	-	-	-	1.13 – 1.21	1.096 – 1.150	1.119 – 1.161
$d_{Cfree\text{-}O}$	μ_1	1.137 – 1.140	1.133 – 1.164	1.124 – 1.150	-	-	-
	μ_2	-	1.126 – 1.149	1.131 – 1.151	1.10 – 1.24	-	-
	μ_3	-	-	-	1.10 – 1.17	1.098 – 1.166	1.113 – 1.153

$[NEt_4]^+[Ag\{M(CO)_6\}_2]^-$ (M = Nb (**1a**))

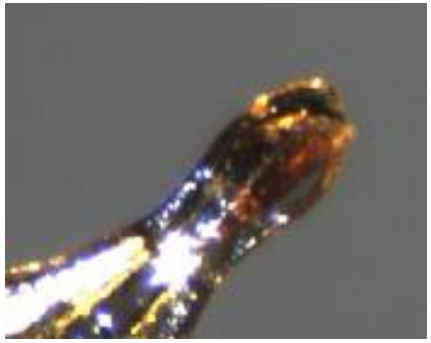


Fig. S8. Crystal of **1a** mounted on a 0.03 mm micromount.

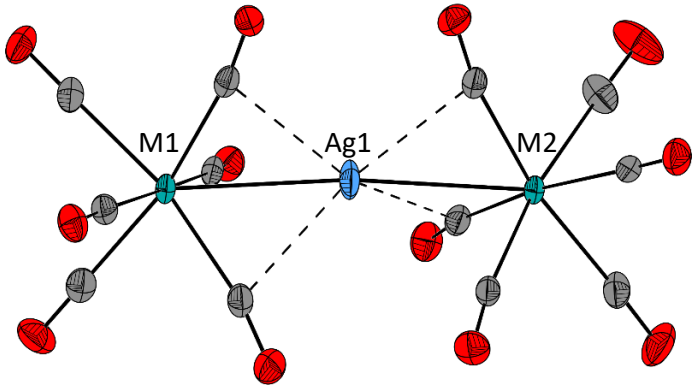


Fig. S9. Atom labels of $\mathbf{1a}^-$ (M = Nb) for the assignment of bond lengths and angles.

Table S15. Range and mean values of bond length [Å] of **1a**$^-$ (M = Nb) and **1b**$^-$ (M = Ta).

	1a$^-$ exp.		**calc. (C_2)** [a]		**1b$^-$ calc. (D_{3d})**[a]	
	range	**av.**	**range**	**av.**	**range**	**av.**
Ag-M	2.836 – 2.847	2.842	2.831		2.818	
Ag-C	2.544 – 2.669	2.608	2.441 – 2.478	2.460	2.639	
C-O	1.137 – 1.157	1.145	1.159 – 1.167	1.162	1.161 – 1.165	1.163
C_{Ag}-O	1.146 – 1.157	1.152	1.166 – 1.167	1.167	1.161	
C_{free}-O	1.137 – 1.140	1.139	1.159 – 1.161	1.160	1.165	
M-C	2.111 – 2.150	2.135	2.123 – 2.140	2.130	2.128 – 2.142	2.135
M-C_{Ag}	2.111 – 2.138	2.145	2.139 – 2.140	2.140	2.128	
M-C_{free}	2.137 – 2.150	2.143	2.123 – 2.130	2.125	2.142	

[a] (RI-)BP86-D3(BJ)/def2-TZVPP

$[NEt_4]^+[Ag_2\{M(CO)_6\}_3]^-$ (M = Nb (**2a**), Ta (**2b**)

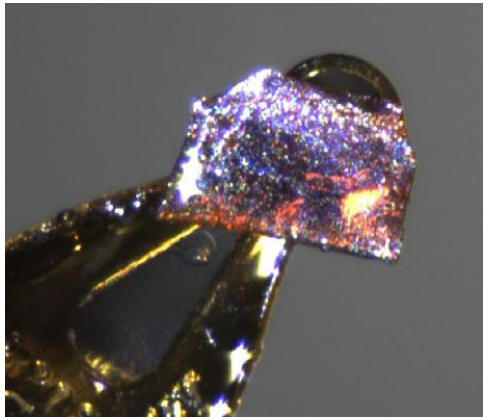


Fig. S10. Crystal of **2a** mounted on a 0.2 mm micromount.

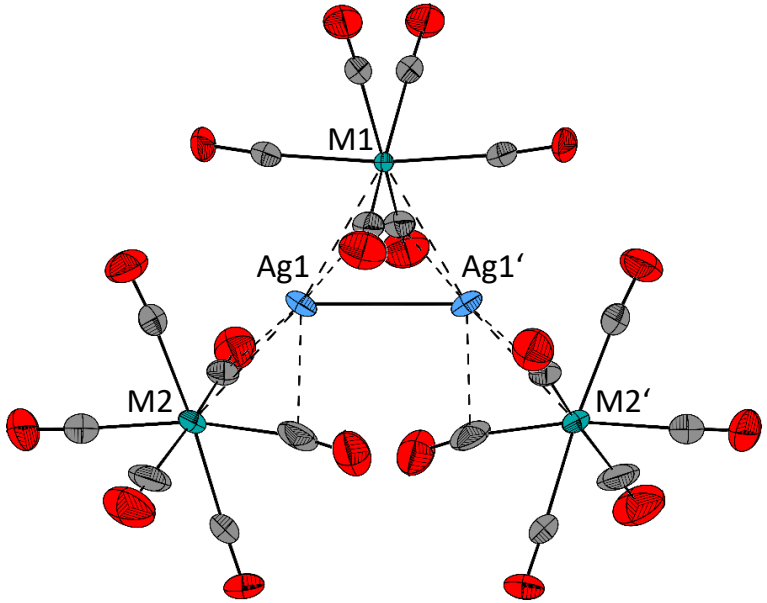


Fig. S11. Atom labels of **2a**$^-$ (M = Nb) or **2b**$^-$ (M = Ta) for the assignment of bond lengths and angles.

Table S16. Range and mean values of bond length [Å] of **2a**$^{-}$ (M = Nb) and **2b**$^{-}$ (M = Ta).

	2a^{-}		**calc. (*C*$_2$)** [a]		**2b**$^{-}$		**calc. (*C*$_2$)**[a]	
	range	**av.**	**range**	**av.**	**range**	**av.**	**range**	**av.**
Ag-Ag	2.889		2.791		2.882		2.784	
Ag-M	2.808 – 2.867	2.838	2.777 – 2.890	2.834	2.816 – 2.871	2.844	2.790 – 2.901	2.846
Ag-C	2.505 – 2.629	2.562	2.327 – 2.640	2.528	2.524 – 2.597	2.563	2.348 – 2.645	2.544
C-O	1.126 – 1.164	1.149	1.156 – 1.165	1.160	1.124 – 1.157	1.143	1.157 – 1.166	1.161
C$_{Ag}$-O	1.152 – 1.164	1.158	1.157 – 1.165	1.162	1.134 – 1.157	1.146	1.158 – 1.166	1.164
C$_{free}$-O	1.126 – 1.150	1.141	1.156 – 1.159	1.157	1.124 – 1.151	1.139	1.157 – 1.160	1.158
M-C	2.107 – 2.164	2.129	2.114 – 2.158	2.134	2.105 – 2.141	2.116	2.119 – 2.159	2.137
M-C$_{Ag}$	2.107 – 2.124	2.116	2.135 – 2.158	2.142	2.105 – 2.114	2.105	2.138 – 2.159	2.144
M-C$_{free}$	2.119 – 2.164	2.140	2.114 – 2.138	2.126	2.110 – 2.141	2.120	2.119 – 2.141	2.130

[a] (RI-)BP86-D3(BJ)/def2-TZVPP

$[Ag_6\{M(CO)_6\}_5]^+[Al(OC(CF_3)_3)_4]^-$ (M = Nb (**3a**))

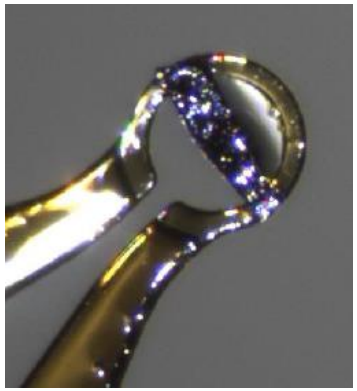


Fig. S12. Crystal of **3a** mounted on a 0.1 mm micromount.

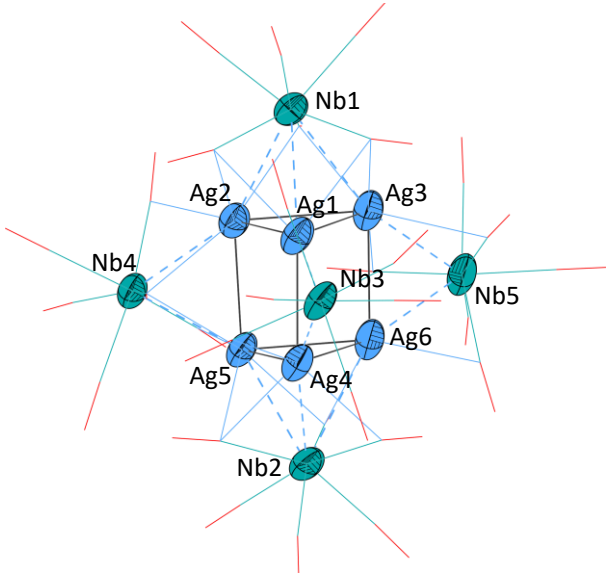


Fig. S13. Atom labels of $\mathbf{3a}^+$ for the assignment of bond lengths and angles.

Due to the poor crystallographic data the given average bond lengths are not reliable, but can be seen as rough guide.

Table S17. Range and mean values of bond length [Å] of **3a**$^+$ (M = Nb).

	3a$^+$		**calc. (D_{3h})**[a]	
	range	**av.**	**range**	**av.**
Ag-Ag	2.776 – 2.948	2.851	2.830 – 2.842	2.838
Ag-M	2.891 – 3.067	2.957	2.873 – 2.964	2.919
Ag-C	2.57 – 2.70	2.62	2.497 – 2.549	2.521
C-O	1.10 – 1.24	1.16	1.144 – 1.164	1.153
C_{Ag}-O	1.13 – 1.21	1.16	1.145 – 1.164	1.160
C_{free}-O	1.10 – 1.24	1.15	1.144 – 1.149	1.146
M-C	2.02 – 2.23	2.13	2.118 – 2.160	2.146
M-C_{Ag}	2.02 – 2.19	2.11	2.150 – 2.160	2.153
M-C_{free}	2.07 – 2.23	2.15	2.118 – 2.149	2.139

[a] (RI-)BP86-D3(BJ)/def2-TZVPP

$[Ag_6\{M(CO)_6\}_4]^{2+}[Al(OC(CF_3)_3)_4]_2^-$ (M = Nb (**4a**), Ta (**4b**))

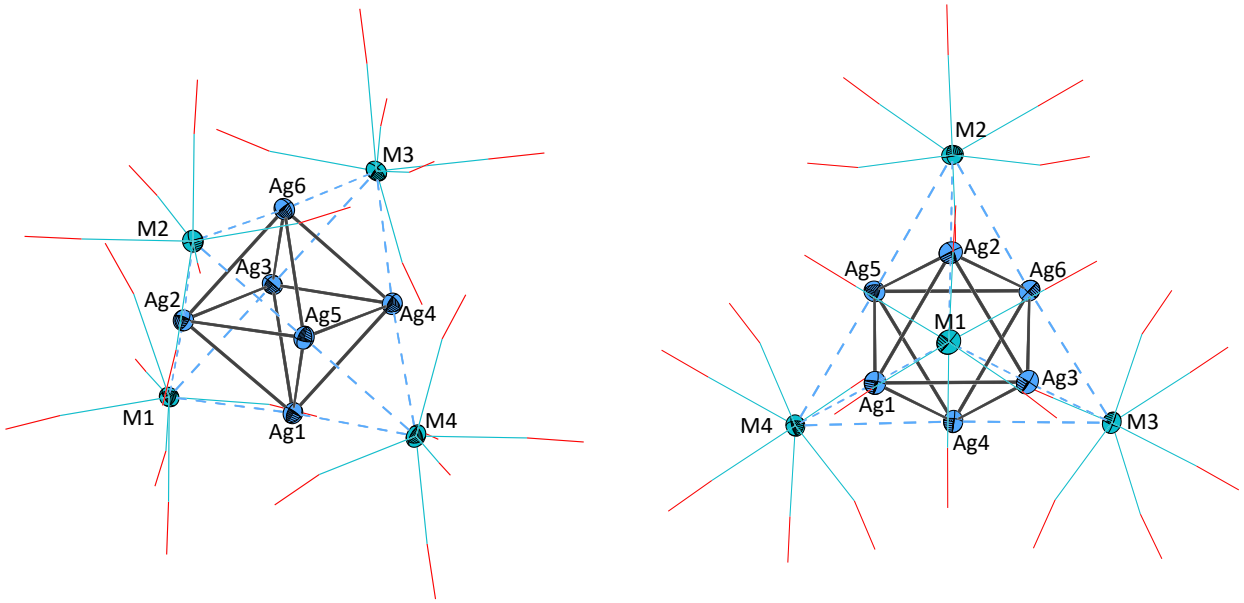


Fig. S14. Atom labels of **4a**$^{2+}$ or **4b**$^{2+}$ (left: side view, right: front view) for the assignment of bond lengths and angles.

Table S18. Range and mean values of bond length [Å] of **4a**$^{2+}$ (M = Nb) and **4b**$^{2+}$ (M = Ta).

	4a^{2+}		**calc. (*T*)**[a]		**4b**$^{2+}$		**calc. (*T*)**[a]	
	range	**av.**	**range**	**av**	**range**	**av.**	**range**	**av.**
Ag-Ag	2.855 – 2.925	2.901	2.907		2.859 – 2.926	2.900	2.904	
Ag-M	2.966 – 3.015	2.986	2.954		2.966 – 3.016	2.984	2.967	
Ag-C	2.592 – 2.701	2.634	2.429		2.582 – 2.706	2.635	2.446	
C-O	1.096 – 1.166	1.128	1.141 – 1.160	1.151	1.113 – 1.161	1.135	1.141 – 1.161	1.151
C_{Ag}-O	1.096 – 1.150	1.132	1.160		1.119 – 1.161	1.147	1.161	
C_{free}-O	1.098 – 1.166	1.124	1.141		1.113 – 1.153	1.123	1.141	
M-C	2.110 – 2.219	2.168	2.151 – 2.167	2.159	2.102 – 2.173	2.142	2.154 – 2.168	2.161
M-C_{Ag}	2.133 – 2.207	2.158	2.151		2.102 – 2.173	2.123	2.154	
M-C_{free}	2.110 – 2.219	2.179	2.167		2.119 – 1.170	2.162	2.168	

[a] (RI-)BP86-D3(BJ)/def2-TZVPP

Single-Crystal Diffraction Results for Compounds 1 – 4

Table S19. Crystallographic data for complexes **1** – **4**.

	1a	**2a**	**2b**	**3a**	**4a**	**4b**
CCDC	1998854	1998851	1998852	1998853	1909279	1998922
Empirical formula	$C_{20}H_{20}AgNNb_2O_{12}$	$C_{26}H_{20}Ag_2NNb_3O_{18}$	$C_{26}H_{20}Ag_2NO_{18}Ta_3$	$C_{61}H_5Ag_6AlF_{46}Nb_5O_{34}$	$C_{80}H_8Ag_6Al_2F_{88}Nb_4O_{32}$	$C_{80}H_8Ag_6Al_2F_{88}O_{32}Ta_4$
Formula weight	760.06	1128.90	1393.02	3294.40	4225.68	4577.85
Temperature/K	100(2)	100(2)	200(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic	orthorhombic	orthorhombic
Space group	$P2_1/c$	$C2/c$	$C2/c$	$P\overline{1}$	$Pbca$	$Pbca$
a/Å	18.187(3)	19.244(3)	19.412(5)	17.242(6)	30.4820(12)	30.459(12)
b/Å	10.524(2)	10.5949(16)	10.642(2)	18.251(4)	21.4374(8)	21.418(12)
c/Å	14.594(3)	18.888(2)	18.956(3)	18.301(4)	36.6092(14)	36.508(17)
α/°	90	90	90	77.593(10)	90	90
β/°	107.735(6)	105.273(3)	105.126(12)	63.291(16)	90	90
γ/°	90	90	90	62.504(10)	90	90
Volume/Å^3	2660.5(9)	3715.0(9)	3780.1(14)	4563(2)	23922.5(16)	23817(19)
Z	4	4	4	2	8	8
ρ_{calc}g/cm^3	1.898	2.018	2.448	2.398	2.347	2.553
μ/mm^{-1}	1.635	2.005	9.739	16.727	1.553	4.848
F(000)	1488	2176	2560	3114	16064.0	17088
Crystal size/mm^3	0.150×0.100×0.050	0.100×0.100×0.030	0.200×0.200×0.050	0.08×0.07×0.02	0.080 × 0.020 × 0.020	0.300×0.100×0.060
Radiation	MoK_α (λ=0.71073)	MoK_α (λ=0.71073)	MoK_α (λ=0.71073)	CuK_α (λ=1.54178)	MoKα (λ = 0.71073)	MoK_α (λ=0.71073)
2Θ range for data collection/°	4.53 to 56.76	4.39 to 50.26	4.35 to 56.78	5.41 to 109.91	2.224 to 50.14	2.23 to 52.86
Index ranges	-24 ≤ h ≤ 24, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19	-17 ≤ h ≤ 22, -12 ≤ k ≤ 12, -22 ≤ l ≤ 21	-25 ≤ h ≤ 25, -14 ≤ k ≤ 14, -25 ≤ l ≤ 24	-17 ≤ h ≤ 17, -18 ≤ k ≤ 19, -19 ≤ l ≤ 19	-36 ≤ h ≤ 36, -25 ≤ k ≤ 25, -43 ≤ l ≤ 43	-38 ≤ h ≤ 38, -26 ≤ k ≤ 26, -45 ≤ l ≤ 45
Reflections collected	58916	16972	39095	58871	743919	542712
Independent reflections	6605 [R_{int} = 0.0411, R_{sigma} = 0.0230]	3314 [R_{int} = 0.0960, R_{sigma} = 0.0853]	4713 [R_{int} = 0.0362, R_{sigma} = 0.0244]	11089 [R_{int} = 0.1317, R_{sigma} = 0.1087]	21232 [R_{int} = 0.0966, R_{sigma} = 0.0312]	24489 [R_{int} = 0.0879, R_{sigma} = 0.0307]
Data/restraints/parameters	6605/0/329	3314/144/274	4713/129/271	11089/7758/1677	21232/50458/3324	24489/43315/3072
Goodness-of-fit on F^2	1.075	1.069	1.156	1.043	1.264	1.215
Final R indexes [I>=2σ (I)]	R_1 = 0.0344, wR_2 = 0.0958	R_1 = 0.0475, wR_2 = 0.0833	R_1 = 0.0352, wR_2 = 0.1181	R_1 = 0.0945, wR_2 = 0.2487	R_1 = 0.0702, wR_2 = 0.1514	R_1 = 0.0485, wR_2 = 0.0917
Final R indexes [all data]	R_1 = 0.0407, wR_2 = 0.1016	R_1 = 0.0906, wR_2 = 0.0939	R_1 = 0.0372, wR_2 = 0.1203	R_1 = 0.1421, wR_2 = 0.2899	R_1 = 0.0804, wR_2 = 0.1559	R_1 = 0.0636, wR_2 = 0.0978
Largest diff. peak/hole / e Å^{-3}	1.50/-1.20	0.73/-1.03	1.60/-1.87	2.21/-1.44	1.46/-1.08	1.70/-1.25

Full Details to the Single-Crystal Structure Determinations

Structure of **1a**

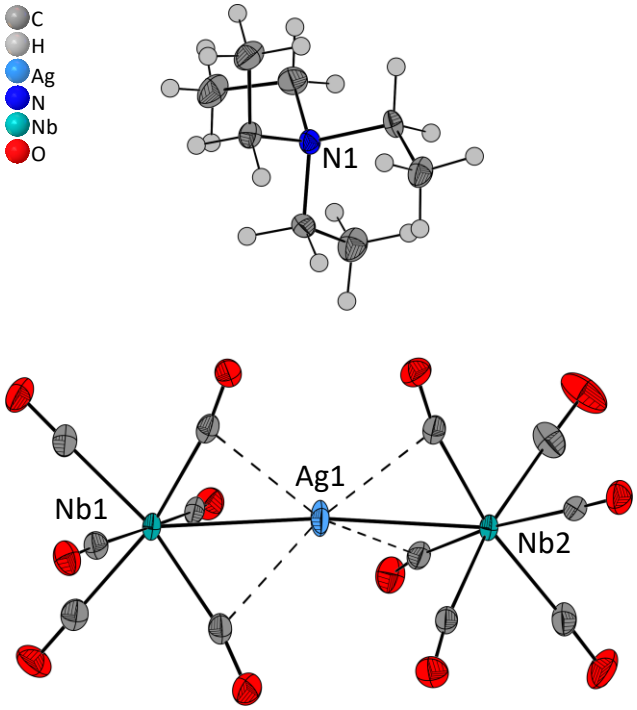


Fig. S15. Molecular structure of **1a**. Thermal ellipsoids are shown at the 50 % probability level.

Structure Tables

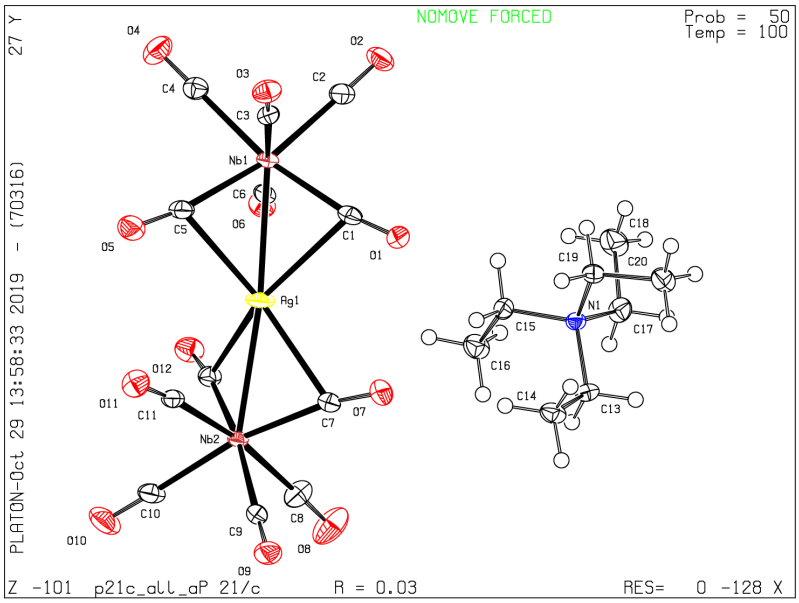


Table 1. Crystal data and structure refinement for p21c_all_a-finalcif.cif

CCDC number	1998854
Empirical formula	$C_{20}H_{20}AgNNb_2O_{12}$
Formula weight	760.06
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	$P2_1/c$ (14)
a [Å]	18.187(3)
b [Å]	10.524(2)
c [Å]	14.594(3)
α [Å]	90
β [Å]	107.735(6)
γ [Å]	90
Volume [Å^3]	2660.5(9)
Z	4
ρ_{calc} [g/cm^3]	1.898
μ [mm^{-1}]	1.635
F(000)	1488
Crystal size [mm^3]	0.150×0.100×0.050
Crystal colour	red
Crystal shape	needle
Radiation	MoK_α (λ=0.71073)
2Θ range [°]	4.53 to 56.76
Index ranges	-24 ≤ h ≤ 24, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	58916
Independent reflections	6605, R_{int} = 0.0411 R_{sigma} = 0.0230
Completeness to θ = 25.242°	100.00
Data / Restraints / Parameters	6605/0/329
Goodness-of-fit on F^2	1.075
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0344, wR_2 = 0.0958
Final *R* indexes [all data]	R_1 = 0.0407, wR_2 = 0.1016
Largest peak/hole [eÅ^3]	1.50/-1.20

Table 2. Bond lengths and angles for p21c_all_a-finalcif.cif.

Atom - Atom	**Length [Å]**
Ag1 - C7	2.544(3)
Ag1 - C5	2.607(3)
Ag1 - C12	2.611(3)
Ag1 - C1	2.669(3)
Ag1 - Nb1	2.8359(5)
Ag1 - Nb2	2.8467(5)
O1 - C1	1.155(4)
C1 - Nb1	2.122(3)
Nb1 - C6	2.130(3)
Nb1 - C5	2.134(3)
Nb1 - C4	2.139(3)
Nb1 - C3	2.139(3)
Nb1 - C2	2.150(3)
N1 - C19	1.514(4)
N1 - C15	1.516(4)
N1 - C13	1.519(4)
N1 - C17	1.521(4)
Nb2 - C7	2.111(3)
Nb2 - C11	2.133(3)
Nb2 - C8	2.136(3)
Nb2 - C12	2.138(3)
Nb2 - C9	2.141(3)
Nb2 - C10	2.150(3)
O2 - C2	1.138(4)
O4 - C4	1.140(4)
C3 - O3	1.139(4)
C5 - O5	1.153(4)
O6 - C6	1.147(4)
O7 - C7	1.157(4)
O8 - C8	1.139(4)
C9 - O9	1.137(4)
C10 - O10	1.139(4)
C11 - O11	1.146(4)
C12 - O12	1.152(4)
C13 - C14	1.516(4)
C15 - C16	1.520(4)
C17 - C18	1.508(5)
C19 - C20	1.514(4)

Atom - Atom - Atom	**Angle [°]**
C7 - Ag1 - C5	145.42(10)
C7 - Ag1 - C12	82.88(10)
C5 - Ag1 - C12	116.42(10)
C7 - Ag1 - C1	94.35(10)
C5 - Ag1 - C1	80.20(10)
C12 - Ag1 - C1	153.47(10)
C7 - Ag1 - Nb1	139.58(7)
C5 - Ag1 - Nb1	45.93(7)
C12 - Ag1 - Nb1	131.99(7)
C1 - Ag1 - Nb1	45.22(7)
C7 - Ag1 - Nb2	45.69(7)
C5 - Ag1 - Nb2	128.47(7)
C12 - Ag1 - Nb2	45.89(7)
C1 - Ag1 - Nb2	139.86(7)
Nb1 - Ag1 - Nb2	174.027(14)
O1 - C1 - Nb1	170.8(3)
O1 - C1 - Ag1	117.5(2)
Nb1 - C1 - Ag1	71.56(9)
C1 - Nb1 - C6	99.79(12)
C1 - Nb1 - C5	105.97(12)
C6 - Nb1 - C5	99.12(12)
C1 - Nb1 - C4	169.03(12)
C6 - Nb1 - C4	85.59(12)
C5 - Nb1 - C4	82.39(12)
C1 - Nb1 - C3	85.09(11)
C6 - Nb1 - C3	173.47(12)
C5 - Nb1 - C3	83.58(12)
C4 - Nb1 - C3	88.89(12)
C1 - Nb1 - C2	84.20(12)
C6 - Nb1 - C2	82.96(12)
C5 - Nb1 - C2	168.99(12)
C4 - Nb1 - C2	87.01(12)
C3 - Nb1 - C2	93.27(12)
C1 - Nb1 - Ag1	63.22(8)
C6 - Nb1 - Ag1	66.40(8)
C5 - Nb1 - Ag1	61.36(8)
C4 - Nb1 - Ag1	127.72(9)

C3 - Nb1 - Ag1	119.96(8)
C2 - Nb1 - Ag1	128.64(9)
C19 - N1 - C15	106.2(2)
C19 - N1 - C13	110.9(2)
C15 - N1 - C13	111.4(2)
C19 - N1 - C17	111.1(2)
C15 - N1 - C17	111.1(2)
C13 - N1 - C17	106.2(2)
C7 - Nb2 - C11	99.47(12)
C7 - Nb2 - C8	84.72(13)
C11 - Nb2 - C8	171.02(13)
C7 - Nb2 - C12	106.80(12)
C11 - Nb2 - C12	98.00(12)
C8 - Nb2 - C12	88.29(13)
C7 - Nb2 - C9	81.82(12)
C11 - Nb2 - C9	84.78(12)
C8 - Nb2 - C9	87.98(13)
C12 - Nb2 - C9	170.25(12)
C7 - Nb2 - C10	169.60(12)
C11 - Nb2 - C10	83.93(13)
C8 - Nb2 - C10	90.61(14)
C12 - Nb2 - C10	82.28(13)
C9 - Nb2 - C10	88.75(12)
C7 - Nb2 - Ag1	59.56(8)
C11 - Nb2 - Ag1	70.73(8)
C8 - Nb2 - Ag1	118.11(11)
C12 - Nb2 - Ag1	61.22(8)
C9 - Nb2 - Ag1	128.32(8)
C10 - Nb2 - Ag1	130.63(9)
O2 - C2 - Nb1	177.4(3)
O4 - C4 - Nb1	179.4(3)
O3 - C3 - Nb1	178.0(3)
O5 - C5 - Nb1	170.7(3)
O5 - C5 - Ag1	116.3(2)
Nb1 - C5 - Ag1	72.71(10)
O6 - C6 - Nb1	172.5(3)
O7 - C7 - Nb2	169.3(3)
O7 - C7 - Ag1	115.8(2)
Nb2 - C7 - Ag1	74.75(10)
O8 - C8 - Nb2	176.4(3)
O9 - C9 - Nb2	177.9(3)
O10 - C10 - Nb2	178.3(3)
O11 - C11 - Nb2	173.1(3)
O12 - C12 - Nb2	171.0(3)
O12 - C12 - Ag1	115.6(2)
Nb2 - C12 - Ag1	72.89(10)
C14 - C13 - N1	115.5(2)
N1 - C15 - C16	115.9(3)
C18 - C17 - N1	115.1(3)
N1 - C19 - C20	115.0(3)

Table 3. Torsion angles for p21c_all_a-finalcif.cif.

Atom - Atom - Atom - Atom	Torsion Angle [°]
C19 - N1 - C13 - C14	53.5(3)
C15 - N1 - C13 - C14	-64.6(3)
C17 - N1 - C13 - C14	174.3(3)
C19 - N1 - C15 - C16	174.5(3)
C13 - N1 - C15 - C16	-64.6(3)
C17 - N1 - C15 - C16	53.5(3)
C19 - N1 - C17 - C18	-62.1(4)
C15 - N1 - C17 - C18	55.9(4)
C13 - N1 - C17 - C18	177.2(3)
C15 - N1 - C19 - C20	177.5(3)
C13 - N1 - C19 - C20	56.3(3)
C17 - N1 - C19 - C20	-61.6(3)

Structure of **1b**

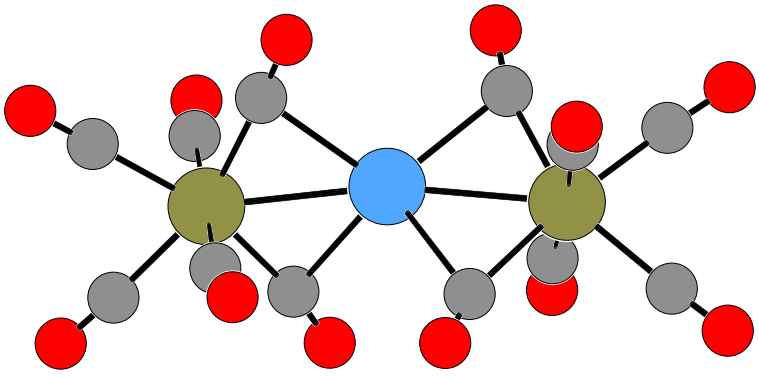


Fig. S16. Enlarged molecule from molecular structure of **1b**.

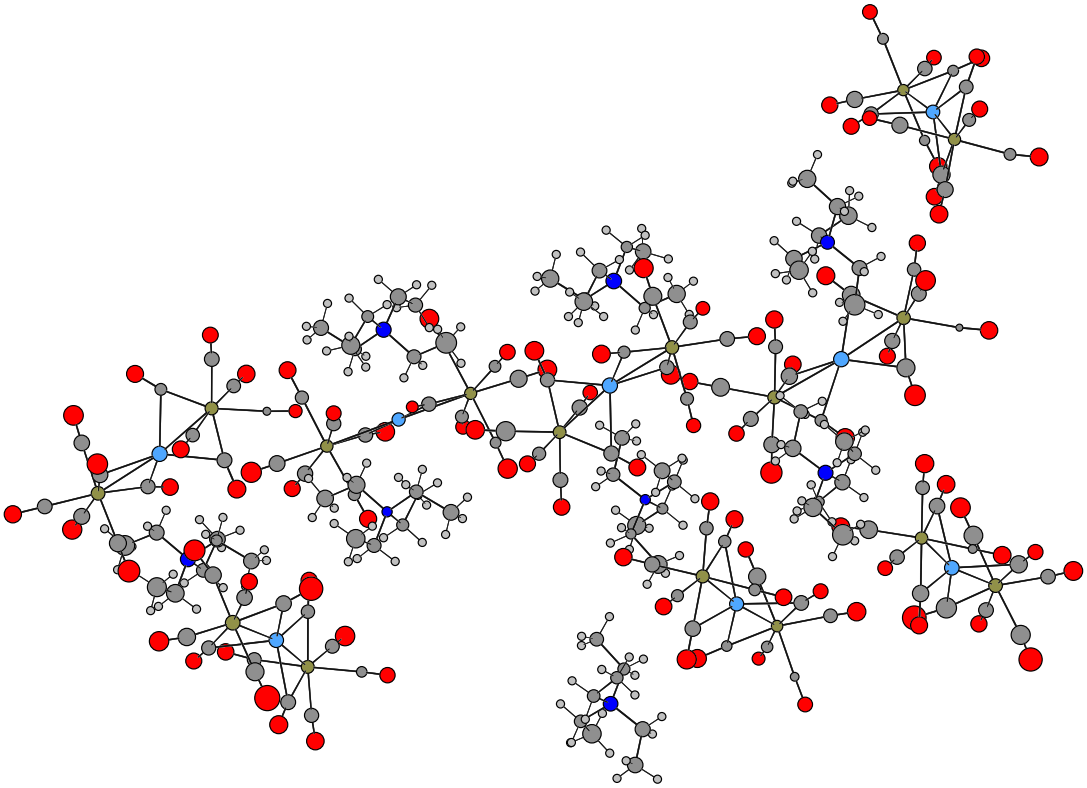


Fig. S17. Molecular structure of **1b**. The molecules are shown isotropically due to poor crystallographic data.

Structure of **2a**

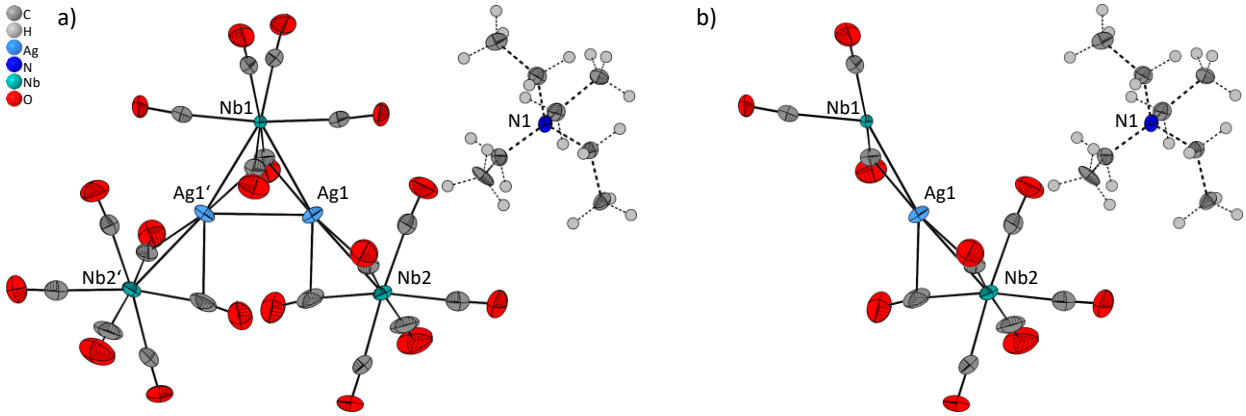


Fig. S18. Molecular structure (a) and asymmetric unit (b) of **2a**. $[NEt_4]^+$ is disordered around its special position. Thermal ellipsoids are shown at the 50 % probability level.

Structure Tables

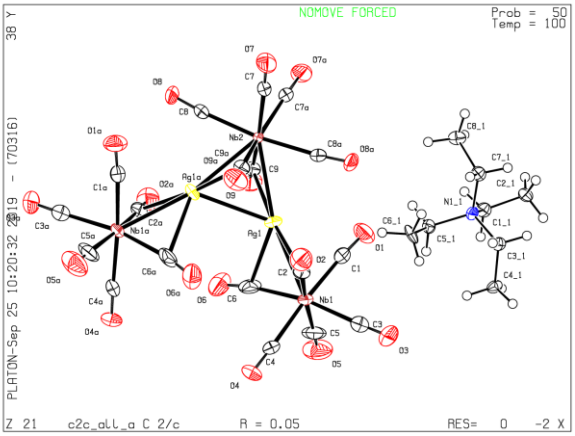


Table 1. Crystal data and structure refinement for c2c_all_a - final-finalcif.cif

CCDC number	1998851
Empirical formula	$C_{26}H_{20}Ag_2NNb_3O_{18}$
Formula weight	1128.90
Temperature [K]	100(2)
Crystal system	monoclinic
Space group (number)	*C2/c* (15)
a [Å]	19.244(3)
b [Å]	10.5949(16)
c [Å]	18.888(2)
α [Å]	90
β [Å]	105.273(3)
γ [Å]	90
Volume [Å^3]	3715.0(9)
Z	4
ρ_{calc} [g/cm^3]	2.018
μ [mm^{-1}]	2.005
F(000)	2176
Crystal size [mm^3]	0.100×0.100×0.030
Crystal colour	red
Crystal shape	block
Radiation	MoK_α (λ=0.71073)
2Θ range [°]	4.39 to 50.26
Index ranges	-17 ≤ h ≤ 22, -12 ≤ k ≤ 12, -22 ≤ l ≤ 21
Reflections collected	16972
Independent reflections	3314, R_{int} = 0.0960, R_{sigma} = 0.0853
Completeness to θ = 25.128°	99.70
Data / Restraints / Parameters	3314/144/274
Goodness-of-fit on F^2	1.069
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0475, wR_2 = 0.0833
Final *R* indexes [all data]	R_1 = 0.0906, wR_2 = 0.0939
Largest peak/hole [eÅ^3]	0.73/-1.03

Table 2. Bond lengths and angles for c2c_all_a - final-finalcif.cif.

Atom - Atom	**Length [Å]**
Ag1 - C6	2.505(7)
Ag1 - C9	2.551(7)
Ag1 - C2	2.629(8)
Ag1 - Nb1	2.8081(8)
Ag1 - Nb2	2.8672(8)
Ag1 - Ag1$^{\#1}$	2.8891(11)
O1 - C1	1.164(8)
C1 - Nb1	2.109(8)
Nb1 - C6	2.107(9)
Nb1 - C4	2.119(8)
Nb1 - C2	2.122(9)
Nb1 - C5	2.141(10)
Nb1 - C3	2.149(9)
Nb2 - C9	2.124(8)
Nb2 - C9$^{\#1}$	2.124(8)
Nb2 - C8$^{\#1}$	2.126(7)
Nb2 - C8	2.126(7)
Nb2 - C7$^{\#1}$	2.164(7)
Nb2 - C7	2.164(7)
O2 - C2	1.157(9)
O5 - C5	1.146(9)
C4 - O4	1.150(8)
C3 - O3	1.133(9)
C6 - O6	1.160(9)
C7 - O7	1.126(8)
C8 - O8	1.149(7)
C9 - O9	1.152(8)
N1_1 - C7_1	1.515(13)
N1_1 - C5_1	1.516(13)
N1_1 - C1_1	1.517(13)
N1_1 - C3_1	1.519(13)
C1_1 - C2_1	1.514(13)
C3_1 - C4_1	1.502(13)
C5_1 - C6_1	1.507(13)
C7_1 - C8_1	1.508(13)
Atom - Atom - Atom	**Angle [°]**
C6 - Ag1 - C9	103.8(3)
C6 - Ag1 - C2	80.8(3)
C9 - Ag1 - C2	174.2(2)
C6 - Ag1 - Nb1	46.3(2)
C9 - Ag1 - Nb1	135.70(18)
C2 - Ag1 - Nb1	45.80(19)
C6 - Ag1 - Nb2	144.1(2)
C9 - Ag1 - Nb2	45.70(17)
C2 - Ag1 - Nb2	131.21(19)
Nb1 - Ag1 - Nb2	167.49(3)
C6 - Ag1 - Ag1$^{\#1}$	91.5(2)
C9 - Ag1 - Ag1$^{\#1}$	62.69(16)
C2 - Ag1 - Ag1$^{\#1}$	121.24(17)

Nb1 - Ag1 - Ag1$^{\#1}$	132.743(18)
Nb2 - Ag1 - Ag1$^{\#1}$	59.747(14)
O1 - C1 - Nb1	175.7(6)
C6 - Nb1 - C1	101.0(3)
C6 - Nb1 - C4	80.9(3)
C1 - Nb1 - C4	175.2(3)
C6 - Nb1 - C2	103.8(3)
C1 - Nb1 - C2	96.5(3)
C4 - Nb1 - C2	87.3(3)
C6 - Nb1 - C5	82.3(3)
C1 - Nb1 - C5	86.0(3)
C4 - Nb1 - C5	90.0(3)
C2 - Nb1 - C5	172.8(3)
C6 - Nb1 - C3	169.5(3)
C1 - Nb1 - C3	86.2(3)
C4 - Nb1 - C3	91.3(3)
C2 - Nb1 - C3	82.8(3)
C5 - Nb1 - C3	90.6(3)
C6 - Nb1 - Ag1	59.26(18)
C1 - Nb1 - Ag1	66.29(19)
C4 - Nb1 - Ag1	118.26(19)
C2 - Nb1 - Ag1	62.63(19)
C5 - Nb1 - Ag1	124.4(2)
C3 - Nb1 - Ag1	131.2(2)
C9 - Nb2 - C9$^{\#1}$	117.8(4)
C9 - Nb2 - C8$^{\#1}$	96.5(3)
C9$^{\#1}$ - Nb2 - C8$^{\#1}$	87.3(3)
C9 - Nb2 - C8	87.3(3)
C9$^{\#1}$ - Nb2 - C8	96.5(3)
C8$^{\#1}$ - Nb2 - C8	172.6(3)
C9 - Nb2 - C7$^{\#1}$	79.8(3)
C9$^{\#1}$ - Nb2 - C7$^{\#1}$	161.3(3)
C8$^{\#1}$ - Nb2 - C7$^{\#1}$	84.4(3)
C8 - Nb2 - C7$^{\#1}$	90.1(2)
C9 - Nb2 - C7	161.3(3)
C9$^{\#1}$ - Nb2 - C7	79.8(3)
C8$^{\#1}$ - Nb2 - C7	90.1(2)
C8 - Nb2 - C7	84.4(3)
C7$^{\#1}$ - Nb2 - C7	83.5(4)
C9 - Nb2 - Ag1	59.26(18)
C9$^{\#1}$ - Nb2 - Ag1	67.60(18)
C8$^{\#1}$ - Nb2 - Ag1	64.41(16)
C8 - Nb2 - Ag1	122.92(17)
C7$^{\#1}$ - Nb2 - Ag1	122.62(18)
C7 - Nb2 - Ag1	138.58(19)
C9 - Nb2 - Ag1$^{\#1}$	67.60(18)
C9$^{\#1}$ - Nb2 - Ag1$^{\#1}$	59.26(18)
C8$^{\#1}$ - Nb2 - Ag1$^{\#1}$	122.92(16)
C8 - Nb2 - Ag1$^{\#1}$	64.41(16)
C7$^{\#1}$ - Nb2 - Ag1$^{\#1}$	138.58(19)
C7 - Nb2 - Ag1$^{\#1}$	122.61(18)
Ag1 - Nb2 - Ag1$^{\#1}$	60.51(3)
O2 - C2 - Nb1	174.9(7)
O2 - C2 - Ag1	113.4(5)
Nb1 - C2 - Ag1	71.6(3)
O5 - C5 - Nb1	177.3(8)
O4 - C4 - Nb1	178.0(6)
O3 - C3 - Nb1	177.6(7)
O6 - C6 - Nb1	170.7(6)
O6 - C6 - Ag1	114.8(5)
Nb1 - C6 - Ag1	74.5(2)
O7 - C7 - Nb2	178.0(6)
O8 - C8 - Nb2	175.2(5)
O9 - C9 - Nb2	170.6(6)
O9 - C9 - Ag1	113.9(5)
Nb2 - C9 - Ag1	75.0(2)
C7_1 - N1_1 - C5_1	111.9(10)
C7_1 - N1_1 - C1_1	110.5(9)
C5_1 - N1_1 - C1_1	106.9(11)
C7_1 - N1_1 - C3_1	106.9(10)
C5_1 - N1_1 - C3_1	110.5(9)
C1_1 - N1_1 - C3_1	110.3(10)
C2_1 - C1_1 - N1_1	116.3(10)
C4_1 - C3_1 - N1_1	116.4(10)
C6_1 - C5_1 - N1_1	116.4(10)
C8_1 - C7_1 - N1_1	116.2(10)

Symmetry transformations used to generate equivalent atoms: #1: 1-X, +Y, 1.5-Z;

Structure of **2b**

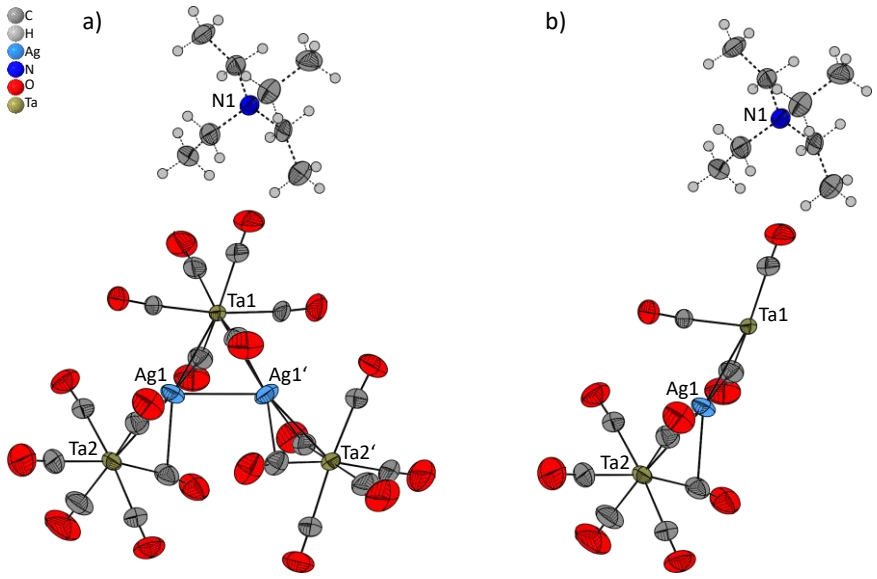


Fig. S19. Molecular structure (a) and asymmetric unit (b) of **2b**. Thermal ellipsoids are shown at the 50 % probability level.

Nb3, Ta3 and the cations $[NEt_4]^+$ are located on a special position in both structures of **2a** and **2b**. **2b** was measured at 200 K, since at 100 K the superlattice was obtained.

Structure Tables

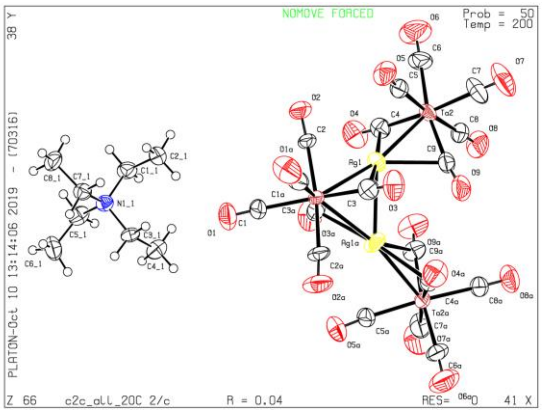


Table 1. Crystal data and structure refinement for c2c_all_200_a-finalcif.cif

CCDC number	1998852
Empirical formula	$C_{26}H_{20}Ag_2NO_{18}Ta_3$
Formula weight	1393.02
Temperature [K]	200(2)
Crystal system	monoclinic
Space group (number)	$C2/c$ (15)
a [Å]	19.412(5)
b [Å]	10.642(2)
c [Å]	18.956(3)
α [Å]	90
β [Å]	105.126(12)
γ [Å]	90
Volume [Å^3]	3780.1(14)
Z	4
ρ_{calc} [g/cm^3]	2.448
μ [mm^{-1}]	9.739
F(000)	2560
Crystal size [mm^3]	0.200×0.200×0.050
Crystal colour	red
Crystal shape	plate
Radiation	MoK_α (λ=0.71073)
2Θ range [°]	4.35 to 56.78
Index ranges	-25 ≤ h ≤ 25, -14 ≤ k ≤ 14, -25 ≤ l ≤ 24
Reflections collected	39095
Independent reflections	4713, R_{int} = 0.0362, R_{sigma} = 0.0244
Completeness to θ = 25.242°	99.90
Data / Restraints / Parameters	4713/129/271
Goodness-of-fit on F^2	1.156
Final R indexes [I≥2σ(I)]	R_1 = 0.0352, wR_2 = 0.1181
Final R indexes [all data]	R_1 = 0.0372, wR_2 = 0.1203
Largest peak/hole [eÅ^3]	1.60/-1.87

Table 2. Bond lengths and angles for c2c_all_200_a-finalcif.cif.

Atom - Atom	Length [Å]
Ag1 - C9	2.524(7)
Ag1 - C3	2.568(7)
Ag1 - C4	2.597(7)
Ag1 - Ta2	2.8166(6)
Ag1 - Ta1	2.8710(7)
Ag1 - Ag1$^{\#1}$	2.8818(12)
Ta1 - C3	2.110(8)
Ta1 - C3$^{\#1}$	2.110(8)
Ta1 - C2$^{\#1}$	2.111(6)
Ta1 - C2	2.111(6)
Ta1 - C1$^{\#1}$	2.141(7)
Ta1 - C1	2.141(7)
O1 - C1	1.124(10)
C5 - O5	1.134(9)
C5 - Ta2	2.114(7)
C4 - O4	1.157(9)
C4 - Ta2	2.091(7)
C3 - O3	1.152(10)
Ta2 - C9	2.105(8)
Ta2 - C6	2.108(9)
Ta2 - C8	2.110(7)
Ta2 - C7	2.128(8)
O2 - C2	1.150(9)
O6 - C6	1.151(12)
C7 - O7	1.131(11)
C8 - O8	1.139(9)
C9 - O9	1.139(10)
N1_1 - C3_1	1.514(12)
N1_1 - C7_1	1.520(13)
N1_1 - C5_1	1.522(12)
N1_1 - C1_1	1.524(13)
C1_1 - C2_1	1.522(17)
C3_1 - C4_1	1.518(15)
C5_1 - C6_1	1.530(17)
C7_1 - C8_1	1.535(14)
Atom - Atom - Atom	**Angle [°]**
C9 - Ag1 - C3	102.8(3)
C9 - Ag1 - C4	80.9(2)
C3 - Ag1 - C4	173.5(2)
C9 - Ag1 - Ta2	46.02(17)
C3 - Ag1 - Ta2	134.61(19)
C4 - Ag1 - Ta2	45.21(16)
C9 - Ag1 - Ta1	143.21(17)
C3 - Ag1 - Ta1	45.23(18)
C4 - Ag1 - Ta1	132.97(17)

Ta2 - Ag1 - Ta1	167.40(3)
C9 - Ag1 - Ag1$^{\#1}$	91.53(18)
C3 - Ag1 - Ag1$^{\#1}$	62.51(18)
C4 - Ag1 - Ag1$^{\#1}$	123.13(17)
Ta2 - Ag1 - Ag1$^{\#1}$	132.679(15)
Ta1 - Ag1 - Ag1$^{\#1}$	59.874(14)
C3 - Ta1 - C3$^{\#1}$	118.4(4)
C3 - Ta1 - C2$^{\#1}$	87.4(3)
C3$^{\#1}$ - Ta1 - C2$^{\#1}$	96.6(3)
C3 - Ta1 - C2	96.6(3)
C3$^{\#1}$ - Ta1 - C2	87.4(3)
C2$^{\#1}$ - Ta1 - C2	172.2(4)
C3 - Ta1 - C1$^{\#1}$	80.3(3)
C3$^{\#1}$ - Ta1 - C1$^{\#1}$	160.4(3)
C2$^{\#1}$ - Ta1 - C1$^{\#1}$	89.8(3)
C2 - Ta1 - C1$^{\#1}$	84.3(3)
C3 - Ta1 - C1	160.4(3)
C3$^{\#1}$ - Ta1 - C1	80.3(3)
C2$^{\#1}$ - Ta1 - C1	84.3(3)
C2 - Ta1 - C1	89.8(3)
C1$^{\#1}$ - Ta1 - C1	81.9(5)
C3 - Ta1 - Ag1$^{\#1}$	67.5(2)
C3$^{\#1}$ - Ta1 - Ag1$^{\#1}$	59.77(19)
C2$^{\#1}$ - Ta1 - Ag1$^{\#1}$	64.63(18)
C2 - Ta1 - Ag1$^{\#1}$	123.05(19)
C1$^{\#1}$ - Ta1 - Ag1$^{\#1}$	138.9(3)
C1 - Ta1 - Ag1$^{\#1}$	123.6(2)
C3 - Ta1 - Ag1	59.77(19)
C3$^{\#1}$ - Ta1 - Ag1	67.5(2)
C2$^{\#1}$ - Ta1 - Ag1	123.05(19)
C2 - Ta1 - Ag1	64.63(18)
C1$^{\#1}$ - Ta1 - Ag1	123.6(2)
C1 - Ta1 - Ag1	138.9(3)
Ag1$^{\#1}$ - Ta1 - Ag1	60.25(3)
O1 - C1 - Ta1	177.4(9)
O5 - C5 - Ta2	175.7(7)
O4 - C4 - Ta2	173.7(7)
O4 - C4 - Ag1	113.3(6)
Ta2 - C4 - Ag1	73.0(2)
O3 - C3 - Ta1	169.6(7)
O3 - C3 - Ag1	114.8(6)
Ta1 - C3 - Ag1	75.0(2)
C4 - Ta2 - C9	104.8(3)
C4 - Ta2 - C6	83.5(4)
C9 - Ta2 - C6	168.6(3)
C4 - Ta2 - C8	87.1(3)
C9 - Ta2 - C8	82.2(3)
C6 - Ta2 - C8	90.6(3)
C4 - Ta2 - C5	96.8(3)
C9 - Ta2 - C5	99.7(3)
C6 - Ta2 - C5	86.9(3)
C8 - Ta2 - C5	175.0(3)
C4 - Ta2 - C7	171.8(4)
C9 - Ta2 - C7	82.3(4)
C6 - Ta2 - C7	88.9(4)
C8 - Ta2 - C7	90.0(3)
C5 - Ta2 - C7	85.7(3)
C4 - Ta2 - Ag1	61.8(2)
C9 - Ta2 - Ag1	59.6(2)
C6 - Ta2 - Ag1	131.8(3)
C8 - Ta2 - Ag1	117.8(2)
C5 - Ta2 - Ag1	66.92(19)
C7 - Ta2 - Ag1	126.1(3)
O2 - C2 - Ta1	175.7(7)
O6 - C6 - Ta2	177.6(9)
O7 - C7 - Ta2	178.3(11)
O8 - C8 - Ta2	178.4(7)
O9 - C9 - Ta2	171.3(7)
O9 - C9 - Ag1	114.4(6)
Ta2 - C9 - Ag1	74.3(2)
C3_1 - N1_1 - C7_1	106.9(10)
C3_1 - N1_1 - C5_1	110.8(10)
C7_1 - N1_1 - C5_1	111.3(10)
C3_1 - N1_1 - C1_1	111.1(9)
C7_1 - N1_1 - C1_1	111.2(10)
C5_1 - N1_1 - C1_1	105.7(11)
C2_1 - C1_1 - N1_1	114.5(11)
N1_1 - C3_1 - C4_1	115.6(10)
N1_1 - C5_1 - C6_1	113.5(13)
N1_1 - C7_1 - C8_1	114.4(10)

Symmetry transformations used to generate equivalent atoms: #1: 1-X, +Y, 0.5-Z;

Table 3. Torsion angles for c2c_all_200_a-finalcif.cif.

Atom - Atom - Atom - Atom	Torsion Angle [°]
C3_1 - N1_1 - C1_1 - C2_1	-53.8(17)
C7_1 - N1_1 - C1_1 - C2_1	65.1(17)
C5_1 - N1_1 - C1_1 - C2_1	-174.0(14)
C7_1 - N1_1 - C3_1 - C4_1	-177.0(12)
C5_1 - N1_1 - C3_1 - C4_1	61.6(15)
C1_1 - N1_1 - C3_1 - C4_1	-55.6(15)
C3_1 - N1_1 - C5_1 - C6_1	61.0(18)
C7_1 - N1_1 - C5_1 - C6_1	-57.8(18)
C1_1 - N1_1 - C5_1 - C6_1	-178.6(15)
C3_1 - N1_1 - C7_1 - C8_1	-176.7(12)
C5_1 - N1_1 - C7_1 - C8_1	-55.7(15)
C1_1 - N1_1 - C7_1 - C8_1	61.9(15)

Structure of **3a**

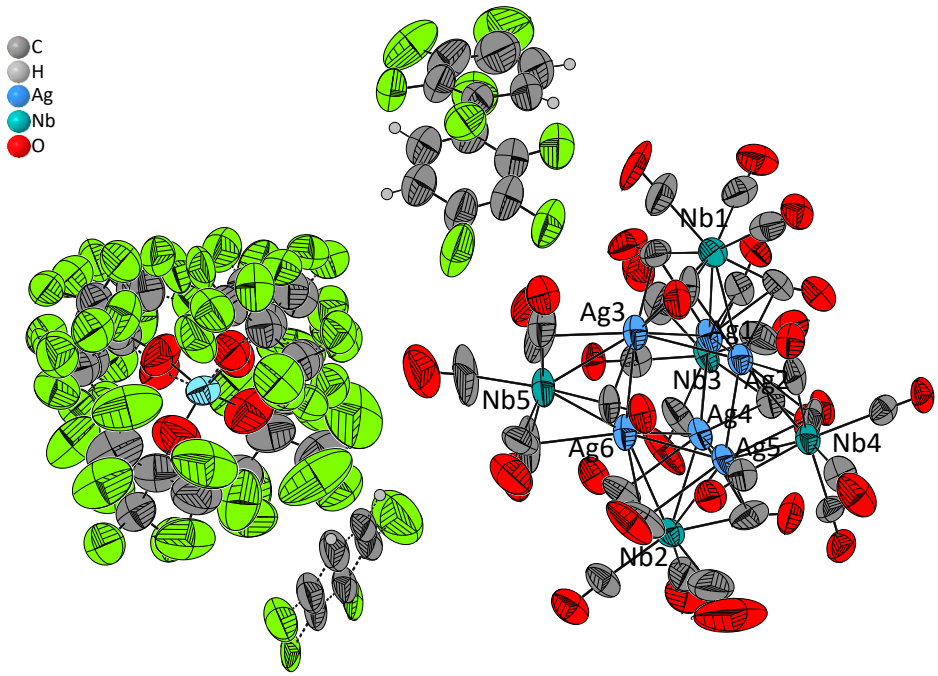


Fig. S20. Molecular structure of **3a**. Thermal ellipsoids are shown at the 50 % probability level.

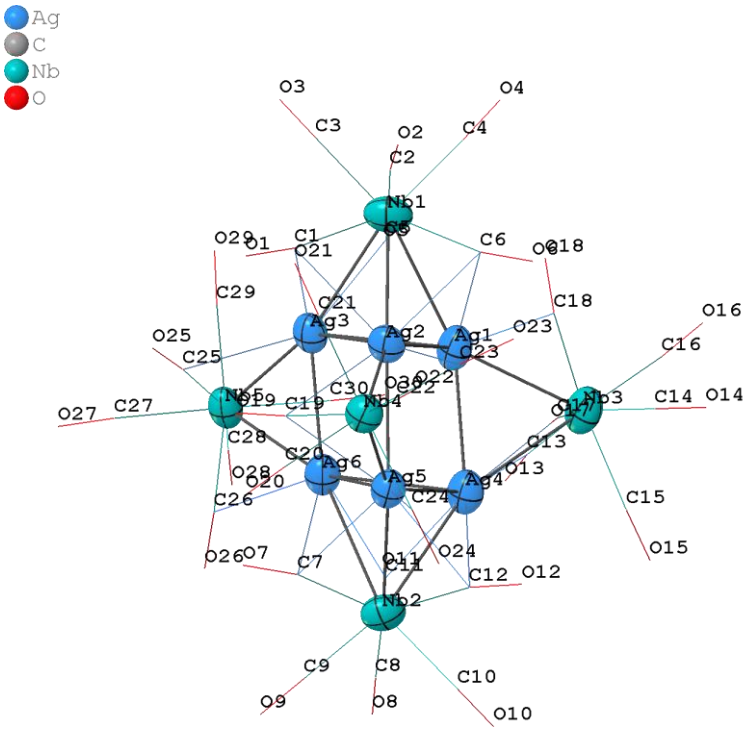


Fig. S21. Enlarged and labled molecular structure of **3a**$^{+}$. Thermal ellipsoids are shown at the 50 % probability level.

Structure Tables

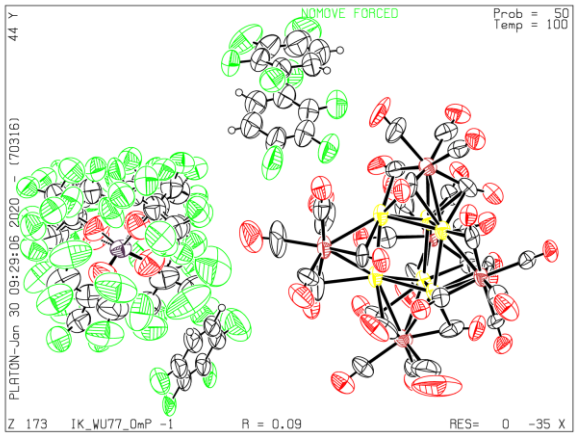


Table 1. Crystal data and structure refinement for IK_WU77_0m-finalcif.cif

CCDC number	1998853
Empirical formula	$C_{61}H_5Ag_6AlF_{46}Nb_5O_{34}$
Formula weight	3294.40
Temperature [K]	100.0
Crystal system	triclinic
Space group (number)	$P\overline{1}$ (2)
a [Å]	17.242(6)
b [Å]	18.251(4)
c [Å]	18.301(4)
α [Å]	77.593(10)
β [Å]	63.291(16)
γ [Å]	62.504(10)
Volume [Å^3]	4563(2)
Z	2
ρ_{calc} [g/cm^3]	2.398
μ [mm^{-1}]	16.727
F(000)	3114
Crystal size [mm^3]	0.08×0.07×0.02
Crystal colour	red
Crystal shape	plate
Radiation	CuK_α (λ=1.54178)
2Θ range [°]	5.41 to 109.91
Index ranges	-17 ≤ h ≤ 17, -18 ≤ k ≤ 19, -19 ≤ l ≤ 19
Reflections collected	58871
Independent reflections	11089, R_{int} = 0.1317, R_{sigma} = 0.1087
Completeness to θ = 54.953°	96.70
Data / Restraints / Parameters	11089/7758/1677
Goodness-of-fit on F^2	1.043
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0945, wR_2 = 0.2487
Final *R* indexes [all data]	R_1 = 0.1421, wR_2 = 0.2899
Largest peak/hole [eÅ^3]	2.21/-1.44

Table 2. Bond lengths and angles for IK_WU77_0m-finalcif.cif.

Atom - Atom	Length [Å]
Ag1 - C6	2.57(3)
Ag1 - C18	2.57(3)
Ag1 - Ag4	2.825(2)
Ag1 - Ag2	2.828(2)
Ag1 - Ag3	2.834(2)
Ag1 - Nb3	2.910(3)
Ag1 - Nb1	3.067(3)
O1 - C1	1.13(3)
Nb1 - C2	2.07(5)
Nb1 - C6	2.07(3)
Nb1 - C5	2.11(3)
Nb1 - C3	2.16(3)
Nb1 - C4	2.17(3)
Nb1 - C1	2.19(4)
Nb1 - Ag3	2.941(3)
Nb1 - Ag2	2.963(2)
Al1 - O1_4	1.637(15)
Al1 - O1_2	1.639(15)
Al1 - O1_8	1.649(18)
Al1 - O1_1	1.671(16)
Al1 - O1_3	1.671(15)
Al1 - O1_7	1.680(17)
C1 - Ag3	2.61(3)
C1 - Ag2	2.64(3)
Ag2 - C23	2.63(2)
Ag2 - C19	2.65(2)
Ag2 - C6	2.69(3)
Ag2 - Ag5	2.833(2)
Ag2 - Nb4	2.901(2)
Ag2 - Ag3	2.928(2)
O2 - C2	1.17(5)
Nb2 - C12	2.02(3)
Nb2 - C7	2.06(3)
Nb2 - C8	2.14(3)
Nb2 - C11	2.17(3)
Nb2 - C9	2.20(4)
Nb2 - C10	2.23(3)
Nb2 - Ag4	2.961(3)
Nb2 - Ag5	2.995(3)
Nb2 - Ag6	3.056(2)
Nb3 - C13	2.07(4)
Nb3 - C16	2.07(4)
Nb3 - C14	2.09(4)
Nb3 - C17	2.10(3)
Nb3 - C18	2.13(4)
Nb3 - C15	2.15(3)
Nb3 - Ag4	2.913(3)
O3 - C3	1.13(3)
Ag3 - C25	2.59(2)
Ag3 - C5	2.59(3)
Ag3 - Ag6	2.776(2)
Ag3 - Nb5	2.891(3)
Nb4 - C24	2.09(3)
Nb4 - C19	2.11(3)
Nb4 - C23	2.13(3)
Nb4 - C20	2.14(3)
Nb4 - C21	2.15(2)

Nb4 - C22	2.15(3)	C4_1 - F8_1	1.338(15)
Nb4 - Ag5	2.935(3)	C4_1 - F7_1	1.339(15)
O4 - C4	1.12(3)	C4_1 - F9_1	1.340(15)
Ag4 - C12	2.58(2)	O1_2 - C1_2	1.36(2)
Ag4 - C11	2.63(3)	C1_2 - C3_2	1.487(17)
Ag4 - C17	2.63(2)	C1_2 - C4_2	1.493(17)
Ag4 - C13	2.70(3)	C1_2 - C2_2	1.497(17)
Ag4 - Ag6	2.813(2)	C2_2 - F2_2	1.330(14)
Ag4 - Ag5	2.948(2)	C2_2 - F3_2	1.335(15)
Nb5 - C30	2.12(3)	C2_2 - F1_2	1.346(15)
Nb5 - C25	2.13(3)	C3_2 - F6_2	1.331(15)
Nb5 - C26	2.14(3)	C3_2 - F5_2	1.335(14)
Nb5 - C28	2.14(4)	C3_2 - F4_2	1.336(15)
Nb5 - C29	2.17(3)	C4_2 - F7_2	1.321(15)
Nb5 - C27	2.21(3)	C4_2 - F8_2	1.329(15)
Nb5 - Ag6	2.952(2)	C4_2 - F9_2	1.342(15)
O5 - C5	1.15(3)	O1_3 - C1_3	1.363(19)
Ag5 - C7	2.57(2)	C1_3 - C2_3	1.488(17)
Ag5 - C12	2.61(2)	C1_3 - C3_3	1.490(17)
Ag5 - C24	2.61(2)	C1_3 - C4_3	1.505(17)
Ag5 - C19	2.68(2)	C2_3 - F3_3	1.329(14)
Ag5 - Ag6	2.878(2)	C2_3 - F2_3	1.341(14)
O6 - C6	1.16(3)	C2_3 - F1_3	1.347(14)
Ag6 - C26	2.57(2)	C3_3 - F4_3	1.326(14)
Ag6 - C7	2.67(2)	C3_3 - F6_3	1.330(14)
Ag6 - C11	2.68(2)	C3_3 - F5_3	1.345(14)
O7 - C7	1.19(3)	C4_3 - F9_3	1.332(14)
C8 - O8	1.17(3)	C4_3 - F8_3	1.333(14)
O9 - C9	1.16(3)	C4_3 - F7_3	1.343(14)
O11 - C11	1.15(3)	O1_4 - C1_4	1.351(19)
O10 - C10	1.10(3)	C1_4 - C2_4	1.487(17)
C12 - O12	1.21(3)	C1_4 - C3_4	1.490(17)
C13 - O13	1.15(4)	C1_4 - C4_4	1.501(17)
C14 - O14	1.20(4)	C2_4 - F1_4	1.327(14)
C15 - O15	1.13(3)	C2_4 - F3_4	1.330(14)
C16 - O16	1.24(3)	C2_4 - F2_4	1.332(14)
C18 - O18	1.17(4)	C3_4 - F5_4	1.333(14)
O17 - C17	1.15(3)	C3_4 - F6_4	1.334(14)
C19 - O19	1.16(3)	C3_4 - F4_4	1.338(14)
C20 - O20	1.11(2)	C4_4 - F8_4	1.326(14)
C21 - O21	1.13(2)	C4_4 - F7_4	1.327(14)
C22 - O22	1.15(3)	C4_4 - F9_4	1.333(14)
C24 - O24	1.20(3)	F1_5 - C1_5	1.359(16)
C23 - O23	1.17(3)	F2_5 - C2_5	1.345(15)
C25 - O25	1.15(3)	F3_5 - C3_5	1.343(16)
C30 - O30	1.18(3)	F4_5 - C4_5	1.353(16)
C29 - O29	1.13(3)	C1_5 - C2_5	1.356(15)
C28 - O28	1.15(3)	C1_5 - C6_5	1.360(15)
C27 - O27	1.10(3)	C2_5 - C3_5	1.358(14)
C26 - O26	1.14(3)	C3_5 - C4_5	1.356(15)
O1_1 - C1_1	1.37(2)	C4_5 - C5_5	1.356(15)
C1_1 - C2_1	1.490(17)	C5_5 - C6_5	1.360(15)
C1_1 - C4_1	1.496(17)	F1_6 - C1_6	1.350(15)
C1_1 - C3_1	1.498(17)	F2_6 - C2_6	1.341(15)
C2_1 - F3_1	1.332(14)	F3_6 - C3_6	1.342(16)
C2_1 - F2_1	1.334(14)	F4_6 - C4_6	1.340(16)
C2_1 - F1_1	1.334(14)	C1_6 - C2_6	1.346(14)
C3_1 - F4_1	1.331(15)	C1_6 - C6_6	1.366(15)
C3_1 - F5_1	1.340(15)	C2_6 - C3_6	1.348(14)
C3_1 - F6_1	1.342(15)	C3_6 - C4_6	1.359(15)

C4_6 - C5_6	1.355(15)
C5_6 - C6_6	1.364(15)
O1_7 - C1_7	1.37(2)
C1_7 - C3_7	1.489(18)
C1_7 - C2_7	1.494(18)
C1_7 - C4_7	1.503(18)
C2_7 - F3_7	1.328(15)
C2_7 - F2_7	1.332(15)
C2_7 - F1_7	1.347(15)
C3_7 - F5_7	1.336(15)
C3_7 - F4_7	1.336(15)
C3_7 - F6_7	1.340(15)
C4_7 - F7_7	1.334(15)
C4_7 - F9_7	1.336(15)
C4_7 - F8_7	1.342(15)
O1_8 - C1_8	1.36(2)
C1_8 - C4_8	1.488(18)
C1_8 - C2_8	1.496(18)
C1_8 - C3_8	1.498(18)
C2_8 - F3_8	1.335(15)
C2_8 - F2_8	1.336(15)
C2_8 - F1_8	1.339(15)
C3_8 - F6_8	1.330(15)
C3_8 - F4_8	1.333(15)
C3_8 - F5_8	1.336(15)
C4_8 - F7_8	1.331(15)
C4_8 - F9_8	1.338(15)
C4_8 - F8_8	1.340(15)
F1_9 - C1_9	1.368(17)
F2_9 - C2_9	1.345(17)
F3_9 - C3_9	1.356(17)
F4_9 - C4_9	1.357(17)
C1_9 - C6_9	1.357(16)
C1_9 - C2_9	1.364(15)
C2_9 - C3_9	1.352(15)
C3_9 - C4_9	1.364(15)
C4_9 - C5_9	1.355(15)
C5_9 - C6_9	1.356(16)

Atom - Atom - Atom	**Angle [°]**
C6 - Ag1 - C18	93.3(13)
C6 - Ag1 - Ag4	135.8(5)
C18 - Ag1 - Ag4	101.7(10)
C6 - Ag1 - Ag2	59.5(7)
C18 - Ag1 - Ag2	151.5(11)
Ag4 - Ag1 - Ag2	93.79(6)
C6 - Ag1 - Ag3	97.0(8)
C18 - Ag1 - Ag3	135.9(8)
Ag4 - Ag1 - Ag3	100.14(7)
Ag2 - Ag1 - Ag3	62.28(6)
C6 - Ag1 - Nb3	108.4(8)
C18 - Ag1 - Nb3	45.1(8)
Ag4 - Ag1 - Nb3	61.03(6)
Ag2 - Ag1 - Nb3	131.13(7)
Ag3 - Ag1 - Nb3	154.56(10)
C6 - Ag1 - Nb1	41.9(7)
C18 - Ag1 - Nb1	106.4(10)
Ag4 - Ag1 - Nb1	151.79(7)
Ag2 - Ag1 - Nb1	60.17(6)
Ag3 - Ag1 - Nb1	59.63(6)
Nb3 - Ag1 - Nb1	143.89(9)
C2 - Nb1 - C6	79.4(18)
C2 - Nb1 - C5	168.6(12)
C6 - Nb1 - C5	105.9(12)
C2 - Nb1 - C3	89.5(16)
C6 - Nb1 - C3	156.8(11)
C5 - Nb1 - C3	81.9(11)
C2 - Nb1 - C4	90.4(13)
C6 - Nb1 - C4	76.9(10)
C5 - Nb1 - C4	81.2(9)
C3 - Nb1 - C4	82.9(10)
C2 - Nb1 - C1	73.6(16)
C6 - Nb1 - C1	116.7(10)
C5 - Nb1 - C1	111.6(10)
C3 - Nb1 - C1	78.7(9)
C4 - Nb1 - C1	155.5(10)
C2 - Nb1 - Ag3	129.9(12)
C6 - Nb1 - Ag3	106.5(7)
C5 - Nb1 - Ag3	58.9(7)
C3 - Nb1 - Ag3	96.2(9)
C4 - Nb1 - Ag3	139.7(7)
C1 - Nb1 - Ag3	59.1(7)
C2 - Nb1 - Ag2	83.6(10)
C6 - Nb1 - Ag2	61.6(7)
C5 - Nb1 - Ag2	107.7(7)
C3 - Nb1 - Ag2	137.8(7)
C4 - Nb1 - Ag2	138.5(7)
C1 - Nb1 - Ag2	59.4(6)
Ag3 - Nb1 - Ag2	59.47(6)
C2 - Nb1 - Ag1	129.3(14)
C6 - Nb1 - Ag1	55.9(8)
C5 - Nb1 - Ag1	60.4(7)
C3 - Nb1 - Ag1	140.7(9)
C4 - Nb1 - Ag1	100.5(8)
C1 - Nb1 - Ag1	104.0(6)
Ag3 - Nb1 - Ag1	56.24(6)
Ag2 - Nb1 - Ag1	55.91(5)
O1_4 - Al1 - O1_2	108.2(16)
O1_4 - Al1 - O1_8	105(2)
O1_4 - Al1 - O1_1	112.2(16)
O1_2 - Al1 - O1_1	109.7(17)
O1_4 - Al1 - O1_3	112.3(13)
O1_2 - Al1 - O1_3	101.2(16)
O1_8 - Al1 - O1_3	104.0(19)
O1_1 - Al1 - O1_3	112.6(15)
O1_4 - Al1 - O1_7	110(2)
O1_8 - Al1 - O1_7	120(3)
O1_3 - Al1 - O1_7	105.9(19)
O1 - C1 - Nb1	170(2)
O1 - C1 - Ag3	113(2)
Nb1 - C1 - Ag3	74.9(9)
O1 - C1 - Ag2	112.4(18)
Nb1 - C1 - Ag2	75.1(10)
Ag3 - C1 - Ag2	67.7(6)
C23 - Ag2 - C1	129.6(8)
C23 - Ag2 - C19	89.4(8)
C1 - Ag2 - C19	87.2(9)
C23 - Ag2 - C6	89.1(8)
C1 - Ag2 - C6	85.8(10)
C19 - Ag2 - C6	169.5(9)

C23 - Ag2 - Ag1	118.0(5)
C1 - Ag2 - Ag1	99.5(7)
C19 - Ag2 - Ag1	133.8(6)
C6 - Ag2 - Ag1	55.4(7)
C23 - Ag2 - Ag5	80.3(5)
C1 - Ag2 - Ag5	136.0(7)
C19 - Ag2 - Ag5	58.3(5)
C6 - Ag2 - Ag5	131.5(7)
Ag1 - Ag2 - Ag5	88.57(7)
C23 - Ag2 - Nb4	44.9(5)
C1 - Ag2 - Nb4	113.6(7)
C19 - Ag2 - Nb4	44.5(6)
C6 - Ag2 - Nb4	132.9(6)
Ag1 - Ag2 - Nb4	145.63(7)
Ag5 - Ag2 - Nb4	61.57(6)
C23 - Ag2 - Ag3	174.6(5)
C1 - Ag2 - Ag3	55.7(6)
C19 - Ag2 - Ag3	90.3(6)
C6 - Ag2 - Ag3	92.1(6)
Ag1 - Ag2 - Ag3	58.96(6)
Ag5 - Ag2 - Ag3	94.93(7)
Nb4 - Ag2 - Ag3	134.67(7)
C23 - Ag2 - Nb1	123.7(5)
C1 - Ag2 - Nb1	45.5(8)
C19 - Ag2 - Nb1	132.2(5)
C6 - Ag2 - Nb1	42.6(6)
Ag1 - Ag2 - Nb1	63.92(6)
Ag5 - Ag2 - Nb1	149.22(8)
Nb4 - Ag2 - Nb1	148.73(8)
Ag3 - Ag2 - Nb1	59.90(6)
O2 - C2 - Nb1	174(6)
C12 - Nb2 - C7	111.1(9)
C12 - Nb2 - C8	78.7(9)
C7 - Nb2 - C8	78.1(9)
C12 - Nb2 - C11	111.8(9)
C7 - Nb2 - C11	109.9(9)
C8 - Nb2 - C11	161.8(9)
C12 - Nb2 - C9	158.6(9)
C7 - Nb2 - C9	80.4(9)
C8 - Nb2 - C9	86.5(9)
C11 - Nb2 - C9	79.0(9)
C12 - Nb2 - C10	78.6(12)
C7 - Nb2 - C10	159.4(11)
C8 - Nb2 - C10	86.5(9)
C11 - Nb2 - C10	81.4(9)
C9 - Nb2 - C10	85.2(12)
C12 - Nb2 - Ag4	58.7(6)
C7 - Nb2 - Ag4	105.7(6)
C8 - Nb2 - Ag4	135.9(6)
C11 - Nb2 - Ag4	59.2(7)
C9 - Nb2 - Ag4	137.6(6)
C10 - Nb2 - Ag4	94.9(9)
C12 - Nb2 - Ag5	58.9(7)
C7 - Nb2 - Ag5	57.6(6)
C8 - Nb2 - Ag5	90.6(6)
C11 - Nb2 - Ag5	107.5(6)
C9 - Nb2 - Ag5	137.4(7)
C10 - Nb2 - Ag5	137.1(10)
Ag4 - Nb2 - Ag5	59.32(6)
C12 - Nb2 - Ag6	103.6(7)
C7 - Nb2 - Ag6	59.1(6)
C8 - Nb2 - Ag6	135.2(6)
C11 - Nb2 - Ag6	58.7(6)
C9 - Nb2 - Ag6	97.8(6)
C10 - Nb2 - Ag6	138.3(7)
Ag4 - Nb2 - Ag6	55.72(5)
Ag5 - Nb2 - Ag6	56.80(5)
C13 - Nb3 - C16	160.1(12)
C13 - Nb3 - C14	78.7(18)
C16 - Nb3 - C14	82.1(18)
C13 - Nb3 - C17	123.6(10)
C16 - Nb3 - C17	76.3(11)
C14 - Nb3 - C17	152.6(15)
C13 - Nb3 - C18	87.8(15)
C16 - Nb3 - C18	85.3(14)
C14 - Nb3 - C18	84.3(13)
C17 - Nb3 - C18	110.0(12)
C13 - Nb3 - C15	87.7(12)
C16 - Nb3 - C15	95.3(10)
C14 - Nb3 - C15	83.9(12)
C17 - Nb3 - C15	81.7(9)
C18 - Nb3 - C15	168.0(11)
C13 - Nb3 - Ag1	85.0(8)
C16 - Nb3 - Ag1	107.0(8)
C14 - Nb3 - Ag1	140.4(10)
C17 - Nb3 - Ag1	63.6(6)
C18 - Nb3 - Ag1	59.0(7)
C15 - Nb3 - Ag1	131.6(6)
C13 - Nb3 - Ag4	63.0(8)
C16 - Nb3 - Ag4	136.8(9)
C14 - Nb3 - Ag4	137.0(16)
C17 - Nb3 - Ag4	60.7(6)
C18 - Nb3 - Ag4	111.5(8)
C15 - Nb3 - Ag4	76.1(7)
Ag1 - Nb3 - Ag4	58.04(6)
O3 - C3 - Nb1	174(3)
C25 - Ag3 - C5	137.3(8)
C25 - Ag3 - C1	94.8(11)
C5 - Ag3 - C1	86.2(10)
C25 - Ag3 - Ag6	78.9(5)
C5 - Ag3 - Ag6	130.7(7)
C1 - Ag3 - Ag6	130.5(5)
C25 - Ag3 - Ag1	158.2(5)
C5 - Ag3 - Ag1	60.3(6)
C1 - Ag3 - Ag1	100.0(8)
Ag6 - Ag3 - Ag1	79.23(6)
C25 - Ag3 - Nb5	45.3(7)
C5 - Ag3 - Nb5	114.5(7)
C1 - Ag3 - Nb5	138.6(8)
Ag6 - Ag3 - Nb5	62.75(6)
Ag1 - Ag3 - Nb5	121.45(8)
C25 - Ag3 - Ag2	119.3(6)
C5 - Ag3 - Ag2	96.7(7)
C1 - Ag3 - Ag2	56.5(6)
Ag6 - Ag3 - Ag2	83.77(6)
Ag1 - Ag3 - Ag2	58.76(5)
Nb5 - Ag3 - Ag2	144.11(7)
C25 - Ag3 - Nb1	136.2(6)
C5 - Ag3 - Nb1	44.3(7)
C1 - Ag3 - Nb1	45.9(8)

Ag6 - Ag3 - Nb1	138.11(8)	Nb3 - Ag4 - Ag5	128.54(9)
Ag1 - Ag3 - Nb1	64.13(7)	C12 - Ag4 - Nb2	42.1(6)
Nb5 - Ag3 - Nb1	155.20(7)	C11 - Ag4 - Nb2	45.3(6)
Ag2 - Ag3 - Nb1	60.63(6)	C17 - Ag4 - Nb2	133.5(6)
C24 - Nb4 - C19	108.6(9)	C13 - Ag4 - Nb2	133.1(10)
C24 - Nb4 - C23	90.9(8)	Ag6 - Ag4 - Nb2	63.85(6)
C19 - Nb4 - C23	122.3(8)	Ag1 - Ag4 - Nb2	138.87(7)
C24 - Nb4 - C20	83.0(8)	Nb3 - Ag4 - Nb2	159.70(8)
C19 - Nb4 - C20	79.2(8)	Ag5 - Ag4 - Nb2	60.91(6)
C23 - Nb4 - C20	158.3(8)	C30 - Nb5 - C25	124.9(9)
C24 - Nb4 - C21	168.8(8)	C30 - Nb5 - C26	103.5(9)
C19 - Nb4 - C21	80.6(9)	C25 - Nb5 - C26	93.4(9)
C23 - Nb4 - C21	89.3(8)	C30 - Nb5 - C28	76.2(9)
C20 - Nb4 - C21	92.7(8)	C25 - Nb5 - C28	158.6(10)
C24 - Nb4 - C22	87.9(9)	C26 - Nb5 - C28	83.8(13)
C19 - Nb4 - C22	150.1(9)	C30 - Nb5 - C29	85.4(10)
C23 - Nb4 - C22	80.7(9)	C25 - Nb5 - C29	88.1(10)
C20 - Nb4 - C22	78.3(9)	C26 - Nb5 - C29	167.8(9)
C21 - Nb4 - C22	81.0(9)	C28 - Nb5 - C29	90.4(14)
C24 - Nb4 - Ag2	111.8(5)	C30 - Nb5 - C27	157.7(10)
C19 - Nb4 - Ag2	61.5(5)	C25 - Nb5 - C27	75.9(11)
C23 - Nb4 - Ag2	60.9(6)	C26 - Nb5 - C27	81.0(9)
C20 - Nb4 - Ag2	140.5(6)	C28 - Nb5 - C27	82.7(11)
C21 - Nb4 - Ag2	78.0(6)	C29 - Nb5 - C27	87.6(10)
C22 - Nb4 - Ag2	136.0(7)	C30 - Nb5 - Ag3	65.3(6)
C24 - Nb4 - Ag5	59.9(5)	C25 - Nb5 - Ag3	59.7(7)
C19 - Nb4 - Ag5	61.5(5)	C26 - Nb5 - Ag3	111.3(6)
C23 - Nb4 - Ag5	86.8(6)	C28 - Nb5 - Ag3	140.8(7)
C20 - Nb4 - Ag5	107.6(6)	C29 - Nb5 - Ag3	79.8(7)
C21 - Nb4 - Ag5	131.3(6)	C27 - Nb5 - Ag3	134.0(9)
C22 - Nb4 - Ag5	145.3(7)	C30 - Nb5 - Ag6	64.6(6)
Ag2 - Nb4 - Ag5	58.07(5)	C25 - Nb5 - Ag6	82.7(6)
O4 - C4 - Nb1	177(3)	C26 - Nb5 - Ag6	58.1(6)
C12 - Ag4 - C11	83.8(9)	C28 - Nb5 - Ag6	113.1(11)
C12 - Ag4 - C17	93.0(8)	C29 - Nb5 - Ag6	134.1(7)
C11 - Ag4 - C17	172.8(7)	C27 - Nb5 - Ag6	132.3(7)
C12 - Ag4 - C13	140.4(8)	Ag3 - Nb5 - Ag6	56.71(6)
C11 - Ag4 - C13	91.3(11)	O5 - C5 - Nb1	169(2)
C17 - Ag4 - C13	87.1(11)	O5 - C5 - Ag3	110.7(17)
C12 - Ag4 - Ag6	97.1(5)	Nb1 - C5 - Ag3	76.8(10)
C11 - Ag4 - Ag6	58.8(5)	C7 - Ag5 - C12	81.1(9)
C17 - Ag4 - Ag6	128.1(5)	C7 - Ag5 - C24	109.1(7)
C13 - Ag4 - Ag6	113.8(6)	C12 - Ag5 - C24	93.6(8)
C12 - Ag4 - Ag1	136.2(6)	C7 - Ag5 - C19	87.3(9)
C11 - Ag4 - Ag1	126.4(6)	C12 - Ag5 - C19	164.4(7)
C17 - Ag4 - Ag1	59.9(5)	C24 - Ag5 - C19	80.4(8)
C13 - Ag4 - Ag1	76.5(9)	C7 - Ag5 - Ag2	129.9(6)
Ag6 - Ag4 - Ag1	78.76(6)	C12 - Ag5 - Ag2	138.0(5)
C12 - Ag4 - Nb3	123.8(6)	C24 - Ag5 - Ag2	99.5(6)
C11 - Ag4 - Nb3	133.7(6)	C19 - Ag5 - Ag2	57.5(5)
C17 - Ag4 - Nb3	44.1(6)	C7 - Ag5 - Ag6	58.3(5)
C13 - Ag4 - Nb3	43.0(9)	C12 - Ag5 - Ag6	94.8(5)
Ag6 - Ag4 - Nb3	135.89(8)	C24 - Ag5 - Ag6	163.4(5)
Ag1 - Ag4 - Nb3	60.93(6)	C19 - Ag5 - Ag6	87.8(6)
C12 - Ag4 - Ag5	55.8(5)	Ag2 - Ag5 - Ag6	83.68(6)
C11 - Ag4 - Ag5	97.5(6)	C7 - Ag5 - Nb4	119.0(6)
C17 - Ag4 - Ag5	86.0(5)	C12 - Ag5 - Nb4	135.6(5)
C13 - Ag4 - Ag5	162.8(8)	C24 - Ag5 - Nb4	43.8(7)
Ag6 - Ag4 - Ag5	59.89(5)	C19 - Ag5 - Nb4	44.0(6)
Ag1 - Ag4 - Ag5	86.40(6)	Ag2 - Ag5 - Nb4	60.36(6)

Ag6 - Ag5 - Nb4	129.53(7)
C7 - Ag5 - Ag4	93.8(6)
C12 - Ag5 - Ag4	54.8(4)
C24 - Ag5 - Ag4	138.0(6)
C19 - Ag5 - Ag4	137.0(4)
Ag2 - Ag5 - Ag4	91.11(6)
Ag6 - Ag5 - Ag4	57.74(5)
Nb4 - Ag5 - Ag4	145.45(7)
C7 - Ag5 - Nb2	42.5(6)
C12 - Ag5 - Nb2	41.6(6)
C24 - Ag5 - Nb2	116.9(6)
C19 - Ag5 - Nb2	129.4(6)
Ag2 - Ag5 - Nb2	143.44(7)
Ag6 - Ag5 - Nb2	62.68(6)
Nb4 - Ag5 - Nb2	153.95(7)
Ag4 - Ag5 - Nb2	59.77(6)
O6 - C6 - Nb1	167(3)
O6 - C6 - Ag1	110(2)
Nb1 - C6 - Ag1	82.1(9)
O6 - C6 - Ag2	111.1(17)
Nb1 - C6 - Ag2	75.8(9)
Ag1 - C6 - Ag2	65.1(6)
C26 - Ag6 - C7	87.9(8)
C26 - Ag6 - C11	86.2(9)
C7 - Ag6 - C11	80.8(8)
C26 - Ag6 - Ag3	102.5(6)
C7 - Ag6 - Ag3	135.1(6)
C11 - Ag6 - Ag3	142.5(5)
C26 - Ag6 - Ag4	142.0(6)
C7 - Ag6 - Ag4	94.9(6)
C11 - Ag6 - Ag4	57.1(6)
Ag3 - Ag6 - Ag4	101.87(7)
C26 - Ag6 - Ag5	141.0(5)
C7 - Ag6 - Ag5	55.0(5)
C11 - Ag6 - Ag5	98.0(6)
Ag3 - Ag6 - Ag5	97.32(7)
Ag4 - Ag6 - Ag5	62.37(5)
C26 - Ag6 - Nb5	44.8(6)
C7 - Ag6 - Nb5	128.3(6)
C11 - Ag6 - Nb5	109.6(6)
Ag3 - Ag6 - Nb5	60.54(6)
Ag4 - Ag6 - Nb5	134.13(7)
Ag5 - Ag6 - Nb5	152.41(8)
C26 - Ag6 - Nb2	101.3(6)
C7 - Ag6 - Nb2	41.4(6)
C11 - Ag6 - Nb2	43.9(6)
Ag3 - Ag6 - Nb2	155.74(8)
Ag4 - Ag6 - Nb2	60.43(6)
Ag5 - Ag6 - Nb2	60.53(6)
Nb5 - Ag6 - Nb2	143.58(8)
O7 - C7 - Nb2	166.6(19)
O7 - C7 - Ag5	112.8(17)
Nb2 - C7 - Ag5	79.9(8)
O7 - C7 - Ag6	108.8(16)
Nb2 - C7 - Ag6	79.5(8)
Ag5 - C7 - Ag6	66.7(5)
O8 - C8 - Nb2	179(2)
O9 - C9 - Nb2	175(2)
O11 - C11 - Nb2	167(2)
O11 - C11 - Ag4	116.9(19)
Nb2 - C11 - Ag4	75.5(9)
O11 - C11 - Ag6	110.9(17)
Nb2 - C11 - Ag6	77.4(8)
Ag4 - C11 - Ag6	64.1(6)
O10 - C10 - Nb2	179(3)
O12 - C12 - Nb2	169(2)
O12 - C12 - Ag4	110.9(17)
Nb2 - C12 - Ag4	79.2(7)
O12 - C12 - Ag5	108.7(18)
Nb2 - C12 - Ag5	79.5(8)
Ag4 - C12 - Ag5	69.3(6)
O13 - C13 - Nb3	170(3)
O13 - C13 - Ag4	113(3)
Nb3 - C13 - Ag4	74.0(8)
O14 - C14 - Nb3	164(5)
O15 - C15 - Nb3	174(2)
O16 - C16 - Nb3	174(3)
O18 - C18 - Nb3	172(3)
O18 - C18 - Ag1	111(2)
Nb3 - C18 - Ag1	75.8(10)
O17 - C17 - Nb3	172.0(17)
O17 - C17 - Ag4	110.7(16)
Nb3 - C17 - Ag4	75.2(8)
O19 - C19 - Nb4	170.5(18)
O19 - C19 - Ag2	110.7(14)
Nb4 - C19 - Ag2	74.0(8)
O19 - C19 - Ag5	114.9(17)
Nb4 - C19 - Ag5	74.5(7)
Ag2 - C19 - Ag5	64.2(5)
O20 - C20 - Nb4	177.2(19)
O21 - C21 - Nb4	178.5(19)
O22 - C22 - Nb4	177(2)
O24 - C24 - Nb4	173.8(17)
O24 - C24 - Ag5	109.8(17)
Nb4 - C24 - Ag5	76.4(7)
O23 - C23 - Nb4	170.8(19)
O23 - C23 - Ag2	114.7(16)
Nb4 - C23 - Ag2	74.2(7)
O25 - C25 - Nb5	172(2)
O25 - C25 - Ag3	112(2)
Nb5 - C25 - Ag3	75.0(7)
O30 - C30 - Nb5	169.3(18)
O29 - C29 - Nb5	176(2)
O28 - C28 - Nb5	165(4)
O27 - C27 - Nb5	173(3)
O26 - C26 - Nb5	172.9(19)
O26 - C26 - Ag6	109.2(17)
Nb5 - C26 - Ag6	77.0(8)
C1_1 - O1_1 - Al1	166(3)
O1_1 - C1_1 - C2_1	109.2(16)
O1_1 - C1_1 - C4_1	108.2(16)
C2_1 - C1_1 - C4_1	111.0(14)
O1_1 - C1_1 - C3_1	110.9(16)
C2_1 - C1_1 - C3_1	108.3(13)
C4_1 - C1_1 - C3_1	109.3(14)
F3_1 - C2_1 - F2_1	104.4(18)
F3_1 - C2_1 - F1_1	107.9(19)
F2_1 - C2_1 - F1_1	108.3(19)
F3_1 - C2_1 - C1_1	110.2(17)
F2_1 - C2_1 - C1_1	114.1(17)

F1_1 - C2_1 - C1_1	111.5(17)
F4_1 - C3_1 - F5_1	105.7(19)
F4_1 - C3_1 - F6_1	108.5(18)
F5_1 - C3_1 - F6_1	105.7(18)
F4_1 - C3_1 - C1_1	111.7(17)
F5_1 - C3_1 - C1_1	112.3(18)
F6_1 - C3_1 - C1_1	112.6(17)
F8_1 - C4_1 - F7_1	108.2(19)
F8_1 - C4_1 - F9_1	106.0(19)
F7_1 - C4_1 - F9_1	107(2)
F8_1 - C4_1 - C1_1	110.9(18)
F7_1 - C4_1 - C1_1	112.8(19)
F9_1 - C4_1 - C1_1	111.6(18)
C1_2 - O1_2 - Al1	177(3)
O1_2 - C1_2 - C3_2	107.6(16)
O1_2 - C1_2 - C4_2	107.1(16)
C3_2 - C1_2 - C4_2	112.1(14)
O1_2 - C1_2 - C2_2	109.7(16)
C3_2 - C1_2 - C2_2	112.3(15)
C4_2 - C1_2 - C2_2	107.9(14)
F2_2 - C2_2 - F3_2	109.5(19)
F2_2 - C2_2 - F1_2	107.7(19)
F3_2 - C2_2 - F1_2	104.8(18)
F2_2 - C2_2 - C1_2	115.3(19)
F3_2 - C2_2 - C1_2	109.1(17)
F1_2 - C2_2 - C1_2	110.0(18)
F6_2 - C3_2 - F5_2	109.4(19)
F6_2 - C3_2 - F4_2	104.7(19)
F5_2 - C3_2 - F4_2	106.4(19)
F6_2 - C3_2 - C1_2	111.9(18)
F5_2 - C3_2 - C1_2	111.8(18)
F4_2 - C3_2 - C1_2	112.3(18)
F7_2 - C4_2 - F8_2	106.1(19)
F7_2 - C4_2 - F9_2	104.3(18)
F8_2 - C4_2 - F9_2	107.7(19)
F7_2 - C4_2 - C1_2	115.3(18)
F8_2 - C4_2 - C1_2	110.2(17)
F9_2 - C4_2 - C1_2	112.6(18)
C1_3 - O1_3 - Al1	158.5(18)
O1_3 - C1_3 - C2_3	113.4(15)
O1_3 - C1_3 - C3_3	109.0(15)
C2_3 - C1_3 - C3_3	109.5(13)
O1_3 - C1_3 - C4_3	107.5(14)
C2_3 - C1_3 - C4_3	107.8(13)
C3_3 - C1_3 - C4_3	109.4(14)
F3_3 - C2_3 - F2_3	105.9(16)
F3_3 - C2_3 - F1_3	108.3(18)
F2_3 - C2_3 - F1_3	108.2(17)
F3_3 - C2_3 - C1_3	112.0(16)
F2_3 - C2_3 - C1_3	113.2(15)
F1_3 - C2_3 - C1_3	109.0(16)
F4_3 - C3_3 - F6_3	107.2(18)
F4_3 - C3_3 - F5_3	108.2(18)
F6_3 - C3_3 - F5_3	109.1(18)
F4_3 - C3_3 - C1_3	112.4(17)
F6_3 - C3_3 - C1_3	111.4(16)
F5_3 - C3_3 - C1_3	108.5(16)
F9_3 - C4_3 - F8_3	107.3(17)
F9_3 - C4_3 - F7_3	107.5(19)
F8_3 - C4_3 - F7_3	112.2(19)
F9_3 - C4_3 - C1_3	109.2(17)
F8_3 - C4_3 - C1_3	111.2(16)
F7_3 - C4_3 - C1_3	109.3(17)
C1_4 - O1_4 - Al1	176(2)
O1_4 - C1_4 - C2_4	107.2(14)
O1_4 - C1_4 - C3_4	109.2(15)
C2_4 - C1_4 - C3_4	111.2(13)
O1_4 - C1_4 - C4_4	109.5(15)
C2_4 - C1_4 - C4_4	109.9(13)
C3_4 - C1_4 - C4_4	109.9(13)
F1_4 - C2_4 - F3_4	106.5(16)
F1_4 - C2_4 - F2_4	105.5(15)
F3_4 - C2_4 - F2_4	106.2(15)
F1_4 - C2_4 - C1_4	111.4(15)
F3_4 - C2_4 - C1_4	113.0(15)
F2_4 - C2_4 - C1_4	113.6(15)
F5_4 - C3_4 - F6_4	105.8(18)
F5_4 - C3_4 - F4_4	109.3(19)
F6_4 - C3_4 - F4_4	106.2(17)
F5_4 - C3_4 - C1_4	110.8(17)
F6_4 - C3_4 - C1_4	113.7(16)
F4_4 - C3_4 - C1_4	110.7(16)
F8_4 - C4_4 - F7_4	108.4(17)
F8_4 - C4_4 - F9_4	108.0(18)
F7_4 - C4_4 - F9_4	105.8(18)
F8_4 - C4_4 - C1_4	109.9(16)
F7_4 - C4_4 - C1_4	112.4(17)
F9_4 - C4_4 - C1_4	112.2(16)
C2_5 - C1_5 - F1_5	119.1(14)
C2_5 - C1_5 - C6_5	120.2(14)
F1_5 - C1_5 - C6_5	120.8(14)
F2_5 - C2_5 - C1_5	120.3(14)
F2_5 - C2_5 - C3_5	119.6(14)
C1_5 - C2_5 - C3_5	120.1(13)
F3_5 - C3_5 - C4_5	119.7(14)
F3_5 - C3_5 - C2_5	120.5(14)
C4_5 - C3_5 - C2_5	119.8(13)
F4_5 - C4_5 - C3_5	119.1(15)
F4_5 - C4_5 - C5_5	120.9(16)
C3_5 - C4_5 - C5_5	120.1(14)
C4_5 - C5_5 - C6_5	120.3(16)
C1_5 - C6_5 - C5_5	119.5(16)
C2_6 - C1_6 - F1_6	117.9(13)
C2_6 - C1_6 - C6_6	119.6(14)
F1_6 - C1_6 - C6_6	122.5(14)
F2_6 - C2_6 - C1_6	120.2(13)
F2_6 - C2_6 - C3_6	118.6(13)
C1_6 - C2_6 - C3_6	121.2(13)
F3_6 - C3_6 - C2_6	120.2(14)
F3_6 - C3_6 - C4_6	120.0(15)
C2_6 - C3_6 - C4_6	119.7(13)
F4_6 - C4_6 - C5_6	123.7(17)
F4_6 - C4_6 - C3_6	116.5(16)
C5_6 - C4_6 - C3_6	119.7(15)
C4_6 - C5_6 - C6_6	120.4(16)
C5_6 - C6_6 - C1_6	119.3(16)
C1_7 - O1_7 - Al1	160(3)
O1_7 - C1_7 - C3_7	111.2(18)
O1_7 - C1_7 - C2_7	108.6(19)
C3_7 - C1_7 - C2_7	111.5(16)

O1_7 - C1_7 - C4_7	110.8(19)
C3_7 - C1_7 - C4_7	109.0(17)
C2_7 - C1_7 - C4_7	105.6(17)
F3_7 - C2_7 - F2_7	109(2)
F3_7 - C2_7 - F1_7	106(2)
F2_7 - C2_7 - F1_7	104(2)
F3_7 - C2_7 - C1_7	113(2)
F2_7 - C2_7 - C1_7	117(2)
F1_7 - C2_7 - C1_7	107(2)
F5_7 - C3_7 - F4_7	105(2)
F5_7 - C3_7 - F6_7	105(2)
F4_7 - C3_7 - F6_7	108(2)
F5_7 - C3_7 - C1_7	113(2)
F4_7 - C3_7 - C1_7	113(2)
F6_7 - C3_7 - C1_7	112.1(19)
F7_7 - C4_7 - F9_7	109(2)
F7_7 - C4_7 - F8_7	107(2)
F9_7 - C4_7 - F8_7	106(2)
F7_7 - C4_7 - C1_7	114(2)
F9_7 - C4_7 - C1_7	111(2)
F8_7 - C4_7 - C1_7	110(2)
C1_8 - O1_8 - Al1	150(3)
O1_8 - C1_8 - C4_8	111(2)
O1_8 - C1_8 - C2_8	109(2)
C4_8 - C1_8 - C2_8	109.1(17)
O1_8 - C1_8 - C3_8	106.5(17)
C4_8 - C1_8 - C3_8	110.8(16)
C2_8 - C1_8 - C3_8	109.5(16)
F3_8 - C2_8 - F2_8	107(2)
F3_8 - C2_8 - F1_8	108(2)
F2_8 - C2_8 - F1_8	107(2)
F3_8 - C2_8 - C1_8	109(2)
F2_8 - C2_8 - C1_8	113(2)
F1_8 - C2_8 - C1_8	112(2)
F6_8 - C3_8 - F4_8	107(2)
F6_8 - C3_8 - F5_8	110(2)
F4_8 - C3_8 - F5_8	108(2)
F6_8 - C3_8 - C1_8	110(2)
F4_8 - C3_8 - C1_8	113(2)
F5_8 - C3_8 - C1_8	108.4(19)
F7_8 - C4_8 - F9_8	107(2)
F7_8 - C4_8 - F8_8	109(2)
F9_8 - C4_8 - F8_8	106(2)
F7_8 - C4_8 - C1_8	112(2)
F9_8 - C4_8 - C1_8	112(2)
F8_8 - C4_8 - C1_8	110(2)
C6_9 - C1_9 - C2_9	120.7(15)
C6_9 - C1_9 - F1_9	120.8(17)
C2_9 - C1_9 - F1_9	118.5(16)
F2_9 - C2_9 - C3_9	122.5(16)
F2_9 - C2_9 - C1_9	117.0(15)
C3_9 - C2_9 - C1_9	120.5(14)
C2_9 - C3_9 - F3_9	125.7(16)
C2_9 - C3_9 - C4_9	118.4(14)
F3_9 - C3_9 - C4_9	115.9(15)
C5_9 - C4_9 - F4_9	121.3(19)
C5_9 - C4_9 - C3_9	121.2(15)
F4_9 - C4_9 - C3_9	117.5(18)
C4_9 - C5_9 - C6_9	120.1(17)
C5_9 - C6_9 - C1_9	119.0(18)

Table 3. Torsion angles for IK_WU77_0m-finalcif.cif.

Atom - Atom - Atom - Atom	Torsion Angle [°]
O1_4 - Al1 - O1_1 - C1_1	25(9)
O1_2 - Al1 - O1_1 - C1_1	-96(9)
O1_3 - Al1 - O1_1 - C1_1	153(9)
Al1 - O1_1 - C1_1 - C2_1	-69(9)
Al1 - O1_1 - C1_1 - C4_1	171(8)
Al1 - O1_1 - C1_1 - C3_1	51(9)
O1_1 - C1_1 - C2_1 - F3_1	80(2)
C4_1 - C1_1 - C2_1 - F3_1	-160.9(19)
C3_1 - C1_1 - C2_1 - F3_1	-41(2)
O1_1 - C1_1 - C2_1 - F2_1	-163(2)
C4_1 - C1_1 - C2_1 - F2_1	-44(2)
C3_1 - C1_1 - C2_1 - F2_1	76(2)
O1_1 - C1_1 - C2_1 - F1_1	-40(2)
C4_1 - C1_1 - C2_1 - F1_1	79(2)
C3_1 - C1_1 - C2_1 - F1_1	-161(2)
O1_1 - C1_1 - C3_1 - F4_1	74(2)
C2_1 - C1_1 - C3_1 - F4_1	-166.3(19)
C4_1 - C1_1 - C3_1 - F4_1	-45(2)
O1_1 - C1_1 - C3_1 - F5_1	-45(2)
C2_1 - C1_1 - C3_1 - F5_1	75(2)
C4_1 - C1_1 - C3_1 - F5_1	-163.8(19)
O1_1 - C1_1 - C3_1 - F6_1	-164(2)
C2_1 - C1_1 - C3_1 - F6_1	-44(2)
C4_1 - C1_1 - C3_1 - F6_1	77(2)
O1_1 - C1_1 - C4_1 - F8_1	-166(2)
C2_1 - C1_1 - C4_1 - F8_1	74(2)
C3_1 - C1_1 - C4_1 - F8_1	-45(2)
O1_1 - C1_1 - C4_1 - F7_1	-45(2)
C2_1 - C1_1 - C4_1 - F7_1	-164(2)
C3_1 - C1_1 - C4_1 - F7_1	76(2)
O1_1 - C1_1 - C4_1 - F9_1	76(2)
C2_1 - C1_1 - C4_1 - F9_1	-44(2)
C3_1 - C1_1 - C4_1 - F9_1	-163.2(18)
O1_2 - C1_2 - C2_2 - F2_2	149(3)
C3_2 - C1_2 - C2_2 - F2_2	29(3)
C4_2 - C1_2 - C2_2 - F2_2	-95(2)
O1_2 - C1_2 - C2_2 - F3_2	25(3)
C3_2 - C1_2 - C2_2 - F3_2	-94(3)
C4_2 - C1_2 - C2_2 - F3_2	141(2)
O1_2 - C1_2 - C2_2 - F1_2	-89(3)
C3_2 - C1_2 - C2_2 - F1_2	151(2)
C4_2 - C1_2 - C2_2 - F1_2	27(2)
O1_2 - C1_2 - C3_2 - F6_2	163(2)
C4_2 - C1_2 - C3_2 - F6_2	45(2)
C2_2 - C1_2 - C3_2 - F6_2	-76(2)
O1_2 - C1_2 - C3_2 - F5_2	-74(2)
C4_2 - C1_2 - C3_2 - F5_2	168(2)
C2_2 - C1_2 - C3_2 - F5_2	47(2)
O1_2 - C1_2 - C3_2 - F4_2	45(2)
C4_2 - C1_2 - C3_2 - F4_2	-72(2)
C2_2 - C1_2 - C3_2 - F4_2	166(2)
O1_2 - C1_2 - C4_2 - F7_2	-74(2)
C3_2 - C1_2 - C4_2 - F7_2	44(2)
C2_2 - C1_2 - C4_2 - F7_2	168.1(19)
O1_2 - C1_2 - C4_2 - F8_2	166(2)
C3_2 - C1_2 - C4_2 - F8_2	-76(2)
C2_2 - C1_2 - C4_2 - F8_2	48(2)
O1_2 - C1_2 - C4_2 - F9_2	46(2)
C3_2 - C1_2 - C4_2 - F9_2	163(2)
C2_2 - C1_2 - C4_2 - F9_2	-72(2)

O1_4 - Al1 - O1_3 - C1_3	75(5)
O1_2 - Al1 - O1_3 - C1_3	-170(5)
O1_8 - Al1 - O1_3 - C1_3	-38(5)
O1_1 - Al1 - O1_3 - C1_3	-53(5)
O1_7 - Al1 - O1_3 - C1_3	-165(5)
Al1 - O1_3 - C1_3 - C2_3	-31(6)
Al1 - O1_3 - C1_3 - C3_3	91(5)
Al1 - O1_3 - C1_3 - C4_3	-151(5)
O1_3 - C1_3 - C2_3 - F3_3	41(2)
C3_3 - C1_3 - C2_3 - F3_3	-81(2)
C4_3 - C1_3 - C2_3 - F3_3	159.9(18)
O1_3 - C1_3 - C2_3 - F2_3	160.6(18)
C3_3 - C1_3 - C2_3 - F2_3	39(2)
C4_3 - C1_3 - C2_3 - F2_3	-80.4(19)
O1_3 - C1_3 - C2_3 - F1_3	-79(2)
C3_3 - C1_3 - C2_3 - F1_3	159.1(17)
C4_3 - C1_3 - C2_3 - F1_3	40(2)
O1_3 - C1_3 - C3_3 - F4_3	36(2)
C2_3 - C1_3 - C3_3 - F4_3	160.8(19)
C4_3 - C1_3 - C3_3 - F4_3	-81(2)
O1_3 - C1_3 - C3_3 - F6_3	156.5(18)
C2_3 - C1_3 - C3_3 - F6_3	-78.9(19)
C4_3 - C1_3 - C3_3 - F6_3	39(2)
O1_3 - C1_3 - C3_3 - F5_3	-83.4(19)
C2_3 - C1_3 - C3_3 - F5_3	41(2)
C4_3 - C1_3 - C3_3 - F5_3	159.2(17)
O1_3 - C1_3 - C4_3 - F9_3	45(2)
C2_3 - C1_3 - C4_3 - F9_3	-78(2)
C3_3 - C1_3 - C4_3 - F9_3	162.8(18)
O1_3 - C1_3 - C4_3 - F8_3	162.8(19)
C2_3 - C1_3 - C4_3 - F8_3	40(2)
C3_3 - C1_3 - C4_3 - F8_3	-79(2)
O1_3 - C1_3 - C4_3 - F7_3	-73(2)
C2_3 - C1_3 - C4_3 - F7_3	164.5(18)
C3_3 - C1_3 - C4_3 - F7_3	45(2)
O1_4 - C1_4 - C2_4 - F1_4	-46(2)
C3_4 - C1_4 - C2_4 - F1_4	-164.9(17)
C4_4 - C1_4 - C2_4 - F1_4	73.2(19)
O1_4 - C1_4 - C2_4 - F3_4	74.3(19)
C3_4 - C1_4 - C2_4 - F3_4	-45(2)
C4_4 - C1_4 - C2_4 - F3_4	-166.9(15)
O1_4 - C1_4 - C2_4 - F2_4	-164.6(17)
C3_4 - C1_4 - C2_4 - F2_4	76.1(19)
C4_4 - C1_4 - C2_4 - F2_4	-45.8(19)
O1_4 - C1_4 - C3_4 - F5_4	-42(2)
C2_4 - C1_4 - C3_4 - F5_4	76(2)
C4_4 - C1_4 - C3_4 - F5_4	-162.2(19)
O1_4 - C1_4 - C3_4 - F6_4	-161(2)
C2_4 - C1_4 - C3_4 - F6_4	-43(2)
C4_4 - C1_4 - C3_4 - F6_4	79(2)
O1_4 - C1_4 - C3_4 - F4_4	79(2)
C2_4 - C1_4 - C3_4 - F4_4	-162.6(19)
C4_4 - C1_4 - C3_4 - F4_4	-41(2)
O1_4 - C1_4 - C4_4 - F8_4	-165.6(19)
C2_4 - C1_4 - C4_4 - F8_4	77(2)
C3_4 - C1_4 - C4_4 - F8_4	-46(2)
O1_4 - C1_4 - C4_4 - F7_4	-45(2)
C2_4 - C1_4 - C4_4 - F7_4	-162.3(17)
C3_4 - C1_4 - C4_4 - F7_4	75(2)
O1_4 - C1_4 - C4_4 - F9_4	74(2)
C2_4 - C1_4 - C4_4 - F9_4	-43(2)
C3_4 - C1_4 - C4_4 - F9_4	-165.8(18)
F1_5 - C1_5 - C2_5 - F2_5	0(2)
C6_5 - C1_5 - C2_5 - F2_5	-179.4(13)
F1_5 - C1_5 - C2_5 - C3_5	179.6(13)
C6_5 - C1_5 - C2_5 - C3_5	0(2)
F2_5 - C2_5 - C3_5 - F3_5	0(2)
C1_5 - C2_5 - C3_5 - F3_5	-179.4(13)
F2_5 - C2_5 - C3_5 - C4_5	179.1(13)
C1_5 - C2_5 - C3_5 - C4_5	0(2)
F3_5 - C3_5 - C4_5 - F4_5	-1(2)
C2_5 - C3_5 - C4_5 - F4_5	-179.9(15)
F3_5 - C3_5 - C4_5 - C5_5	179.8(14)
C2_5 - C3_5 - C4_5 - C5_5	0(2)
F4_5 - C4_5 - C5_5 - C6_5	179.8(16)
C3_5 - C4_5 - C5_5 - C6_5	-1(2)
C2_5 - C1_5 - C6_5 - C5_5	0(2)
F1_5 - C1_5 - C6_5 - C5_5	-179.7(14)
C4_5 - C5_5 - C6_5 - C1_5	0(2)
F1_6 - C1_6 - C2_6 - F2_6	0(2)
C6_6 - C1_6 - C2_6 - F2_6	-179.7(13)
F1_6 - C1_6 - C2_6 - C3_6	179.7(14)
C6_6 - C1_6 - C2_6 - C3_6	0(2)
F2_6 - C2_6 - C3_6 - F3_6	0(2)
C1_6 - C2_6 - C3_6 - F3_6	-180.0(14)
F2_6 - C2_6 - C3_6 - C4_6	178.9(14)
C1_6 - C2_6 - C3_6 - C4_6	-1(3)
F3_6 - C3_6 - C4_6 - F4_6	-3(2)
C2_6 - C3_6 - C4_6 - F4_6	178.3(16)
F3_6 - C3_6 - C4_6 - C5_6	-179.2(14)
C2_6 - C3_6 - C4_6 - C5_6	2(3)
F4_6 - C4_6 - C5_6 - C6_6	-178.1(16)
C3_6 - C4_6 - C5_6 - C6_6	-2(3)
C4_6 - C5_6 - C6_6 - C1_6	1(3)
C2_6 - C1_6 - C6_6 - C5_6	0(2)
F1_6 - C1_6 - C6_6 - C5_6	-179.7(14)
O1_4 - Al1 - O1_7 - C1_7	114(11)
O1_8 - Al1 - O1_7 - C1_7	-124(10)
O1_3 - Al1 - O1_7 - C1_7	-7(11)
Al1 - O1_7 - C1_7 - C3_7	178(10)
Al1 - O1_7 - C1_7 - C2_7	55(11)
Al1 - O1_7 - C1_7 - C4_7	-60(11)
O1_7 - C1_7 - C2_7 - F3_7	37(3)
C3_7 - C1_7 - C2_7 - F3_7	-85(3)
C4_7 - C1_7 - C2_7 - F3_7	156(3)
O1_7 - C1_7 - C2_7 - F2_7	164(3)
C3_7 - C1_7 - C2_7 - F2_7	41(3)
C4_7 - C1_7 - C2_7 - F2_7	-77(3)
O1_7 - C1_7 - C2_7 - F1_7	-79(3)
C3_7 - C1_7 - C2_7 - F1_7	158(3)
C4_7 - C1_7 - C2_7 - F1_7	40(3)
O1_7 - C1_7 - C3_7 - F5_7	-70(3)
C2_7 - C1_7 - C3_7 - F5_7	51(3)
C4_7 - C1_7 - C3_7 - F5_7	168(3)
O1_7 - C1_7 - C3_7 - F4_7	49(3)
C2_7 - C1_7 - C3_7 - F4_7	170(3)
C4_7 - C1_7 - C3_7 - F4_7	-73(3)
O1_7 - C1_7 - C3_7 - F6_7	171(3)
C2_7 - C1_7 - C3_7 - F6_7	-68(3)
C4_7 - C1_7 - C3_7 - F6_7	49(3)

O1_7 - C1_7 - C4_7 - F7_7	-56(4)
C3_7 - C1_7 - C4_7 - F7_7	67(4)
C2_7 - C1_7 - C4_7 - F7_7	-173(3)
O1_7 - C1_7 - C4_7 - F9_7	67(4)
C3_7 - C1_7 - C4_7 - F9_7	-170(3)
C2_7 - C1_7 - C4_7 - F9_7	-50(3)
O1_7 - C1_7 - C4_7 - F8_7	-176(3)
C3_7 - C1_7 - C4_7 - F8_7	-53(3)
C2_7 - C1_7 - C4_7 - F8_7	67(3)
O1_4 - Al1 - O1_8 - C1_8	100(7)
O1_3 - Al1 - O1_8 - C1_8	-141(7)
O1_7 - Al1 - O1_8 - C1_8	-24(8)
Al1 - O1_8 - C1_8 - C4_8	-40(7)
Al1 - O1_8 - C1_8 - C2_8	81(7)
Al1 - O1_8 - C1_8 - C3_8	-161(7)
O1_8 - C1_8 - C2_8 - F3_8	28(3)
C4_8 - C1_8 - C2_8 - F3_8	151(3)
C3_8 - C1_8 - C2_8 - F3_8	-88(3)
O1_8 - C1_8 - C2_8 - F2_8	148(3)
C4_8 - C1_8 - C2_8 - F2_8	-90(3)
C3_8 - C1_8 - C2_8 - F2_8	31(3)
O1_8 - C1_8 - C2_8 - F1_8	-91(3)
C4_8 - C1_8 - C2_8 - F1_8	31(3)
C3_8 - C1_8 - C2_8 - F1_8	153(3)
O1_8 - C1_8 - C3_8 - F6_8	165(3)
C4_8 - C1_8 - C3_8 - F6_8	44(3)
C2_8 - C1_8 - C3_8 - F6_8	-76(3)
O1_8 - C1_8 - C3_8 - F4_8	46(3)
C4_8 - C1_8 - C3_8 - F4_8	-75(3)
C2_8 - C1_8 - C3_8 - F4_8	164(3)
O1_8 - C1_8 - C3_8 - F5_8	-74(3)
C4_8 - C1_8 - C3_8 - F5_8	165(3)
C2_8 - C1_8 - C3_8 - F5_8	44(3)
O1_8 - C1_8 - C4_8 - F7_8	-81(3)
C2_8 - C1_8 - C4_8 - F7_8	158(3)
C3_8 - C1_8 - C4_8 - F7_8	37(3)
O1_8 - C1_8 - C4_8 - F9_8	39(3)
C2_8 - C1_8 - C4_8 - F9_8	-82(3)
C3_8 - C1_8 - C4_8 - F9_8	158(3)
O1_8 - C1_8 - C4_8 - F8_8	158(3)
C2_8 - C1_8 - C4_8 - F8_8	37(3)
C3_8 - C1_8 - C4_8 - F8_8	-84(3)
C6_9 - C1_9 - C2_9 - F2_9	179.7(14)
F1_9 - C1_9 - C2_9 - F2_9	0(2)
C6_9 - C1_9 - C2_9 - C3_9	0(3)
F1_9 - C1_9 - C2_9 - C3_9	-179.9(14)
F2_9 - C2_9 - C3_9 - F3_9	0(2)
C1_9 - C2_9 - C3_9 - F3_9	180.0(14)
F2_9 - C2_9 - C3_9 - C4_9	-179.6(14)
C1_9 - C2_9 - C3_9 - C4_9	1(2)
C2_9 - C3_9 - C4_9 - C5_9	-1(2)
F3_9 - C3_9 - C4_9 - C5_9	179.6(14)
C2_9 - C3_9 - C4_9 - F4_9	-180.0(15)
F3_9 - C3_9 - C4_9 - F4_9	1(2)
F4_9 - C4_9 - C5_9 - C6_9	-179.8(16)
C3_9 - C4_9 - C5_9 - C6_9	1(3)
C4_9 - C5_9 - C6_9 - C1_9	-1(2)
C2_9 - C1_9 - C6_9 - C5_9	1(2)
F1_9 - C1_9 - C6_9 - C5_9	-179.8(14)

Structure of **4b**

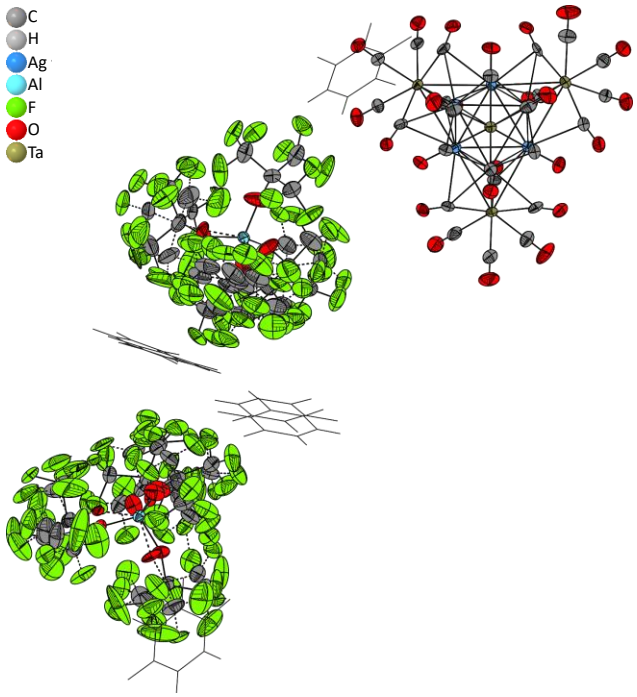


Fig. S22. Molecular structure of **4b**. Thermal ellipsoids are shown at the 50 % probability level. Solvent molecules (4FB) are displayed as wire frame and were partly disordered twice. Disorders of the anions are included with dashed bonds.

Four 4FB molecules were detected in the orthorhombic (*Pbca*) structure of **4b**. Fragments of the anions were disordered twice or three times.

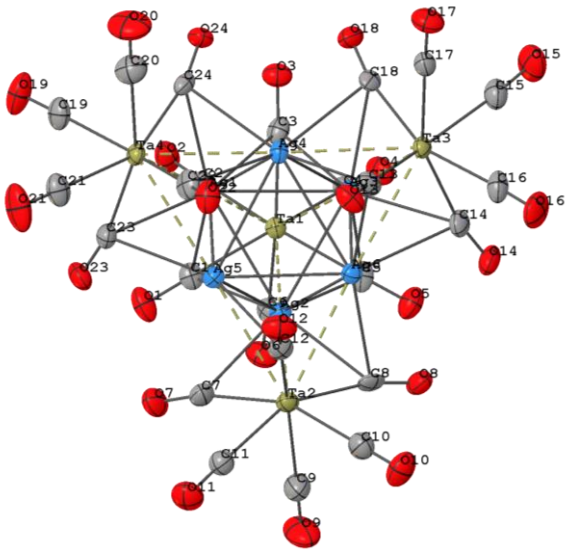


Fig. S23. Enlarged and labled molecular structure of **4b**$^{2+}$. Thermal ellipsoids are shown at the 50 % probability level.

Structure Tables

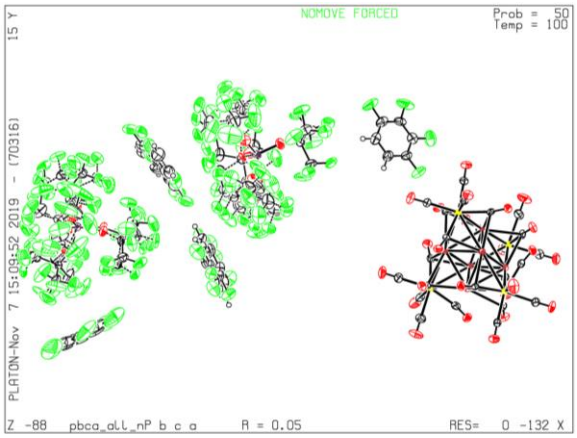


Table 1. Crystal data and structure refinement for pbca_all_new_d-finalcif.cif

CCDC number	1998922
Empirical formula	$C_{80}H_8Ag_6Al_2F_{88}O_{32}Ta_4$
Formula weight	4577.85
Temperature [K]	100(2)
Crystal system	orthorhombic
Space group (number)	*Pbca* (61)
a [Å]	30.459(12)
b [Å]	21.418(12)
c [Å]	36.508(17)
α [Å]	90
β [Å]	90
γ [Å]	90
Volume [Å^3]	23817(19)
Z	8
ρ_{calc} [g/cm^3]	2.553
μ [mm^{-1}]	4.848
F(000)	17088
Crystal size [mm^3]	0.300×0.100×0.060
Crystal colour	red
Crystal shape	needle
Radiation	MoK_α (λ=0.71073)
2Θ range [°]	2.23 to 52.86
Index ranges	-38 ≤ h ≤ 38, -26 ≤ k ≤ 26, -45 ≤ l ≤ 45
Reflections collected	542712
Independent reflections	24489 R_{int} = 0.0879, R_{sigma} = 0.0307
Completeness to θ = 25.242°	100.00
Data / Restraints / Parameters	24489/43315/3072
Goodness-of-fit on F^2	1.215
Final *R* indexes [I≥2σ(I)]	R_1 = 0.0485, wR_2 = 0.0917
Final *R* indexes [all data]	R_1 = 0.0636, wR_2 = 0.0978
Largest peak/hole [eÅ^3]	1.70/-1.25

Table 2. Bond lengths and angles for pbca_all_new_d-finalcif.cif.

Atom - Atom	Length [Å]
O1_1 - C1_1	1.331(9)
O1_1 - Al1	1.685(7)
C1_1 - C4_1	1.539(10)
C1_1 - C3_1	1.540(10)
C1_1 - C2_1	1.546(9)
C2_1 - F3_1	1.323(9)
C2_1 - F2_1	1.323(9)
C2_1 - F1_1	1.328(9)
C3_1 - F4_1	1.323(9)
C3_1 - F6_1	1.336(10)
C3_1 - F5_1	1.337(9)
C4_1 - F8_1	1.319(10)
C4_1 - F9_1	1.324(10)
C4_1 - F7_1	1.332(9)
F1_5 - C1_5	1.354(9)
F2_5 - C2_5	1.337(9)
F3_5 - C3_5	1.330(9)
F4_5 - C4_5	1.343(9)
C1_5 - C6_5	1.341(10)
C1_5 - C2_5	1.367(10)
C2_5 - C3_5	1.363(10)
C3_5 - C4_5	1.359(10)
C4_5 - C5_5	1.369(10)
C5_5 - C6_5	1.382(10)
O1_15 - C1_15	1.345(13)
O1_15 - Al2	1.698(11)
C1_15 - C2_15	1.529(12)
C1_15 - C4_15	1.538(12)
C1_15 - C3_15	1.539(13)
C2_15 - F3_15	1.305(13)
C2_15 - F2_15	1.308(13)
C2_15 - F1_15	1.336(13)
C3_15 - F6_15	1.300(13)
C3_15 - F5_15	1.320(13)
C3_15 - F4_15	1.328(13)
C4_15 - F9_15	1.304(13)
C4_15 - F8_15	1.317(12)
C4_15 - F7_15	1.332(13)
F1_14 - C1_14	1.351(12)
F2_14 - C2_14	1.342(13)
F3_14 - C3_14	1.345(13)
F4_14 - C4_14	1.334(12)
C1_14 - C2_14	1.364(12)
C1_14 - C6_14	1.364(13)
C2_14 - C3_14	1.364(12)
C3_14 - C4_14	1.359(13)
C4_14 - C5_14	1.358(13)
C5_14 - C6_14	1.370(13)
F1_13 - C1_13	1.353(13)
F2_13 - C2_13	1.349(12)

F3_13 - C3_13	1.336(11)	C2_9 - F2_9	1.322(13)
F4_13 - C4_13	1.348(13)	C2_9 - F1_9	1.341(13)
C1_13 - C2_13	1.354(12)	C3_9 - F4_9	1.312(13)
C1_13 - C6_13	1.363(12)	C3_9 - F5_9	1.315(13)
C2_13 - C3_13	1.365(12)	C3_9 - F6_9	1.328(13)
C3_13 - C4_13	1.366(12)	C4_9 - F8_9	1.319(13)
C4_13 - C5_13	1.360(12)	C4_9 - F7_9	1.327(13)
C5_13 - C6_13	1.369(13)	C4_9 - F9_9	1.331(13)
O1_12 - C1_12	1.328(12)	O1_8 - C1_8	1.343(12)
O1_12 - Al2	1.664(10)	O1_8 - Al1	1.684(10)
C1_12 - C3_12	1.532(12)	C1_8 - C2_8	1.533(12)
C1_12 - C2_12	1.535(12)	C1_8 - C4_8	1.543(12)
C1_12 - C4_12	1.542(12)	C1_8 - C3_8	1.544(12)
C2_12 - F1_12	1.305(13)	C2_8 - F1_8	1.318(13)
C2_12 - F3_12	1.317(13)	C2_8 - F3_8	1.326(13)
C2_12 - F2_12	1.332(13)	C2_8 - F2_8	1.332(13)
C3_12 - F6_12	1.310(13)	C3_8 - F4_8	1.320(12)
C3_12 - F5_12	1.312(13)	C3_8 - F6_8	1.321(12)
C3_12 - F4_12	1.324(13)	C3_8 - F5_8	1.323(13)
C4_12 - F7_12	1.309(12)	C4_8 - F7_8	1.318(12)
C4_12 - F8_12	1.321(12)	C4_8 - F8_8	1.318(12)
C4_12 - F9_12	1.323(13)	C4_8 - F9_8	1.319(13)
O1_11 - C1_11	1.339(12)	O1_7 - C1_7	1.345(13)
O1_11 - Al2	1.687(9)	O1_7 - Al1	1.677(12)
C1_11 - C4_11	1.529(12)	C1_7 - C3_7	1.534(13)
C1_11 - C3_11	1.530(12)	C1_7 - C2_7	1.538(13)
C1_11 - C2_11	1.531(12)	C1_7 - C4_7	1.538(13)
C2_11 - F2_11	1.300(13)	C2_7 - F3_7	1.315(13)
C2_11 - F3_11	1.312(12)	C2_7 - F2_7	1.322(13)
C2_11 - F1_11	1.318(13)	C2_7 - F1_7	1.328(13)
C3_11 - F6_11	1.318(13)	C3_7 - F4_7	1.313(13)
C3_11 - F5_11	1.325(13)	C3_7 - F6_7	1.327(13)
C3_11 - F4_11	1.332(13)	C3_7 - F5_7	1.328(14)
C4_11 - F7_11	1.284(12)	C4_7 - F8_7	1.313(13)
C4_11 - F9_11	1.313(12)	C4_7 - F9_7	1.321(13)
C4_11 - F8_11	1.341(12)	C4_7 - F7_7	1.323(13)
O1_10 - C1_10	1.348(12)	F1_6 - C1_6	1.350(11)
O1_10 - Al2	1.756(10)	F2_6 - C2_6	1.338(11)
C1_10 - C3_10	1.532(12)	F3_6 - C3_6	1.338(11)
C1_10 - C2_10	1.545(12)	F4_6 - C4_6	1.344(11)
C1_10 - C4_10	1.553(12)	C1_6 - C2_6	1.361(11)
C2_10 - F2_10	1.318(13)	C1_6 - C6_6	1.362(12)
C2_10 - F3_10	1.321(12)	C2_6 - C3_6	1.371(11)
C2_10 - F1_10	1.331(13)	C3_6 - C4_6	1.358(11)
C3_10 - F4_10	1.308(13)	C4_6 - C5_6	1.368(11)
C3_10 - F5_10	1.319(12)	C5_6 - C6_6	1.357(12)
C3_10 - F6_10	1.321(12)	O1_4 - C1_4	1.350(13)
C4_10 - F8_10	1.318(12)	O1_4 - Al2	1.734(11)
C4_10 - F9_10	1.333(12)	C1_4 - C4_4	1.531(13)
C4_10 - F7_10	1.339(12)	C1_4 - C3_4	1.541(13)
O1_9 - C1_9	1.353(12)	C1_4 - C2_4	1.548(13)
O1_9 - Al1	1.744(11)	C2_4 - F3_4	1.307(13)
C1_9 - C3_9	1.538(12)	C2_4 - F1_4	1.338(13)
C1_9 - C2_9	1.540(12)	C2_4 - F2_4	1.343(14)
C1_9 - C4_9	1.542(12)	C3_4 - F4_4	1.312(13)
C2_9 - F3_9	1.296(12)	C3_4 - F6_4	1.318(13)

C3_4 - F5_4	1.337(14)	Ta2 - C8	2.115(10)
C4_4 - F8_4	1.301(13)	Ta2 - C12	2.121(9)
C4_4 - F7_4	1.325(13)	Ta2 - C7	2.133(9)
C4_4 - F9_4	1.330(14)	Ta2 - C10	2.150(10)
O1_3 - C1_3	1.347(12)	Ta2 - C9	2.159(11)
O1_3 - Al2	1.704(11)	Ta2 - C11	2.162(9)
C1_3 - C4_3	1.535(12)	Ta2 - Ag2	2.9787(13)
C1_3 - C3_3	1.538(12)	Ta2 - Ag6	2.9854(12)
C1_3 - C2_3	1.540(12)	Ta2 - Ag5	3.0073(13)
C2_3 - F3_3	1.317(12)	O2 - C2	1.136(10)
C2_3 - F2_3	1.320(12)	Ag2 - C7	2.626(9)
C2_3 - F1_3	1.335(12)	Ag2 - C8	2.648(8)
C3_3 - F5_3	1.297(13)	Ag2 - C5	2.650(9)
C3_3 - F4_3	1.311(12)	Ag2 - Ag5	2.8876(13)
C3_3 - F6_3	1.330(13)	Ag2 - Ag3	2.8919(13)
C4_3 - F8_3	1.304(13)	Ag2 - Ag6	2.9083(12)
C4_3 - F7_3	1.311(13)	Al2 - O1_20	1.75(2)
C4_3 - F9_3	1.315(13)	Ta3 - C18	2.123(9)
O1_2 - C1_2	1.325(11)	Ta3 - C14	2.125(9)
O1_2 - Al2	1.680(10)	Ta3 - C13	2.132(9)
C1_2 - C4_2	1.539(11)	Ta3 - C16	2.159(10)
C1_2 - C2_2	1.542(12)	Ta3 - C15	2.161(10)
C1_2 - C3_2	1.543(12)	Ta3 - C17	2.162(9)
C2_2 - F3_2	1.317(12)	Ta3 - Ag4	2.9658(17)
C2_2 - F2_2	1.318(12)	Ta3 - Ag6	2.9868(12)
C2_2 - F1_2	1.323(12)	Ta3 - Ag3	2.9903(12)
C3_2 - F5_2	1.306(12)	O3 - C3	1.154(11)
C3_2 - F4_2	1.317(12)	C3 - Ag3	2.627(9)
C3_2 - F6_2	1.327(12)	Ag3 - C18	2.628(8)
C4_2 - F8_2	1.313(12)	Ag3 - C5	2.649(9)
C4_2 - F9_2	1.324(12)	Ag3 - C14	2.672(9)
C4_2 - F7_2	1.329(12)	Ag3 - Ag6	2.8819(13)
Ta1 - C1	2.123(9)	Ag3 - Ag4	2.9222(13)
Ta1 - C3	2.124(9)	Ta4 - C24	2.102(9)
Ta1 - C5	2.124(9)	Ta4 - C22	2.119(10)
Ta1 - C2	2.160(9)	Ta4 - C23	2.129(9)
Ta1 - C4	2.167(9)	Ta4 - C20	2.156(11)
Ta1 - C6	2.173(9)	Ta4 - C19	2.166(10)
Ta1 - Ag1	2.9685(13)	Ta4 - C21	2.170(10)
Ta1 - Ag2	2.9732(12)	Ta4 - Ag4	2.9671(16)
Ta1 - Ag3	2.9879(11)	Ta4 - Ag5	3.0155(13)
O1 - C1	1.142(10)	Ag4 - C13	2.597(9)
C1 - Ag1	2.591(8)	Ag4 - C24	2.626(8)
C1 - Ag2	2.652(9)	Ag4 - C18	2.668(9)
Ag1 - C24	2.620(8)	Ag4 - C22	2.706(9)
Ag1 - C3	2.652(9)	Ag4 - Ag5	2.9193(13)
Ag1 - C23	2.663(9)	Ag4 - Ag6	2.9259(14)
Ag1 - Ag4	2.8590(12)	O4 - C4	1.115(10)
Ag1 - Ag3	2.9053(17)	Ag5 - C23	2.582(9)
Ag1 - Ag2	2.9093(14)	Ag5 - C12	2.615(9)
Ag1 - Ag5	2.9203(13)	Ag5 - Ag6	2.8627(17)
Ag1 - Ta4	2.9755(12)	O5 - C5	1.142(10)
Al1 - O1_18	1.684(10)	Ag6 - C8	2.585(9)
Al1 - O1_19	1.700(11)	Ag6 - C13	2.588(9)
Al1 - O1_21	1.731(13)	Ag6 - C14	2.691(9)
Al1 - O1_22	1.81(3)	O6 - C6	1.122(10)

C9 - O9	1.128(12)
O8 - C8	1.154(11)
C7 - O7	1.143(11)
O13 - C13	1.137(10)
C12 - O12	1.153(11)
C11 - O11	1.119(11)
C10 - O10	1.135(11)
C16 - O16	1.118(11)
O15 - C15	1.123(12)
C14 - O14	1.135(11)
C20 - O20	1.113(12)
C21 - O21	1.122(11)
C22 - O22	1.153(11)
C23 - O23	1.150(10)
C24 - O24	1.161(10)
C19 - O19	1.120(11)
C18 - O18	1.144(10)
C17 - O17	1.125(10)
F1_16 - C1_16	1.343(13)
F2_16 - C2_16	1.340(14)
F3_16 - C3_16	1.348(13)
F4_16 - C4_16	1.345(13)
C1_16 - C6_16	1.362(13)
C1_16 - C2_16	1.364(13)
C2_16 - C3_16	1.365(13)
C3_16 - C4_16	1.365(13)
C4_16 - C5_16	1.359(14)
C5_16 - C6_16	1.365(14)
F1_17 - C1_17	1.341(14)
F2_17 - C2_17	1.339(14)
F3_17 - C3_17	1.341(14)
F4_17 - C4_17	1.343(14)
C1_17 - C2_17	1.362(13)
C1_17 - C6_17	1.365(14)
C2_17 - C3_17	1.365(13)
C3_17 - C4_17	1.358(13)
C4_17 - C5_17	1.363(14)
C5_17 - C6_17	1.362(14)
O1_18 - C1_18	1.337(12)
C1_18 - C3_18	1.537(13)
C1_18 - C4_18	1.538(12)
C1_18 - C2_18	1.547(12)
C2_18 - F2_18	1.298(13)
C2_18 - F1_18	1.304(13)
C2_18 - F3_18	1.315(13)
C3_18 - F4_18	1.315(13)
C3_18 - F6_18	1.322(13)
C3_18 - F5_18	1.322(13)
C4_18 - F9_18	1.306(13)
C4_18 - F8_18	1.317(13)
C4_18 - F7_18	1.324(13)
O1_19 - C1_19	1.353(13)
C1_19 - C4_19	1.539(13)
C1_19 - C3_19	1.542(12)
C1_19 - C2_19	1.547(13)
C2_19 - F2_19	1.318(13)
C2_19 - F3_19	1.323(14)
C2_19 - F1_19	1.327(13)
C3_19 - F4_19	1.318(13)
C3_19 - F6_19	1.319(13)
C3_19 - F5_19	1.323(13)
C4_19 - F8_19	1.315(13)
C4_19 - F7_19	1.324(13)
C4_19 - F9_19	1.324(13)
O1_20 - C1_20	1.346(14)
C1_20 - C4_20	1.537(13)
C1_20 - C2_20	1.542(13)
C1_20 - C3_20	1.544(13)
C2_20 - F3_20	1.325(13)
C2_20 - F2_20	1.327(13)
C2_20 - F1_20	1.329(13)
C3_20 - F6_20	1.318(13)
C3_20 - F5_20	1.326(13)
C3_20 - F4_20	1.327(13)
C4_20 - F9_20	1.315(13)
C4_20 - F7_20	1.318(13)
C4_20 - F8_20	1.324(13)
O1_21 - C1_21	1.363(13)
C1_21 - C3_21	1.537(13)
C1_21 - C4_21	1.541(13)
C1_21 - C2_21	1.542(13)
C2_21 - F1_21	1.321(13)
C2_21 - F2_21	1.323(13)
C2_21 - F3_21	1.327(13)
C3_21 - F6_21	1.325(13)
C3_21 - F5_21	1.325(13)
C3_21 - F4_21	1.326(13)
C4_21 - F7_21	1.318(13)
C4_21 - F8_21	1.322(13)
C4_21 - F9_21	1.330(13)
O1_22 - C1_22	1.347(15)
C1_22 - C4_22	1.535(13)
C1_22 - C3_22	1.540(13)
C1_22 - C2_22	1.541(13)
C2_22 - F2_22	1.320(14)
C2_22 - F3_22	1.322(14)
C2_22 - F1_22	1.322(14)
C3_22 - F6_22	1.318(14)
C3_22 - F5_22	1.321(14)
C3_22 - F4_22	1.326(14)
C4_22 - F7_22	1.318(14)
C4_22 - F9_22	1.324(14)
C4_22 - F8_22	1.324(14)

Atom - Atom - Atom	**Angle [°]**
C1_1 - O1_1 - Al1	156.4(7)
O1_1 - C1_1 - C4_1	110.8(8)
O1_1 - C1_1 - C3_1	107.6(7)
C4_1 - C1_1 - C3_1	107.7(7)
O1_1 - C1_1 - C2_1	112.8(7)
C4_1 - C1_1 - C2_1	109.0(6)
C3_1 - C1_1 - C2_1	108.7(7)

F3_1 - C2_1 - F2_1	107.0(8)
F3_1 - C2_1 - F1_1	107.3(8)
F2_1 - C2_1 - F1_1	107.3(8)
F3_1 - C2_1 - C1_1	111.3(7)
F2_1 - C2_1 - C1_1	112.6(7)
F1_1 - C2_1 - C1_1	111.1(7)
F4_1 - C3_1 - F6_1	107.6(8)
F4_1 - C3_1 - F5_1	106.9(8)
F6_1 - C3_1 - F5_1	107.7(9)
F4_1 - C3_1 - C1_1	111.7(8)
F6_1 - C3_1 - C1_1	112.0(7)
F5_1 - C3_1 - C1_1	110.7(8)
F8_1 - C4_1 - F9_1	107.4(8)
F8_1 - C4_1 - F7_1	106.9(8)
F9_1 - C4_1 - F7_1	108.9(8)
F8_1 - C4_1 - C1_1	113.5(7)
F9_1 - C4_1 - C1_1	109.3(8)
F7_1 - C4_1 - C1_1	110.8(7)
C6_5 - C1_5 - F1_5	122.3(9)
C6_5 - C1_5 - C2_5	121.9(8)
F1_5 - C1_5 - C2_5	115.8(9)
F2_5 - C2_5 - C3_5	122.2(9)
F2_5 - C2_5 - C1_5	118.6(8)
C3_5 - C2_5 - C1_5	119.2(8)
F3_5 - C3_5 - C4_5	119.9(8)
F3_5 - C3_5 - C2_5	120.2(8)
C4_5 - C3_5 - C2_5	119.9(8)
F4_5 - C4_5 - C3_5	119.2(8)
F4_5 - C4_5 - C5_5	120.3(8)
C3_5 - C4_5 - C5_5	120.5(8)
C4_5 - C5_5 - C6_5	119.5(9)
C1_5 - C6_5 - C5_5	119.0(9)
C1_15 - O1_15 - Al2	146.2(18)
O1_15 - C1_15 - C2_15	106.1(12)
O1_15 - C1_15 - C4_15	113.5(13)
C2_15 - C1_15 - C4_15	110.5(11)
O1_15 - C1_15 - C3_15	107.4(14)
C2_15 - C1_15 - C3_15	112.1(11)
C4_15 - C1_15 - C3_15	107.3(10)
F3_15 - C2_15 - F2_15	107.4(14)
F3_15 - C2_15 - F1_15	106.5(16)
F2_15 - C2_15 - F1_15	104.5(16)
F3_15 - C2_15 - C1_15	113.9(13)
F2_15 - C2_15 - C1_15	113.6(13)
F1_15 - C2_15 - C1_15	110.3(14)
F6_15 - C3_15 - F5_15	109.2(15)
F6_15 - C3_15 - F4_15	108.8(15)
F5_15 - C3_15 - F4_15	105.3(15)
F6_15 - C3_15 - C1_15	112.6(13)
F5_15 - C3_15 - C1_15	109.7(12)
F4_15 - C3_15 - C1_15	111.1(13)
F9_15 - C4_15 - F8_15	112.7(15)
F9_15 - C4_15 - F7_15	100.6(13)
F8_15 - C4_15 - F7_15	108.2(15)
F9_15 - C4_15 - C1_15	110.3(12)
F8_15 - C4_15 - C1_15	112.1(11)
F7_15 - C4_15 - C1_15	112.3(12)
F1_14 - C1_14 - C2_14	119.2(14)
F1_14 - C1_14 - C6_14	119.6(15)
C2_14 - C1_14 - C6_14	121.2(13)
F2_14 - C2_14 - C1_14	120.6(13)
F2_14 - C2_14 - C3_14	118.8(13)
C1_14 - C2_14 - C3_14	120.6(13)
F3_14 - C3_14 - C4_14	120.0(13)
F3_14 - C3_14 - C2_14	122.1(13)
C4_14 - C3_14 - C2_14	117.9(13)
F4_14 - C4_14 - C5_14	120.0(15)
F4_14 - C4_14 - C3_14	118.1(14)
C5_14 - C4_14 - C3_14	121.9(13)
C4_14 - C5_14 - C6_14	120.1(15)
C1_14 - C6_14 - C5_14	118.2(15)
F1_13 - C1_13 - C2_13	118.4(12)
F1_13 - C1_13 - C6_13	120.8(12)
C2_13 - C1_13 - C6_13	120.7(12)
F2_13 - C2_13 - C1_13	119.2(11)
F2_13 - C2_13 - C3_13	121.1(11)
C1_13 - C2_13 - C3_13	119.8(12)
F3_13 - C3_13 - C2_13	119.4(11)
F3_13 - C3_13 - C4_13	119.9(11)
C2_13 - C3_13 - C4_13	120.7(11)
F4_13 - C4_13 - C5_13	123.5(13)
F4_13 - C4_13 - C3_13	117.8(12)
C5_13 - C4_13 - C3_13	118.7(13)
C4_13 - C5_13 - C6_13	121.3(14)
C1_13 - C6_13 - C5_13	118.8(13)
C1_12 - O1_12 - Al2	155.1(12)
O1_12 - C1_12 - C3_12	109.2(11)
O1_12 - C1_12 - C2_12	112.0(12)
C3_12 - C1_12 - C2_12	108.8(10)
O1_12 - C1_12 - C4_12	107.3(10)
C3_12 - C1_12 - C4_12	110.1(10)
C2_12 - C1_12 - C4_12	109.4(10)
F1_12 - C2_12 - F3_12	107.9(15)
F1_12 - C2_12 - F2_12	107.4(16)
F3_12 - C2_12 - F2_12	104.0(15)
F1_12 - C2_12 - C1_12	114.1(12)
F3_12 - C2_12 - C1_12	110.9(13)
F2_12 - C2_12 - C1_12	111.9(12)
F6_12 - C3_12 - F5_12	108.6(14)
F6_12 - C3_12 - F4_12	104.5(16)
F5_12 - C3_12 - F4_12	106.1(14)
F6_12 - C3_12 - C1_12	114.6(12)
F5_12 - C3_12 - C1_12	113.2(11)
F4_12 - C3_12 - C1_12	109.2(12)
F7_12 - C4_12 - F8_12	107.5(13)
F7_12 - C4_12 - F9_12	108.1(13)
F8_12 - C4_12 - F9_12	107.6(13)
F7_12 - C4_12 - C1_12	111.3(11)
F8_12 - C4_12 - C1_12	111.3(11)
F9_12 - C4_12 - C1_12	111.0(11)
C1_11 - O1_11 - Al2	149.6(11)
O1_11 - C1_11 - C4_11	114.2(10)

O1_11 - C1_11 - C3_11	104.7(11)
C4_11 - C1_11 - C3_11	109.0(10)
O1_11 - C1_11 - C2_11	109.6(11)
C4_11 - C1_11 - C2_11	106.8(9)
C3_11 - C1_11 - C2_11	112.8(11)
F2_11 - C2_11 - F3_11	102.6(13)
F2_11 - C2_11 - F1_11	101.0(14)
F3_11 - C2_11 - F1_11	117.7(17)
F2_11 - C2_11 - C1_11	111.9(12)
F3_11 - C2_11 - C1_11	110.9(12)
F1_11 - C2_11 - C1_11	111.9(12)
F6_11 - C3_11 - F5_11	111.0(16)
F6_11 - C3_11 - F4_11	108.3(16)
F5_11 - C3_11 - F4_11	109.6(16)
F6_11 - C3_11 - C1_11	112.6(14)
F5_11 - C3_11 - C1_11	107.8(13)
F4_11 - C3_11 - C1_11	107.5(12)
F7_11 - C4_11 - F9_11	107.1(14)
F7_11 - C4_11 - F8_11	106.7(12)
F9_11 - C4_11 - F8_11	110.4(14)
F7_11 - C4_11 - C1_11	112.0(10)
F9_11 - C4_11 - C1_11	109.6(12)
F8_11 - C4_11 - C1_11	110.9(11)
C1_10 - O1_10 - Al2	155.0(11)
O1_10 - C1_10 - C3_10	112.3(10)
O1_10 - C1_10 - C2_10	109.0(11)
C3_10 - C1_10 - C2_10	108.2(10)
O1_10 - C1_10 - C4_10	109.6(10)
C3_10 - C1_10 - C4_10	109.9(9)
C2_10 - C1_10 - C4_10	107.7(9)
F2_10 - C2_10 - F3_10	108.3(14)
F2_10 - C2_10 - F1_10	103.9(14)
F3_10 - C2_10 - F1_10	105.3(13)
F2_10 - C2_10 - C1_10	114.5(12)
F3_10 - C2_10 - C1_10	113.1(12)
F1_10 - C2_10 - C1_10	110.9(12)
F4_10 - C3_10 - F5_10	106.9(14)
F4_10 - C3_10 - F6_10	108.1(14)
F5_10 - C3_10 - F6_10	105.9(13)
F4_10 - C3_10 - C1_10	111.8(11)
F5_10 - C3_10 - C1_10	110.9(12)
F6_10 - C3_10 - C1_10	112.8(11)
F8_10 - C4_10 - F9_10	110.1(12)
F8_10 - C4_10 - F7_10	110.0(13)
F9_10 - C4_10 - F7_10	107.4(13)
F8_10 - C4_10 - C1_10	112.3(11)
F9_10 - C4_10 - C1_10	107.6(10)
F7_10 - C4_10 - C1_10	109.2(11)
C1_9 - O1_9 - Al1	153.6(13)
O1_9 - C1_9 - C3_9	111.1(11)
O1_9 - C1_9 - C2_9	110.6(12)
C3_9 - C1_9 - C2_9	107.1(10)
O1_9 - C1_9 - C4_9	111.6(12)
C3_9 - C1_9 - C4_9	109.1(11)
C2_9 - C1_9 - C4_9	107.2(10)
F3_9 - C2_9 - F2_9	109.8(15)
F3_9 - C2_9 - F1_9	110.0(15)
F2_9 - C2_9 - F1_9	105.3(15)
F3_9 - C2_9 - C1_9	111.8(12)
F2_9 - C2_9 - C1_9	113.6(13)
F1_9 - C2_9 - C1_9	106.1(13)
F4_9 - C3_9 - F5_9	104.6(15)
F4_9 - C3_9 - F6_9	110.5(15)
F5_9 - C3_9 - F6_9	107.9(15)
F4_9 - C3_9 - C1_9	109.6(12)
F5_9 - C3_9 - C1_9	111.4(12)
F6_9 - C3_9 - C1_9	112.4(13)
F8_9 - C4_9 - F7_9	108.4(15)
F8_9 - C4_9 - F9_9	106.0(15)
F7_9 - C4_9 - F9_9	110.1(16)
F8_9 - C4_9 - C1_9	112.5(12)
F7_9 - C4_9 - C1_9	109.0(13)
F9_9 - C4_9 - C1_9	110.7(12)
C1_8 - O1_8 - Al1	159.4(13)
O1_8 - C1_8 - C2_8	107.4(11)
O1_8 - C1_8 - C4_8	110.1(11)
C2_8 - C1_8 - C4_8	109.3(10)
O1_8 - C1_8 - C3_8	110.6(11)
C2_8 - C1_8 - C3_8	110.0(10)
C4_8 - C1_8 - C3_8	109.4(10)
F1_8 - C2_8 - F3_8	107.3(14)
F1_8 - C2_8 - F2_8	106.0(14)
F3_8 - C2_8 - F2_8	108.0(15)
F1_8 - C2_8 - C1_8	114.0(12)
F3_8 - C2_8 - C1_8	110.7(11)
F2_8 - C2_8 - C1_8	110.6(13)
F4_8 - C3_8 - F6_8	107.9(13)
F4_8 - C3_8 - F5_8	107.4(14)
F6_8 - C3_8 - F5_8	105.9(15)
F4_8 - C3_8 - C1_8	112.1(11)
F6_8 - C3_8 - C1_8	113.4(12)
F5_8 - C3_8 - C1_8	109.8(12)
F7_8 - C4_8 - F8_8	109.7(14)
F7_8 - C4_8 - F9_8	106.5(14)
F8_8 - C4_8 - F9_8	107.4(15)
F7_8 - C4_8 - C1_8	108.7(11)
F8_8 - C4_8 - C1_8	112.7(12)
F9_8 - C4_8 - C1_8	111.7(12)
C1_7 - O1_7 - Al1	149.4(19)
O1_7 - C1_7 - C3_7	112.7(15)
O1_7 - C1_7 - C2_7	105.5(12)
C3_7 - C1_7 - C2_7	108.6(12)
O1_7 - C1_7 - C4_7	109.2(14)
C3_7 - C1_7 - C4_7	109.8(12)
C2_7 - C1_7 - C4_7	110.9(11)
F3_7 - C2_7 - F2_7	109.4(14)
F3_7 - C2_7 - F1_7	105.2(16)
F2_7 - C2_7 - F1_7	108.2(17)
F3_7 - C2_7 - C1_7	112.0(13)
F2_7 - C2_7 - C1_7	110.3(13)
F1_7 - C2_7 - C1_7	111.4(15)
F4_7 - C3_7 - F6_7	107.7(16)

F4_7 - C3_7 - F5_7	107.1(17)
F6_7 - C3_7 - F5_7	105.1(18)
F4_7 - C3_7 - C1_7	112.2(15)
F6_7 - C3_7 - C1_7	113.5(15)
F5_7 - C3_7 - C1_7	110.8(15)
F8_7 - C4_7 - F9_7	108.6(16)
F8_7 - C4_7 - F7_7	106.7(15)
F9_7 - C4_7 - F7_7	108.2(16)
F8_7 - C4_7 - C1_7	113.2(14)
F9_7 - C4_7 - C1_7	110.4(14)
F7_7 - C4_7 - C1_7	109.6(13)
F1_6 - C1_6 - C2_6	118.4(10)
F1_6 - C1_6 - C6_6	121.5(11)
C2_6 - C1_6 - C6_6	120.1(10)
F2_6 - C2_6 - C1_6	119.4(10)
F2_6 - C2_6 - C3_6	120.8(10)
C1_6 - C2_6 - C3_6	119.8(9)
F3_6 - C3_6 - C4_6	119.7(9)
F3_6 - C3_6 - C2_6	120.5(9)
C4_6 - C3_6 - C2_6	119.8(9)
F4_6 - C4_6 - C3_6	119.1(9)
F4_6 - C4_6 - C5_6	120.6(9)
C3_6 - C4_6 - C5_6	120.3(9)
C6_6 - C5_6 - C4_6	119.8(11)
C5_6 - C6_6 - C1_6	120.2(12)
C1_4 - O1_4 - Al2	151.8(15)
O1_4 - C1_4 - C4_4	109.7(12)
O1_4 - C1_4 - C3_4	109.0(12)
C4_4 - C1_4 - C3_4	111.3(12)
O1_4 - C1_4 - C2_4	113.2(13)
C4_4 - C1_4 - C2_4	107.8(11)
C3_4 - C1_4 - C2_4	105.8(11)
F3_4 - C2_4 - F1_4	116.5(17)
F3_4 - C2_4 - F2_4	109.4(17)
F1_4 - C2_4 - F2_4	101.7(16)
F3_4 - C2_4 - C1_4	108.0(13)
F1_4 - C2_4 - C1_4	113.3(14)
F2_4 - C2_4 - C1_4	107.4(15)
F4_4 - C3_4 - F6_4	107.0(16)
F4_4 - C3_4 - F5_4	110.9(19)
F6_4 - C3_4 - F5_4	105.7(17)
F4_4 - C3_4 - C1_4	109.7(15)
F6_4 - C3_4 - C1_4	115.3(14)
F5_4 - C3_4 - C1_4	108.2(15)
F8_4 - C4_4 - F7_4	115.5(16)
F8_4 - C4_4 - F9_4	100.6(17)
F7_4 - C4_4 - F9_4	104.9(17)
F8_4 - C4_4 - C1_4	114.2(13)
F7_4 - C4_4 - C1_4	111.6(12)
F9_4 - C4_4 - C1_4	108.8(14)
C1_3 - O1_3 - Al2	156.9(16)
O1_3 - C1_3 - C4_3	109.7(12)
O1_3 - C1_3 - C3_3	109.4(12)
C4_3 - C1_3 - C3_3	107.7(10)
O1_3 - C1_3 - C2_3	110.4(12)
C4_3 - C1_3 - C2_3	110.2(10)
C3_3 - C1_3 - C2_3	109.4(9)
F3_3 - C2_3 - F2_3	106.6(14)
F3_3 - C2_3 - F1_3	108.2(13)
F2_3 - C2_3 - F1_3	106.5(13)
F3_3 - C2_3 - C1_3	110.8(11)
F2_3 - C2_3 - C1_3	113.1(11)
F1_3 - C2_3 - C1_3	111.3(11)
F5_3 - C3_3 - F4_3	102.8(13)
F5_3 - C3_3 - F6_3	108.4(15)
F4_3 - C3_3 - F6_3	110.9(14)
F5_3 - C3_3 - C1_3	113.6(12)
F4_3 - C3_3 - C1_3	111.7(11)
F6_3 - C3_3 - C1_3	109.3(12)
F8_3 - C4_3 - F7_3	106.3(14)
F8_3 - C4_3 - F9_3	102.9(16)
F7_3 - C4_3 - F9_3	111.3(15)
F8_3 - C4_3 - C1_3	114.5(13)
F7_3 - C4_3 - C1_3	112.0(11)
F9_3 - C4_3 - C1_3	109.5(11)
C1_2 - O1_2 - Al2	161.3(13)
O1_2 - C1_2 - C4_2	111.4(10)
O1_2 - C1_2 - C2_2	110.4(10)
C4_2 - C1_2 - C2_2	108.7(9)
O1_2 - C1_2 - C3_2	107.6(11)
C4_2 - C1_2 - C3_2	108.8(9)
C2_2 - C1_2 - C3_2	110.0(9)
F3_2 - C2_2 - F2_2	106.0(14)
F3_2 - C2_2 - F1_2	106.1(13)
F2_2 - C2_2 - F1_2	107.3(13)
F3_2 - C2_2 - C1_2	112.1(11)
F2_2 - C2_2 - C1_2	112.2(12)
F1_2 - C2_2 - C1_2	112.7(12)
F5_2 - C3_2 - F4_2	107.8(12)
F5_2 - C3_2 - F6_2	107.1(12)
F4_2 - C3_2 - F6_2	107.8(12)
F5_2 - C3_2 - C1_2	110.9(10)
F4_2 - C3_2 - C1_2	110.5(11)
F6_2 - C3_2 - C1_2	112.6(10)
F8_2 - C4_2 - F9_2	107.8(11)
F8_2 - C4_2 - F7_2	106.7(13)
F9_2 - C4_2 - F7_2	106.3(13)
F8_2 - C4_2 - C1_2	112.5(10)
F9_2 - C4_2 - C1_2	112.2(10)
F7_2 - C4_2 - C1_2	110.9(11)
C1 - Ta1 - C3	111.8(3)
C1 - Ta1 - C5	113.5(3)
C3 - Ta1 - C5	110.9(3)
C1 - Ta1 - C2	79.7(3)
C3 - Ta1 - C2	77.7(3)
C5 - Ta1 - C2	157.9(3)
C1 - Ta1 - C4	156.5(3)
C3 - Ta1 - C4	80.9(3)
C5 - Ta1 - C4	77.5(3)
C2 - Ta1 - C4	84.2(3)
C1 - Ta1 - C6	75.9(3)
C3 - Ta1 - C6	160.7(3)

C5 - Ta1 - C6	79.9(3)
C2 - Ta1 - C6	86.8(3)
C4 - Ta1 - C6	86.3(3)
C1 - Ta1 - Ag1	58.4(2)
C3 - Ta1 - Ag1	60.1(2)
C5 - Ta1 - Ag1	108.2(2)
C2 - Ta1 - Ag1	93.8(2)
C4 - Ta1 - Ag1	140.3(2)
C6 - Ta1 - Ag1	133.3(2)
C1 - Ta1 - Ag2	60.0(2)
C3 - Ta1 - Ag2	107.5(2)
C5 - Ta1 - Ag2	59.9(2)
C2 - Ta1 - Ag2	138.6(2)
C4 - Ta1 - Ag2	137.0(2)
C6 - Ta1 - Ag2	91.6(2)
Ag1 - Ta1 - Ag2	58.63(2)
C1 - Ta1 - Ag3	106.9(2)
C3 - Ta1 - Ag3	59.0(2)
C5 - Ta1 - Ag3	59.6(2)
C2 - Ta1 - Ag3	135.8(2)
C4 - Ta1 - Ag3	96.6(2)
C6 - Ta1 - Ag3	137.4(2)
Ag1 - Ta1 - Ag3	58.39(4)
Ag2 - Ta1 - Ag3	58.04(2)
O1 - C1 - Ta1	167.3(7)
O1 - C1 - Ag1	113.9(6)
Ta1 - C1 - Ag1	77.3(3)
O1 - C1 - Ag2	113.0(7)
Ta1 - C1 - Ag2	76.1(3)
Ag1 - C1 - Ag2	67.4(2)
C1 - Ag1 - C24	154.5(3)
C1 - Ag1 - C3	84.2(3)
C24 - Ag1 - C3	92.9(3)
C1 - Ag1 - C23	89.9(3)
C24 - Ag1 - C23	84.0(3)
C3 - Ag1 - C23	159.5(3)
C1 - Ag1 - Ag4	148.4(2)
C24 - Ag1 - Ag4	57.08(18)
C3 - Ag1 - Ag4	99.36(19)
C23 - Ag1 - Ag4	95.9(2)
C1 - Ag1 - Ag3	97.5(2)
C24 - Ag1 - Ag3	101.96(18)
C3 - Ag1 - Ag3	56.21(19)
C23 - Ag1 - Ag3	144.21(19)
Ag4 - Ag1 - Ag3	60.92(3)
C1 - Ag1 - Ag2	57.3(2)
C24 - Ag1 - Ag2	148.02(18)
C3 - Ag1 - Ag2	96.2(2)
C23 - Ag1 - Ag2	97.07(19)
Ag4 - Ag1 - Ag2	91.15(3)
Ag3 - Ag1 - Ag2	59.65(2)
C1 - Ag1 - Ag5	99.2(2)
C24 - Ag1 - Ag5	97.41(19)
C3 - Ag1 - Ag5	145.46(19)
C23 - Ag1 - Ag5	54.86(19)
Ag4 - Ag1 - Ag5	60.67(3)
Ag3 - Ag1 - Ag5	89.36(3)
Ag2 - Ag1 - Ag5	59.38(3)
C1 - Ag1 - Ta1	44.25(19)
C24 - Ag1 - Ta1	136.7(2)
C3 - Ag1 - Ta1	43.96(19)
C23 - Ag1 - Ta1	134.1(2)
Ag4 - Ag1 - Ta1	122.03(4)
Ag3 - Ag1 - Ta1	61.142(19)
Ag2 - Ag1 - Ta1	60.76(2)
Ag5 - Ag1 - Ta1	120.14(3)
C1 - Ag1 - Ta4	133.62(19)
C24 - Ag1 - Ta4	43.5(2)
C3 - Ag1 - Ta4	136.5(2)
C23 - Ag1 - Ta4	43.9(2)
Ag4 - Ag1 - Ta4	61.10(4)
Ag3 - Ag1 - Ta4	122.00(2)
Ag2 - Ag1 - Ta4	120.86(3)
Ag5 - Ag1 - Ta4	61.51(2)
Ta1 - Ag1 - Ta4	176.80(2)
O1_7 - Al1 - O1_8	111.6(12)
O1_7 - Al1 - O1_1	118.8(10)
O1_8 - Al1 - O1_1	98.4(7)
O1_18 - Al1 - O1_1	102.9(7)
O1_18 - Al1 - O1_19	113.9(9)
O1_1 - Al1 - O1_19	118.9(6)
O1_18 - Al1 - O1_21	107.4(11)
O1_1 - Al1 - O1_21	102.4(9)
O1_19 - Al1 - O1_21	110.1(12)
O1_7 - Al1 - O1_9	110.2(10)
O1_8 - Al1 - O1_9	102.2(9)
O1_1 - Al1 - O1_9	113.8(7)
O1_1 - Al1 - O1_22	100.0(16)
C8 - Ta2 - C12	114.1(3)
C8 - Ta2 - C7	111.8(3)
C12 - Ta2 - C7	111.4(4)
C8 - Ta2 - C10	78.7(3)
C12 - Ta2 - C10	78.3(4)
C7 - Ta2 - C10	158.9(4)
C8 - Ta2 - C9	77.0(4)
C12 - Ta2 - C9	157.4(4)
C7 - Ta2 - C9	79.9(4)
C10 - Ta2 - C9	85.1(4)
C8 - Ta2 - C11	155.3(3)
C12 - Ta2 - C11	80.3(3)
C7 - Ta2 - C11	78.4(4)
C10 - Ta2 - C11	85.2(4)
C9 - Ta2 - C11	83.1(4)
C8 - Ta2 - Ag2	59.8(2)
C12 - Ta2 - Ag2	108.6(2)
C7 - Ta2 - Ag2	59.1(2)
C10 - Ta2 - Ag2	137.4(3)
C9 - Ta2 - Ag2	94.0(3)
C11 - Ta2 - Ag2	137.1(2)
C8 - Ta2 - Ag6	57.9(2)
C12 - Ta2 - Ag6	62.6(2)
C7 - Ta2 - Ag6	108.4(2)

C10 - Ta2 - Ag6	92.7(3)
C9 - Ta2 - Ag6	134.3(3)
C11 - Ta2 - Ag6	142.4(2)
Ag2 - Ta2 - Ag6	58.37(3)
C8 - Ta2 - Ag5	105.5(2)
C12 - Ta2 - Ag5	58.3(2)
C7 - Ta2 - Ag5	62.2(2)
C10 - Ta2 - Ag5	134.5(3)
C9 - Ta2 - Ag5	140.3(3)
C11 - Ta2 - Ag5	99.2(2)
Ag2 - Ta2 - Ag5	57.68(3)
Ag6 - Ta2 - Ag5	57.07(3)
O2 - C2 - Ta1	178.2(8)
C7 - Ag2 - C8	83.7(3)
C7 - Ag2 - C5	153.1(3)
C8 - Ag2 - C5	90.9(3)
C7 - Ag2 - C1	92.1(3)
C8 - Ag2 - C1	160.3(3)
C5 - Ag2 - C1	84.1(3)
C7 - Ag2 - Ag5	59.8(2)
C8 - Ag2 - Ag5	95.9(2)
C5 - Ag2 - Ag5	147.1(2)
C1 - Ag2 - Ag5	98.61(18)
C7 - Ag2 - Ag3	149.8(2)
C8 - Ag2 - Ag3	96.8(2)
C5 - Ag2 - Ag3	56.9(2)
C1 - Ag2 - Ag3	96.4(2)
Ag5 - Ag2 - Ag3	90.27(3)
C7 - Ag2 - Ag6	98.0(2)
C8 - Ag2 - Ag6	55.22(19)
C5 - Ag2 - Ag6	100.42(19)
C1 - Ag2 - Ag6	144.47(19)
Ag5 - Ag2 - Ag6	59.20(4)
Ag3 - Ag2 - Ag6	59.59(3)
C7 - Ag2 - Ag1	103.1(2)
C8 - Ag2 - Ag1	144.41(19)
C5 - Ag2 - Ag1	96.6(2)
C1 - Ag2 - Ag1	55.31(19)
Ag5 - Ag2 - Ag1	60.50(2)
Ag3 - Ag2 - Ag1	60.11(3)
Ag6 - Ag2 - Ag1	89.19(3)
C7 - Ag2 - Ta1	135.7(2)
C8 - Ag2 - Ta1	134.8(2)
C5 - Ag2 - Ta1	43.93(19)
C1 - Ag2 - Ta1	43.88(19)
Ag5 - Ag2 - Ta1	121.09(3)
Ag3 - Ag2 - Ta1	61.24(3)
Ag6 - Ag2 - Ta1	120.82(3)
Ag1 - Ag2 - Ta1	60.60(3)
C7 - Ag2 - Ta2	44.2(2)
C8 - Ag2 - Ta2	43.7(2)
C5 - Ag2 - Ta2	134.4(2)
C1 - Ag2 - Ta2	136.29(19)
Ag5 - Ag2 - Ta2	61.66(2)
Ag3 - Ag2 - Ta2	120.43(3)
Ag6 - Ag2 - Ta2	60.93(2)
Ag1 - Ag2 - Ta2	122.16(4)
Ta1 - Ag2 - Ta2	177.13(2)
O1_12 - Al2 - O1_2	115.7(8)
O1_11 - Al2 - O1_15	113.2(10)
O1_12 - Al2 - O1_3	112.1(9)
O1_2 - Al2 - O1_3	104.3(10)
O1_12 - Al2 - O1_4	106.6(9)
O1_2 - Al2 - O1_4	114.2(10)
O1_3 - Al2 - O1_4	103.3(10)
O1_11 - Al2 - O1_20	99.9(12)
O1_15 - Al2 - O1_20	109.5(14)
O1_11 - Al2 - O1_10	109.3(7)
O1_15 - Al2 - O1_10	114.2(9)
O1_20 - Al2 - O1_10	109.8(12)
C18 - Ta3 - C14	110.6(3)
C18 - Ta3 - C13	113.9(3)
C14 - Ta3 - C13	111.6(4)
C18 - Ta3 - C16	159.9(3)
C14 - Ta3 - C16	77.3(4)
C13 - Ta3 - C16	78.0(3)
C18 - Ta3 - C15	75.7(4)
C14 - Ta3 - C15	81.0(4)
C13 - Ta3 - C15	157.8(3)
C16 - Ta3 - C15	87.7(4)
C18 - Ta3 - C17	80.4(3)
C14 - Ta3 - C17	157.1(3)
C13 - Ta3 - C17	79.8(3)
C16 - Ta3 - C17	86.3(4)
C15 - Ta3 - C17	82.5(4)
C18 - Ta3 - Ag4	60.6(2)
C14 - Ta3 - Ag4	109.6(2)
C13 - Ta3 - Ag4	58.6(2)
C16 - Ta3 - Ag4	135.8(3)
C15 - Ta3 - Ag4	136.1(3)
C17 - Ta3 - Ag4	93.3(2)
C18 - Ta3 - Ag6	107.5(2)
C14 - Ta3 - Ag6	60.8(2)
C13 - Ta3 - Ag6	57.9(2)
C16 - Ta3 - Ag6	92.5(3)
C15 - Ta3 - Ag6	140.6(3)
C17 - Ta3 - Ag6	136.8(2)
Ag4 - Ta3 - Ag6	58.88(3)
C18 - Ta3 - Ag3	59.0(2)
C14 - Ta3 - Ag3	60.2(2)
C13 - Ta3 - Ag3	105.6(2)
C16 - Ta3 - Ag3	135.8(3)
C15 - Ta3 - Ag3	96.5(3)
C17 - Ta3 - Ag3	137.9(2)
Ag4 - Ta3 - Ag3	58.76(3)
Ag6 - Ta3 - Ag3	57.65(3)
O3 - C3 - Ta1	168.3(7)
O3 - C3 - Ag3	113.6(6)
Ta1 - C3 - Ag3	77.1(3)
O3 - C3 - Ag1	112.0(6)
Ta1 - C3 - Ag1	76.0(3)
Ag3 - C3 - Ag1	66.8(2)

C3 - Ag3 - C18	89.6(3)	C22 - Ta4 - C21	79.0(3)
C3 - Ag3 - C5	83.1(3)	C23 - Ta4 - C21	80.1(4)
C18 - Ag3 - C5	155.6(3)	C20 - Ta4 - C21	84.7(4)
C3 - Ag3 - C14	155.4(3)	C19 - Ta4 - C21	84.9(4)
C18 - Ag3 - C14	82.4(3)	C24 - Ta4 - Ag4	59.5(2)
C5 - Ag3 - C14	94.7(3)	C22 - Ta4 - Ag4	61.6(2)
C3 - Ag3 - Ag6	146.8(2)	C23 - Ta4 - Ag4	106.0(2)
C18 - Ag3 - Ag6	97.7(2)	C20 - Ta4 - Ag4	93.2(3)
C5 - Ag3 - Ag6	101.1(2)	C19 - Ta4 - Ag4	135.0(2)
C14 - Ag3 - Ag6	57.8(2)	C21 - Ta4 - Ag4	140.1(3)
C3 - Ag3 - Ag2	97.1(2)	C24 - Ta4 - Ag1	59.2(2)
C18 - Ag3 - Ag2	147.4(2)	C22 - Ta4 - Ag1	109.1(2)
C5 - Ag3 - Ag2	56.9(2)	C23 - Ta4 - Ag1	60.2(2)
C14 - Ag3 - Ag2	102.1(2)	C20 - Ta4 - Ag1	135.0(3)
Ag6 - Ag3 - Ag2	60.49(3)	C19 - Ta4 - Ag1	91.0(2)
C3 - Ag3 - Ag1	57.0(2)	C21 - Ta4 - Ag1	140.1(3)
C18 - Ag3 - Ag1	98.70(19)	Ag4 - Ta4 - Ag1	57.514(19)
C5 - Ag3 - Ag1	96.70(19)	C24 - Ta4 - Ag5	107.7(2)
C14 - Ag3 - Ag1	147.2(2)	C22 - Ta4 - Ag5	60.8(2)
Ag6 - Ag3 - Ag1	89.78(3)	C23 - Ta4 - Ag5	57.2(2)
Ag2 - Ag3 - Ag1	60.24(4)	C20 - Ta4 - Ag5	137.5(3)
C3 - Ag3 - Ag4	98.34(18)	C19 - Ta4 - Ag5	134.2(3)
C18 - Ag3 - Ag4	57.2(2)	C21 - Ta4 - Ag5	97.8(3)
C5 - Ag3 - Ag4	146.9(2)	Ag4 - Ta4 - Ag5	58.408(18)
C14 - Ag3 - Ag4	96.8(2)	Ag1 - Ta4 - Ag5	58.34(2)
Ag6 - Ag3 - Ag4	60.54(3)	C13 - Ag4 - C24	157.7(3)
Ag2 - Ag3 - Ag4	90.23(3)	C13 - Ag4 - C18	85.3(3)
Ag1 - Ag3 - Ag4	58.76(2)	C24 - Ag4 - C18	93.2(3)
C3 - Ag3 - Ta1	43.9(2)	C13 - Ag4 - C22	90.1(3)
C18 - Ag3 - Ta1	133.47(19)	C24 - Ag4 - C22	83.0(3)
C5 - Ag3 - Ta1	43.77(19)	C18 - Ag4 - C22	157.7(3)
C14 - Ag3 - Ta1	138.4(2)	C13 - Ag4 - Ag1	145.3(2)
Ag6 - Ag3 - Ta1	121.21(3)	C24 - Ag4 - Ag1	56.87(18)
Ag2 - Ag3 - Ta1	60.72(3)	C18 - Ag4 - Ag1	98.91(18)
Ag1 - Ag3 - Ta1	60.47(3)	C22 - Ag4 - Ag1	97.3(2)
Ag4 - Ag3 - Ta1	119.21(4)	C13 - Ag4 - Ag5	96.7(2)
C3 - Ag3 - Ta3	133.4(2)	C24 - Ag4 - Ag5	97.30(19)
C18 - Ag3 - Ta3	43.82(19)	C18 - Ag4 - Ag5	144.76(18)
C5 - Ag3 - Ta3	138.29(19)	C22 - Ag4 - Ag5	57.5(2)
C14 - Ag3 - Ta3	43.6(2)	Ag1 - Ag4 - Ag5	60.70(3)
Ag6 - Ag3 - Ta3	61.11(2)	C13 - Ag4 - Ag3	96.1(2)
Ag2 - Ag3 - Ta3	121.60(3)	C24 - Ag4 - Ag3	101.36(18)
Ag1 - Ag3 - Ta3	118.95(3)	C18 - Ag4 - Ag3	55.86(18)
Ag4 - Ag3 - Ta3	60.20(4)	C22 - Ag4 - Ag3	146.5(2)
Ta1 - Ag3 - Ta3	177.27(3)	Ag1 - Ag4 - Ag3	60.32(4)
C24 - Ta4 - C22	113.6(3)	Ag5 - Ag4 - Ag3	89.05(3)
C24 - Ta4 - C23	113.3(3)	C13 - Ag4 - Ag6	55.5(2)
C22 - Ta4 - C23	109.9(4)	C24 - Ag4 - Ag6	146.50(18)
C24 - Ta4 - C20	76.9(3)	C18 - Ag4 - Ag6	95.78(19)
C22 - Ta4 - C20	78.4(4)	C22 - Ag4 - Ag6	99.5(2)
C23 - Ta4 - C20	160.7(4)	Ag1 - Ag4 - Ag6	89.82(3)
C24 - Ta4 - C19	77.2(3)	Ag5 - Ag4 - Ag6	58.65(4)
C22 - Ta4 - C19	159.9(3)	Ag3 - Ag4 - Ag6	59.05(2)
C23 - Ta4 - C19	78.7(4)	C13 - Ag4 - Ta3	44.5(2)
C20 - Ta4 - C19	88.2(4)	C24 - Ag4 - Ta3	137.0(2)
C24 - Ta4 - C21	154.5(4)	C18 - Ag4 - Ta3	43.88(19)

C22 - Ag4 - Ta3	134.4(2)	C13 - Ag6 - Ag3	97.3(2)
Ag1 - Ag4 - Ta3	121.35(3)	C14 - Ag6 - Ag3	57.2(2)
Ag5 - Ag4 - Ta3	119.54(4)	Ag5 - Ag6 - Ag3	90.97(3)
Ag3 - Ag4 - Ta3	61.04(2)	C8 - Ag6 - Ag2	57.26(19)
Ag6 - Ag4 - Ta3	60.918(18)	C13 - Ag6 - Ag2	145.6(2)
C13 - Ag4 - Ta4	133.6(2)	C14 - Ag6 - Ag2	101.3(2)
C24 - Ag4 - Ta4	43.6(2)	Ag5 - Ag6 - Ag2	60.04(3)
C18 - Ag4 - Ta4	136.80(19)	Ag3 - Ag6 - Ag2	59.92(3)
C22 - Ag4 - Ta4	43.6(2)	C8 - Ag6 - Ag4	147.10(19)
Ag1 - Ag4 - Ta4	61.39(3)	C13 - Ag6 - Ag4	55.8(2)
Ag5 - Ag4 - Ta4	61.62(3)	C14 - Ag6 - Ag4	96.3(2)
Ag3 - Ag4 - Ta4	121.71(3)	Ag5 - Ag6 - Ag4	60.56(2)
Ag6 - Ag4 - Ta4	120.26(2)	Ag3 - Ag6 - Ag4	60.41(4)
Ta3 - Ag4 - Ta4	177.25(2)	Ag2 - Ag6 - Ag4	89.84(3)
O4 - C4 - Ta1	177.5(8)	C8 - Ag6 - Ta2	43.9(2)
C23 - Ag5 - C12	152.6(3)	C13 - Ag6 - Ta2	135.7(2)
C23 - Ag5 - Ag6	147.3(2)	C14 - Ag6 - Ta2	134.9(2)
C12 - Ag5 - Ag6	60.1(2)	Ag5 - Ag6 - Ta2	61.85(3)
C23 - Ag5 - Ag2	99.5(2)	Ag3 - Ag6 - Ta2	120.54(3)
C12 - Ag5 - Ag2	98.5(2)	Ag2 - Ag6 - Ta2	60.70(3)
Ag6 - Ag5 - Ag2	60.76(2)	Ag4 - Ag6 - Ta2	122.41(4)
C23 - Ag5 - Ag4	96.3(2)	C8 - Ag6 - Ta3	134.7(2)
C12 - Ag5 - Ag4	104.2(2)	C13 - Ag6 - Ta3	44.3(2)
Ag6 - Ag5 - Ag4	60.79(3)	C14 - Ag6 - Ta3	43.6(2)
Ag2 - Ag5 - Ag4	90.38(3)	Ag5 - Ag6 - Ta3	120.74(4)
C23 - Ag5 - Ag1	57.5(2)	Ag3 - Ag6 - Ta3	61.23(3)
C12 - Ag5 - Ag1	149.8(2)	Ag2 - Ag6 - Ta3	121.15(3)
Ag6 - Ag5 - Ag1	89.86(3)	Ag4 - Ag6 - Ta3	60.20(3)
Ag2 - Ag5 - Ag1	60.12(3)	Ta2 - Ag6 - Ta3	177.21(2)
Ag4 - Ag5 - Ag1	58.63(3)	O6 - C6 - Ta1	176.1(8)
C23 - Ag5 - Ta2	134.9(2)	O9 - C9 - Ta2	179.5(11)
C12 - Ag5 - Ta2	43.6(2)	O8 - C8 - Ta2	167.8(7)
Ag6 - Ag5 - Ta2	61.080(18)	O8 - C8 - Ag6	111.6(6)
Ag2 - Ag5 - Ta2	60.66(2)	Ta2 - C8 - Ag6	78.2(3)
Ag4 - Ag5 - Ta2	121.87(4)	O8 - C8 - Ag2	113.4(6)
Ag1 - Ag5 - Ta2	120.78(4)	Ta2 - C8 - Ag2	76.5(3)
C23 - Ag5 - Ta4	43.9(2)	Ag6 - C8 - Ag2	67.5(2)
C12 - Ag5 - Ta4	136.5(2)	O7 - C7 - Ta2	167.5(8)
Ag6 - Ag5 - Ta4	120.75(3)	O7 - C7 - Ag2	113.2(7)
Ag2 - Ag5 - Ta4	120.23(3)	Ta2 - C7 - Ag2	76.7(3)
Ag4 - Ag5 - Ta4	59.97(3)	O13 - C13 - Ta3	167.4(7)
Ag1 - Ag5 - Ta4	60.14(3)	O13 - C13 - Ag6	111.5(6)
Ta2 - Ag5 - Ta4	178.14(3)	Ta3 - C13 - Ag6	77.8(3)
O5 - C5 - Ta1	167.6(7)	O13 - C13 - Ag4	113.8(7)
O5 - C5 - Ag3	112.9(6)	Ta3 - C13 - Ag4	77.0(3)
Ta1 - C5 - Ag3	76.6(3)	Ag6 - C13 - Ag4	68.7(2)
O5 - C5 - Ag2	114.4(7)	O12 - C12 - Ta2	168.4(8)
Ta1 - C5 - Ag2	76.1(3)	O12 - C12 - Ag5	112.8(7)
Ag3 - C5 - Ag2	66.14(19)	Ta2 - C12 - Ag5	78.1(3)
C8 - Ag6 - C13	157.1(3)	O11 - C11 - Ta2	177.2(8)
C8 - Ag6 - C14	91.1(3)	O10 - C10 - Ta2	178.8(9)
C13 - Ag6 - C14	83.6(3)	O16 - C16 - Ta3	176.7(9)
C8 - Ag6 - Ag5	97.9(2)	O15 - C15 - Ta3	175.9(9)
C13 - Ag6 - Ag5	98.3(2)	O14 - C14 - Ta3	168.2(7)
C14 - Ag6 - Ag5	147.9(2)	O14 - C14 - Ag3	113.9(7)
C8 - Ag6 - Ag3	98.46(19)	Ta3 - C14 - Ag3	76.2(3)

O14 - C14 - Ag6	113.6(7)
Ta3 - C14 - Ag6	75.6(3)
Ag3 - C14 - Ag6	65.0(2)
O20 - C20 - Ta4	178.8(10)
O21 - C21 - Ta4	178.9(9)
O22 - C22 - Ta4	168.8(7)
O22 - C22 - Ag4	114.5(6)
Ta4 - C22 - Ag4	74.8(3)
O23 - C23 - Ta4	167.9(7)
O23 - C23 - Ag5	111.8(6)
Ta4 - C23 - Ag5	78.9(3)
O23 - C23 - Ag1	112.9(6)
Ta4 - C23 - Ag1	75.9(3)
Ag5 - C23 - Ag1	67.7(2)
O24 - C24 - Ta4	166.0(7)
O24 - C24 - Ag1	114.1(6)
Ta4 - C24 - Ag1	77.3(3)
O24 - C24 - Ag4	114.7(6)
Ta4 - C24 - Ag4	76.9(3)
Ag1 - C24 - Ag4	66.05(19)
O19 - C19 - Ta4	178.7(10)
O18 - C18 - Ta3	168.0(7)
O18 - C18 - Ag3	112.3(6)
Ta3 - C18 - Ag3	77.2(3)
O18 - C18 - Ag4	114.5(6)
Ta3 - C18 - Ag4	75.5(3)
Ag3 - C18 - Ag4	67.0(2)
O17 - C17 - Ta3	178.5(8)
F1_16 - C1_16 - C6_16	120.6(15)
F1_16 - C1_16 - C2_16	119.7(15)
C6_16 - C1_16 - C2_16	119.7(14)
F2_16 - C2_16 - C1_16	119.5(14)
F2_16 - C2_16 - C3_16	120.6(15)
C1_16 - C2_16 - C3_16	119.9(14)
F3_16 - C3_16 - C2_16	121.5(15)
F3_16 - C3_16 - C4_16	118.3(15)
C2_16 - C3_16 - C4_16	120.2(13)
F4_16 - C4_16 - C5_16	121.6(16)
F4_16 - C4_16 - C3_16	118.4(15)
C5_16 - C4_16 - C3_16	120.0(14)
C4_16 - C5_16 - C6_16	119.7(17)
C1_16 - C6_16 - C5_16	120.6(16)
F1_17 - C1_17 - C2_17	118.9(17)
F1_17 - C1_17 - C6_17	120.4(18)
C2_17 - C1_17 - C6_17	120.7(15)
F2_17 - C2_17 - C1_17	119.7(17)
F2_17 - C2_17 - C3_17	120.4(17)
C1_17 - C2_17 - C3_17	119.9(15)
F3_17 - C3_17 - C4_17	120.1(17)
F3_17 - C3_17 - C2_17	120.3(17)
C4_17 - C3_17 - C2_17	119.6(15)
F4_17 - C4_17 - C3_17	119.3(17)
F4_17 - C4_17 - C5_17	120.3(18)
C3_17 - C4_17 - C5_17	120.3(15)
C6_17 - C5_17 - C4_17	120.5(18)
C5_17 - C6_17 - C1_17	119.0(18)
C1_18 - O1_18 - Al1	144.1(11)
O1_18 - C1_18 - C3_18	111.4(12)
O1_18 - C1_18 - C4_18	110.7(11)
C3_18 - C1_18 - C4_18	109.2(11)
O1_18 - C1_18 - C2_18	107.0(11)
C3_18 - C1_18 - C2_18	108.2(11)
C4_18 - C1_18 - C2_18	110.3(11)
F2_18 - C2_18 - F1_18	108.1(16)
F2_18 - C2_18 - F3_18	108.4(16)
F1_18 - C2_18 - F3_18	106.3(18)
F2_18 - C2_18 - C1_18	114.6(13)
F1_18 - C2_18 - C1_18	110.7(13)
F3_18 - C2_18 - C1_18	108.4(13)
F4_18 - C3_18 - F6_18	110.4(18)
F4_18 - C3_18 - F5_18	103.8(17)
F6_18 - C3_18 - F5_18	108.0(17)
F4_18 - C3_18 - C1_18	112.3(14)
F6_18 - C3_18 - C1_18	109.4(14)
F5_18 - C3_18 - C1_18	112.7(15)
F9_18 - C4_18 - F8_18	105.3(15)
F9_18 - C4_18 - F7_18	111.7(17)
F8_18 - C4_18 - F7_18	106.3(15)
F9_18 - C4_18 - C1_18	109.4(13)
F8_18 - C4_18 - C1_18	115.6(13)
F7_18 - C4_18 - C1_18	108.4(13)
C1_19 - O1_19 - Al1	148.3(13)
O1_19 - C1_19 - C4_19	111.9(13)
O1_19 - C1_19 - C3_19	105.0(11)
C4_19 - C1_19 - C3_19	110.0(11)
O1_19 - C1_19 - C2_19	113.9(13)
C4_19 - C1_19 - C2_19	107.5(11)
C3_19 - C1_19 - C2_19	108.6(11)
F2_19 - C2_19 - F3_19	107.4(17)
F2_19 - C2_19 - F1_19	111.7(16)
F3_19 - C2_19 - F1_19	105.9(17)
F2_19 - C2_19 - C1_19	111.6(15)
F3_19 - C2_19 - C1_19	110.3(15)
F1_19 - C2_19 - C1_19	109.8(14)
F4_19 - C3_19 - F6_19	107.1(15)
F4_19 - C3_19 - F5_19	107.3(17)
F6_19 - C3_19 - F5_19	107.3(17)
F4_19 - C3_19 - C1_19	113.0(13)
F6_19 - C3_19 - C1_19	111.8(14)
F5_19 - C3_19 - C1_19	110.0(13)
F8_19 - C4_19 - F7_19	106.1(17)
F8_19 - C4_19 - F9_19	108.6(16)
F7_19 - C4_19 - F9_19	107.5(17)
F8_19 - C4_19 - C1_19	115.6(15)
F7_19 - C4_19 - C1_19	109.9(13)
F9_19 - C4_19 - C1_19	108.8(13)
C1_20 - O1_20 - Al2	148(2)
O1_20 - C1_20 - C4_20	111.0(15)
O1_20 - C1_20 - C2_20	109.2(16)
C4_20 - C1_20 - C2_20	109.2(12)
O1_20 - C1_20 - C3_20	109.3(16)
C4_20 - C1_20 - C3_20	108.4(12)

C2_20 - C1_20 - C3_20	109.7(12)
F3_20 - C2_20 - F2_20	108.7(15)
F3_20 - C2_20 - F1_20	105.5(16)
F2_20 - C2_20 - F1_20	108.8(16)
F3_20 - C2_20 - C1_20	109.8(13)
F2_20 - C2_20 - C1_20	112.6(14)
F1_20 - C2_20 - C1_20	111.2(13)
F6_20 - C3_20 - F5_20	107.8(17)
F6_20 - C3_20 - F4_20	108.1(17)
F5_20 - C3_20 - F4_20	105.8(16)
F6_20 - C3_20 - C1_20	112.4(14)
F5_20 - C3_20 - C1_20	110.3(15)
F4_20 - C3_20 - C1_20	112.2(14)
F9_20 - C4_20 - F7_20	106.0(18)
F9_20 - C4_20 - F8_20	107.3(18)
F7_20 - C4_20 - F8_20	107.5(15)
F9_20 - C4_20 - C1_20	112.5(16)
F7_20 - C4_20 - C1_20	110.3(15)
F8_20 - C4_20 - C1_20	112.8(15)
C1_21 - O1_21 - Al1	149.9(18)
O1_21 - C1_21 - C3_21	110.2(13)
O1_21 - C1_21 - C4_21	112.3(14)
C3_21 - C1_21 - C4_21	109.4(11)
O1_21 - C1_21 - C2_21	108.4(13)
C3_21 - C1_21 - C2_21	108.9(11)
C4_21 - C1_21 - C2_21	107.6(12)
F1_21 - C2_21 - F2_21	108.5(16)
F1_21 - C2_21 - F3_21	106.0(17)
F2_21 - C2_21 - F3_21	108.4(17)
F1_21 - C2_21 - C1_21	110.3(14)
F2_21 - C2_21 - C1_21	111.5(14)
F3_21 - C2_21 - C1_21	111.8(15)
F6_21 - C3_21 - F5_21	104.8(16)
F6_21 - C3_21 - F4_21	107.8(16)
F5_21 - C3_21 - F4_21	106.4(17)
F6_21 - C3_21 - C1_21	115.1(15)
F5_21 - C3_21 - C1_21	111.4(14)
F4_21 - C3_21 - C1_21	110.9(14)
F7_21 - C4_21 - F8_21	106.4(16)
F7_21 - C4_21 - F9_21	107.8(16)
F8_21 - C4_21 - F9_21	108.1(17)
F7_21 - C4_21 - C1_21	112.1(14)
F8_21 - C4_21 - C1_21	111.1(14)
F9_21 - C4_21 - C1_21	111.2(14)
C1_22 - O1_22 - Al1	147(3)
O1_22 - C1_22 - C4_22	110.8(19)
O1_22 - C1_22 - C3_22	109.5(19)
C4_22 - C1_22 - C3_22	110.4(16)
O1_22 - C1_22 - C2_22	108.4(19)
C4_22 - C1_22 - C2_22	108.6(15)
C3_22 - C1_22 - C2_22	109.1(15)
F2_22 - C2_22 - F3_22	107(2)
F2_22 - C2_22 - F1_22	108(2)
F3_22 - C2_22 - F1_22	108(2)
F2_22 - C2_22 - C1_22	112.2(18)
F3_22 - C2_22 - C1_22	110.5(18)
F1_22 - C2_22 - C1_22	111.0(18)
F6_22 - C3_22 - F5_22	109(2)
F6_22 - C3_22 - F4_22	107(2)
F5_22 - C3_22 - F4_22	107(2)
F6_22 - C3_22 - C1_22	112.5(19)
F5_22 - C3_22 - C1_22	110.8(19)
F4_22 - C3_22 - C1_22	110.2(19)
F7_22 - C4_22 - F9_22	107(2)
F7_22 - C4_22 - F8_22	108(2)
F9_22 - C4_22 - F8_22	107(2)
F7_22 - C4_22 - C1_22	111.6(19)
F9_22 - C4_22 - C1_22	110.1(19)
F8_22 - C4_22 - C1_22	112.6(19)

Table 3. Torsion angles for pbca_all_new_d-finalcif.cif.

Atom - Atom - Atom - Atom	Torsion Angle [°]
Al1 - O1_1 - C1_1 - C4_1	-95(2)
Al1 - O1_1 - C1_1 - C3_1	148(2)
Al1 - O1_1 - C1_1 - C2_1	28(3)
O1_1 - C1_1 - C2_1 - F3_1	40.1(11)
C4_1 - C1_1 - C2_1 - F3_1	163.7(8)
C3_1 - C1_1 - C2_1 - F3_1	-79.1(10)
O1_1 - C1_1 - C2_1 - F2_1	160.2(9)
C4_1 - C1_1 - C2_1 - F2_1	-76.2(9)
C3_1 - C1_1 - C2_1 - F2_1	40.9(10)
O1_1 - C1_1 - C2_1 - F1_1	-79.4(10)
C4_1 - C1_1 - C2_1 - F1_1	44.2(10)
C3_1 - C1_1 - C2_1 - F1_1	161.3(8)
O1_1 - C1_1 - C3_1 - F4_1	40.3(10)
C4_1 - C1_1 - C3_1 - F4_1	-79.2(9)
C2_1 - C1_1 - C3_1 - F4_1	162.8(7)
O1_1 - C1_1 - C3_1 - F6_1	161.1(8)
C4_1 - C1_1 - C3_1 - F6_1	41.6(9)
C2_1 - C1_1 - C3_1 - F6_1	-76.4(9)
O1_1 - C1_1 - C3_1 - F5_1	-78.7(10)
C4_1 - C1_1 - C3_1 - F5_1	161.8(8)
C2_1 - C1_1 - C3_1 - F5_1	43.8(10)
O1_1 - C1_1 - C4_1 - F8_1	167.4(8)
C3_1 - C1_1 - C4_1 - F8_1	-75.1(9)
C2_1 - C1_1 - C4_1 - F8_1	42.7(10)
O1_1 - C1_1 - C4_1 - F9_1	47.6(10)
C3_1 - C1_1 - C4_1 - F9_1	165.1(8)
C2_1 - C1_1 - C4_1 - F9_1	-77.1(9)
O1_1 - C1_1 - C4_1 - F7_1	-72.3(10)
C3_1 - C1_1 - C4_1 - F7_1	45.2(10)
C2_1 - C1_1 - C4_1 - F7_1	162.9(8)
C6_5 - C1_5 - C2_5 - F2_5	178.5(8)
F1_5 - C1_5 - C2_5 - F2_5	0.0(12)
C6_5 - C1_5 - C2_5 - C3_5	-1.0(14)
F1_5 - C1_5 - C2_5 - C3_5	-179.5(8)
F2_5 - C2_5 - C3_5 - F3_5	0.0(13)
C1_5 - C2_5 - C3_5 - F3_5	179.5(8)
F2_5 - C2_5 - C3_5 - C4_5	-178.8(8)
C1_5 - C2_5 - C3_5 - C4_5	0.7(14)
F3_5 - C3_5 - C4_5 - F4_5	1.4(13)

C2_5 - C3_5 - C4_5 - F4_5	-179.8(8)
F3_5 - C3_5 - C4_5 - C5_5	-178.8(8)
C2_5 - C3_5 - C4_5 - C5_5	0.0(14)
F4_5 - C4_5 - C5_5 - C6_5	179.4(9)
C3_5 - C4_5 - C5_5 - C6_5	-0.4(14)
F1_5 - C1_5 - C6_5 - C5_5	178.9(8)
C2_5 - C1_5 - C6_5 - C5_5	0.5(15)
C4_5 - C5_5 - C6_5 - C1_5	0.2(14)
Al2 - O1_15 - C1_15 - C2_15	167(3)
Al2 - O1_15 - C1_15 - C4_15	46(4)
Al2 - O1_15 - C1_15 - C3_15	-73(4)
O1_15 - C1_15 - C2_15 - F3_15	39(2)
C4_15 - C1_15 - C2_15 - F3_15	162.3(16)
C3_15 - C1_15 - C2_15 - F3_15	-78.1(18)
O1_15 - C1_15 - C2_15 - F2_15	162.3(17)
C4_15 - C1_15 - C2_15 - F2_15	-74.3(16)
C3_15 - C1_15 - C2_15 - F2_15	45.3(17)
O1_15 - C1_15 - C2_15 - F1_15	-80.8(19)
C4_15 - C1_15 - C2_15 - F1_15	42.7(18)
C3_15 - C1_15 - C2_15 - F1_15	162.2(15)
O1_15 - C1_15 - C3_15 - F6_15	169.5(16)
C2_15 - C1_15 - C3_15 - F6_15	-74.3(17)
C4_15 - C1_15 - C3_15 - F6_15	47.1(17)
O1_15 - C1_15 - C3_15 - F5_15	-68.7(18)
C2_15 - C1_15 - C3_15 - F5_15	47.5(17)
C4_15 - C1_15 - C3_15 - F5_15	168.9(14)
O1_15 - C1_15 - C3_15 - F4_15	47.2(18)
C2_15 - C1_15 - C3_15 - F4_15	163.4(14)
C4_15 - C1_15 - C3_15 - F4_15	-75.2(15)
O1_15 - C1_15 - C4_15 - F9_15	32.1(19)
C2_15 - C1_15 - C4_15 - F9_15	-86.9(15)
C3_15 - C1_15 - C4_15 - F9_15	150.6(14)
O1_15 - C1_15 - C4_15 - F8_15	158.6(18)
C2_15 - C1_15 - C4_15 - F8_15	39.6(18)
C3_15 - C1_15 - C4_15 - F8_15	-82.8(17)
O1_15 - C1_15 - C4_15 - F7_15	-79.3(18)
C2_15 - C1_15 - C4_15 - F7_15	161.7(13)
C3_15 - C1_15 - C4_15 - F7_15	39.2(15)
F1_14 - C1_14 - C2_14 - F2_14	-0.8(19)
C6_14 - C1_14 - C2_14 - F2_14	179.8(12)
F1_14 - C1_14 - C2_14 - C3_14	-179.8(12)
C6_14 - C1_14 - C2_14 - C3_14	1(2)
F2_14 - C2_14 - C3_14 - F3_14	0(2)
C1_14 - C2_14 - C3_14 - F3_14	179.2(12)
F2_14 - C2_14 - C3_14 - C4_14	-178.9(12)
C1_14 - C2_14 - C3_14 - C4_14	0(2)
F3_14 - C3_14 - C4_14 - F4_14	1(2)
C2_14 - C3_14 - C4_14 - F4_14	-179.7(12)
F3_14 - C3_14 - C4_14 - C5_14	-179.7(12)
C2_14 - C3_14 - C4_14 - C5_14	-1(2)
F4_14 - C4_14 - C5_14 - C6_14	179.3(13)
C3_14 - C4_14 - C5_14 - C6_14	0(2)
F1_14 - C1_14 - C6_14 - C5_14	179.4(12)
C2_14 - C1_14 - C6_14 - C5_14	-1(2)
C4_14 - C5_14 - C6_14 - C1_14	1(2)
F1_13 - C1_13 - C2_13 - F2_13	-2.2(17)
C6_13 - C1_13 - C2_13 - F2_13	-179.4(11)
F1_13 - C1_13 - C2_13 - C3_13	179.0(11)
C6_13 - C1_13 - C2_13 - C3_13	2(2)
F2_13 - C2_13 - C3_13 - F3_13	0.2(17)
C1_13 - C2_13 - C3_13 - F3_13	179.0(10)
F2_13 - C2_13 - C3_13 - C4_13	179.4(10)
C1_13 - C2_13 - C3_13 - C4_13	-1.8(19)
F3_13 - C3_13 - C4_13 - F4_13	0.0(18)
C2_13 - C3_13 - C4_13 - F4_13	-179.2(12)
F3_13 - C3_13 - C4_13 - C5_13	179.6(10)
C2_13 - C3_13 - C4_13 - C5_13	0.4(19)
F4_13 - C4_13 - C5_13 - C6_13	-179.4(13)
C3_13 - C4_13 - C5_13 - C6_13	1(2)
F1_13 - C1_13 - C6_13 - C5_13	-177.5(11)
C2_13 - C1_13 - C6_13 - C5_13	0(2)
C4_13 - C5_13 - C6_13 - C1_13	-1(2)
Al2 - O1_12 - C1_12 - C3_12	49(4)
Al2 - O1_12 - C1_12 - C2_12	-72(4)
Al2 - O1_12 - C1_12 - C4_12	168(3)
O1_12 - C1_12 - C2_12 - F1_12	-73.0(18)
C3_12 - C1_12 - C2_12 - F1_12	166.1(15)
C4_12 - C1_12 - C2_12 - F1_12	45.8(18)
O1_12 - C1_12 - C2_12 - F3_12	49.1(18)
C3_12 - C1_12 - C2_12 - F3_12	-71.8(17)
C4_12 - C1_12 - C2_12 - F3_12	167.9(15)
O1_12 - C1_12 - C2_12 - F2_12	164.8(16)
C3_12 - C1_12 - C2_12 - F2_12	44.0(18)
C4_12 - C1_12 - C2_12 - F2_12	-76.4(17)
O1_12 - C1_12 - C3_12 - F6_12	166.9(16)
C2_12 - C1_12 - C3_12 - F6_12	-70.5(17)
C4_12 - C1_12 - C3_12 - F6_12	49.3(17)
O1_12 - C1_12 - C3_12 - F5_12	-67.9(16)
C2_12 - C1_12 - C3_12 - F5_12	54.7(16)
C4_12 - C1_12 - C3_12 - F5_12	174.6(13)
O1_12 - C1_12 - C3_12 - F4_12	50.1(18)
C2_12 - C1_12 - C3_12 - F4_12	172.7(15)
C4_12 - C1_12 - C3_12 - F4_12	-67.5(17)
O1_12 - C1_12 - C4_12 - F7_12	-63.7(16)
C3_12 - C1_12 - C4_12 - F7_12	55.1(15)
C2_12 - C1_12 - C4_12 - F7_12	174.6(13)
O1_12 - C1_12 - C4_12 - F8_12	176.5(13)
C3_12 - C1_12 - C4_12 - F8_12	-64.8(14)
C2_12 - C1_12 - C4_12 - F8_12	54.7(14)
O1_12 - C1_12 - C4_12 - F9_12	56.8(16)
C3_12 - C1_12 - C4_12 - F9_12	175.5(13)
C2_12 - C1_12 - C4_12 - F9_12	-65.0(15)
Al2 - O1_11 - C1_11 - C4_11	-1(3)
Al2 - O1_11 - C1_11 - C3_11	-120(3)
Al2 - O1_11 - C1_11 - C2_11	119(2)
O1_11 - C1_11 - C2_11 - F2_11	162.2(14)
C4_11 - C1_11 - C2_11 - F2_11	-73.6(15)
C3_11 - C1_11 - C2_11 - F2_11	46.0(17)
O1_11 - C1_11 - C2_11 - F3_11	48.4(19)
C4_11 - C1_11 - C2_11 - F3_11	172.5(16)
C3_11 - C1_11 - C2_11 - F3_11	-67.8(19)
O1_11 - C1_11 - C2_11 - F1_11	-85.2(17)

C4_11 - C1_11 - C2_11 - F1_11	39.0(17)
C3_11 - C1_11 - C2_11 - F1_11	158.6(15)
O1_11 - C1_11 - C3_11 - F6_11	166.4(16)
C4_11 - C1_11 - C3_11 - F6_11	43.8(18)
C2_11 - C1_11 - C3_11 - F6_11	-74.6(18)
O1_11 - C1_11 - C3_11 - F5_11	-70.9(15)
C4_11 - C1_11 - C3_11 - F5_11	166.5(14)
C2_11 - C1_11 - C3_11 - F5_11	48.1(17)
O1_11 - C1_11 - C3_11 - F4_11	47.2(16)
C4_11 - C1_11 - C3_11 - F4_11	-75.4(16)
C2_11 - C1_11 - C3_11 - F4_11	166.2(15)
O1_11 - C1_11 - C4_11 - F7_11	-62.8(16)
C3_11 - C1_11 - C4_11 - F7_11	53.9(15)
C2_11 - C1_11 - C4_11 - F7_11	176.0(13)
O1_11 - C1_11 - C4_11 - F9_11	55.9(17)
C3_11 - C1_11 - C4_11 - F9_11	172.6(14)
C2_11 - C1_11 - C4_11 - F9_11	-65.3(15)
O1_11 - C1_11 - C4_11 - F8_11	178.1(14)
C3_11 - C1_11 - C4_11 - F8_11	-65.2(15)
C2_11 - C1_11 - C4_11 - F8_11	56.9(15)
Al2 - O1_10 - C1_10 - C3_10	-160(2)
Al2 - O1_10 - C1_10 - C2_10	80(3)
Al2 - O1_10 - C1_10 - C4_10	-38(3)
O1_10 - C1_10 - C2_10 - F2_10	-160.5(14)
C3_10 - C1_10 - C2_10 - F2_10	77.1(15)
C4_10 - C1_10 - C2_10 - F2_10	-41.7(16)
O1_10 - C1_10 - C2_10 - F3_10	74.7(15)
C3_10 - C1_10 - C2_10 - F3_10	-47.7(16)
C4_10 - C1_10 - C2_10 - F3_10	-166.4(13)
O1_10 - C1_10 - C2_10 - F1_10	-43.4(16)
C3_10 - C1_10 - C2_10 - F1_10	-165.7(13)
C4_10 - C1_10 - C2_10 - F1_10	75.5(14)
O1_10 - C1_10 - C3_10 - F4_10	69.0(16)
C2_10 - C1_10 - C3_10 - F4_10	-170.7(13)
C4_10 - C1_10 - C3_10 - F4_10	-53.3(15)
O1_10 - C1_10 - C3_10 - F5_10	-50.2(16)
C2_10 - C1_10 - C3_10 - F5_10	70.1(15)
C4_10 - C1_10 - C3_10 - F5_10	-172.5(13)
O1_10 - C1_10 - C3_10 - F6_10	-168.8(14)
C2_10 - C1_10 - C3_10 - F6_10	-48.5(16)
C4_10 - C1_10 - C3_10 - F6_10	68.9(16)
O1_10 - C1_10 - C4_10 - F8_10	-172.2(13)
C3_10 - C1_10 - C4_10 - F8_10	-48.3(15)
C2_10 - C1_10 - C4_10 - F8_10	69.4(14)
O1_10 - C1_10 - C4_10 - F9_10	66.4(13)
C3_10 - C1_10 - C4_10 - F9_10	-169.7(11)
C2_10 - C1_10 - C4_10 - F9_10	-52.0(13)
O1_10 - C1_10 - C4_10 - F7_10	-49.9(15)
C3_10 - C1_10 - C4_10 - F7_10	74.0(14)
C2_10 - C1_10 - C4_10 - F7_10	-168.3(12)
Al1 - O1_9 - C1_9 - C3_9	177(3)
Al1 - O1_9 - C1_9 - C2_9	59(3)
Al1 - O1_9 - C1_9 - C4_9	-61(3)
O1_9 - C1_9 - C2_9 - F3_9	69.4(16)
C3_9 - C1_9 - C2_9 - F3_9	-51.8(15)
C4_9 - C1_9 - C2_9 - F3_9	-168.8(13)
O1_9 - C1_9 - C2_9 - F2_9	-165.8(16)
C3_9 - C1_9 - C2_9 - F2_9	73.0(17)
C4_9 - C1_9 - C2_9 - F2_9	-43.9(17)
O1_9 - C1_9 - C2_9 - F1_9	-50.5(17)
C3_9 - C1_9 - C2_9 - F1_9	-171.7(14)
C4_9 - C1_9 - C2_9 - F1_9	71.3(15)
O1_9 - C1_9 - C3_9 - F4_9	72.1(18)
C2_9 - C1_9 - C3_9 - F4_9	-167.0(15)
C4_9 - C1_9 - C3_9 - F4_9	-51.3(18)
O1_9 - C1_9 - C3_9 - F5_9	-43.2(18)
C2_9 - C1_9 - C3_9 - F5_9	77.7(16)
C4_9 - C1_9 - C3_9 - F5_9	-166.6(14)
O1_9 - C1_9 - C3_9 - F6_9	-164.5(16)
C2_9 - C1_9 - C3_9 - F6_9	-43.6(17)
C4_9 - C1_9 - C3_9 - F6_9	72.1(17)
O1_9 - C1_9 - C4_9 - F8_9	-161.9(16)
C3_9 - C1_9 - C4_9 - F8_9	-38.8(18)
C2_9 - C1_9 - C4_9 - F8_9	76.9(16)
O1_9 - C1_9 - C4_9 - F7_9	-41.6(18)
C3_9 - C1_9 - C4_9 - F7_9	81.6(17)
C2_9 - C1_9 - C4_9 - F7_9	-162.8(15)
O1_9 - C1_9 - C4_9 - F9_9	79.6(17)
C3_9 - C1_9 - C4_9 - F9_9	-157.2(15)
C2_9 - C1_9 - C4_9 - F9_9	-41.6(17)
Al1 - O1_8 - C1_8 - C2_8	-153(4)
Al1 - O1_8 - C1_8 - C4_8	88(4)
Al1 - O1_8 - C1_8 - C3_8	-33(4)
O1_8 - C1_8 - C2_8 - F1_8	-43.2(17)
C4_8 - C1_8 - C2_8 - F1_8	76.3(16)
C3_8 - C1_8 - C2_8 - F1_8	-163.6(13)
O1_8 - C1_8 - C2_8 - F3_8	77.8(17)
C4_8 - C1_8 - C2_8 - F3_8	-162.7(14)
C3_8 - C1_8 - C2_8 - F3_8	-42.6(17)
O1_8 - C1_8 - C2_8 - F2_8	-162.6(15)
C4_8 - C1_8 - C2_8 - F2_8	-43.1(17)
C3_8 - C1_8 - C2_8 - F2_8	77.0(16)
O1_8 - C1_8 - C3_8 - F4_8	79.2(15)
C2_8 - C1_8 - C3_8 - F4_8	-162.4(13)
C4_8 - C1_8 - C3_8 - F4_8	-42.3(15)
O1_8 - C1_8 - C3_8 - F6_8	-158.4(14)
C2_8 - C1_8 - C3_8 - F6_8	-39.9(16)
C4_8 - C1_8 - C3_8 - F6_8	80.2(15)
O1_8 - C1_8 - C3_8 - F5_8	-40.2(18)
C2_8 - C1_8 - C3_8 - F5_8	78.3(16)
C4_8 - C1_8 - C3_8 - F5_8	-161.6(15)
O1_8 - C1_8 - C4_8 - F7_8	-42.7(16)
C2_8 - C1_8 - C4_8 - F7_8	-160.5(13)
C3_8 - C1_8 - C4_8 - F7_8	79.0(14)
O1_8 - C1_8 - C4_8 - F8_8	-164.5(15)
C2_8 - C1_8 - C4_8 - F8_8	77.6(16)
C3_8 - C1_8 - C4_8 - F8_8	-42.8(16)
O1_8 - C1_8 - C4_8 - F9_8	74.5(17)
C2_8 - C1_8 - C4_8 - F9_8	-43.4(17)
C3_8 - C1_8 - C4_8 - F9_8	-163.9(14)
Al1 - O1_7 - C1_7 - C3_7	-58(4)
Al1 - O1_7 - C1_7 - C2_7	-177(4)

Al1 - O1_7 - C1_7 - C4_7	64(4)
O1_7 - C1_7 - C2_7 - F3_7	45(2)
C3_7 - C1_7 - C2_7 - F3_7	-75.7(18)
C4_7 - C1_7 - C2_7 - F3_7	163.4(16)
O1_7 - C1_7 - C2_7 - F2_7	167.4(18)
C3_7 - C1_7 - C2_7 - F2_7	46.4(17)
C4_7 - C1_7 - C2_7 - F2_7	-74.4(17)
O1_7 - C1_7 - C2_7 - F1_7	-72(2)
C3_7 - C1_7 - C2_7 - F1_7	166.7(16)
C4_7 - C1_7 - C2_7 - F1_7	45.9(19)
O1_7 - C1_7 - C3_7 - F4_7	43(2)
C2_7 - C1_7 - C3_7 - F4_7	159.5(17)
C4_7 - C1_7 - C3_7 - F4_7	-79.0(18)
O1_7 - C1_7 - C3_7 - F6_7	165(2)
C2_7 - C1_7 - C3_7 - F6_7	-78(2)
C4_7 - C1_7 - C3_7 - F6_7	43(2)
O1_7 - C1_7 - C3_7 - F5_7	-77(2)
C2_7 - C1_7 - C3_7 - F5_7	39.8(19)
C4_7 - C1_7 - C3_7 - F5_7	161.3(16)
O1_7 - C1_7 - C4_7 - F8_7	160.6(18)
C3_7 - C1_7 - C4_7 - F8_7	-75.3(18)
C2_7 - C1_7 - C4_7 - F8_7	44.8(18)
O1_7 - C1_7 - C4_7 - F9_7	39(2)
C3_7 - C1_7 - C4_7 - F9_7	162.7(17)
C2_7 - C1_7 - C4_7 - F9_7	-77.2(18)
O1_7 - C1_7 - C4_7 - F7_7	-80.5(19)
C3_7 - C1_7 - C4_7 - F7_7	43.6(17)
C2_7 - C1_7 - C4_7 - F7_7	163.7(15)
F1_6 - C1_6 - C2_6 - F2_6	0.2(17)
C6_6 - C1_6 - C2_6 - F2_6	179.2(11)
F1_6 - C1_6 - C2_6 - C3_6	-179.2(10)
C6_6 - C1_6 - C2_6 - C3_6	-0.2(19)
F2_6 - C2_6 - C3_6 - F3_6	0.9(17)
C1_6 - C2_6 - C3_6 - F3_6	-179.6(10)
F2_6 - C2_6 - C3_6 - C4_6	179.9(10)
C1_6 - C2_6 - C3_6 - C4_6	-0.6(19)
F3_6 - C3_6 - C4_6 - F4_6	-0.2(17)
C2_6 - C3_6 - C4_6 - F4_6	-179.2(11)
F3_6 - C3_6 - C4_6 - C5_6	179.9(10)
C2_6 - C3_6 - C4_6 - C5_6	0.9(18)
F4_6 - C4_6 - C5_6 - C6_6	179.9(11)
C3_6 - C4_6 - C5_6 - C6_6	-0.3(18)
C4_6 - C5_6 - C6_6 - C1_6	-1(2)
F1_6 - C1_6 - C6_6 - C5_6	179.8(11)
C2_6 - C1_6 - C6_6 - C5_6	1(2)
Al2 - O1_4 - C1_4 - C4_4	-26(4)
Al2 - O1_4 - C1_4 - C3_4	-148(3)
Al2 - O1_4 - C1_4 - C2_4	94(4)
O1_4 - C1_4 - C2_4 - F3_4	54(2)
C4_4 - C1_4 - C2_4 - F3_4	175.1(17)
C3_4 - C1_4 - C2_4 - F3_4	-65.7(18)
O1_4 - C1_4 - C2_4 - F1_4	-77.1(19)
C4_4 - C1_4 - C2_4 - F1_4	44.5(19)
C3_4 - C1_4 - C2_4 - F1_4	163.7(16)
O1_4 - C1_4 - C2_4 - F2_4	171.4(17)
C4_4 - C1_4 - C2_4 - F2_4	-67.0(18)
C3_4 - C1_4 - C2_4 - F2_4	52.2(18)
O1_4 - C1_4 - C3_4 - F4_4	42(2)
C4_4 - C1_4 - C3_4 - F4_4	-80(2)
C2_4 - C1_4 - C3_4 - F4_4	163.5(18)
O1_4 - C1_4 - C3_4 - F6_4	162.3(19)
C4_4 - C1_4 - C3_4 - F6_4	41(2)
C2_4 - C1_4 - C3_4 - F6_4	-75.7(19)
O1_4 - C1_4 - C3_4 - F5_4	-79.6(19)
C4_4 - C1_4 - C3_4 - F5_4	159.3(17)
C2_4 - C1_4 - C3_4 - F5_4	42.4(19)
O1_4 - C1_4 - C4_4 - F8_4	169(2)
C3_4 - C1_4 - C4_4 - F8_4	-70(2)
C2_4 - C1_4 - C4_4 - F8_4	46(2)
O1_4 - C1_4 - C4_4 - F7_4	-57(2)
C3_4 - C1_4 - C4_4 - F7_4	63.4(19)
C2_4 - C1_4 - C4_4 - F7_4	179.0(16)
O1_4 - C1_4 - C4_4 - F9_4	58(2)
C3_4 - C1_4 - C4_4 - F9_4	178.6(18)
C2_4 - C1_4 - C4_4 - F9_4	-65.7(19)
Al2 - O1_3 - C1_3 - C4_3	-79(4)
Al2 - O1_3 - C1_3 - C3_3	163(4)
Al2 - O1_3 - C1_3 - C2_3	43(4)
O1_3 - C1_3 - C2_3 - F3_3	72.5(17)
C4_3 - C1_3 - C2_3 - F3_3	-166.2(13)
C3_3 - C1_3 - C2_3 - F3_3	-47.9(15)
O1_3 - C1_3 - C2_3 - F2_3	-167.8(16)
C4_3 - C1_3 - C2_3 - F2_3	-46.5(16)
C3_3 - C1_3 - C2_3 - F2_3	71.7(16)
O1_3 - C1_3 - C2_3 - F1_3	-48.0(17)
C4_3 - C1_3 - C2_3 - F1_3	73.3(15)
C3_3 - C1_3 - C2_3 - F1_3	-168.4(13)
O1_3 - C1_3 - C3_3 - F5_3	-48.5(17)
C4_3 - C1_3 - C3_3 - F5_3	-167.7(14)
C2_3 - C1_3 - C3_3 - F5_3	72.5(15)
O1_3 - C1_3 - C3_3 - F4_3	67.2(18)
C4_3 - C1_3 - C3_3 - F4_3	-52.0(17)
C2_3 - C1_3 - C3_3 - F4_3	-171.8(14)
O1_3 - C1_3 - C3_3 - F6_3	-169.8(15)
C4_3 - C1_3 - C3_3 - F6_3	71.0(15)
C2_3 - C1_3 - C3_3 - F6_3	-48.7(15)
O1_3 - C1_3 - C4_3 - F8_3	-166.8(16)
C3_3 - C1_3 - C4_3 - F8_3	-47.8(17)
C2_3 - C1_3 - C4_3 - F8_3	71.5(16)
O1_3 - C1_3 - C4_3 - F7_3	-45.7(18)
C3_3 - C1_3 - C4_3 - F7_3	73.3(16)
C2_3 - C1_3 - C4_3 - F7_3	-167.5(14)
O1_3 - C1_3 - C4_3 - F9_3	78.3(18)
C3_3 - C1_3 - C4_3 - F9_3	-162.7(15)
C2_3 - C1_3 - C4_3 - F9_3	-43.5(17)
Al2 - O1_2 - C1_2 - C4_2	-5(5)
Al2 - O1_2 - C1_2 - C2_2	116(4)
Al2 - O1_2 - C1_2 - C3_2	-124(4)
O1_2 - C1_2 - C2_2 - F3_2	74.5(16)
C4_2 - C1_2 - C2_2 - F3_2	-163.1(13)
C3_2 - C1_2 - C2_2 - F3_2	-44.2(16)
O1_2 - C1_2 - C2_2 - F2_2	-166.3(14)

C4_2 - C1_2 - C2_2 - F2_2	-43.9(15)
C3_2 - C1_2 - C2_2 - F2_2	75.0(14)
O1_2 - C1_2 - C2_2 - F1_2	-45.1(17)
C4_2 - C1_2 - C2_2 - F1_2	77.3(15)
C3_2 - C1_2 - C2_2 - F1_2	-163.7(13)
O1_2 - C1_2 - C3_2 - F5_2	-42.4(15)
C4_2 - C1_2 - C3_2 - F5_2	-163.2(11)
C2_2 - C1_2 - C3_2 - F5_2	77.9(13)
O1_2 - C1_2 - C3_2 - F4_2	77.1(14)
C4_2 - C1_2 - C3_2 - F4_2	-43.8(14)
C2_2 - C1_2 - C3_2 - F4_2	-162.7(12)
O1_2 - C1_2 - C3_2 - F6_2	-162.4(13)
C4_2 - C1_2 - C3_2 - F6_2	76.8(13)
C2_2 - C1_2 - C3_2 - F6_2	-42.1(14)
O1_2 - C1_2 - C4_2 - F8_2	-158.8(13)
C2_2 - C1_2 - C4_2 - F8_2	79.4(14)
C3_2 - C1_2 - C4_2 - F8_2	-40.3(14)
O1_2 - C1_2 - C4_2 - F9_2	79.4(15)
C2_2 - C1_2 - C4_2 - F9_2	-42.4(14)
C3_2 - C1_2 - C4_2 - F9_2	-162.1(12)
O1_2 - C1_2 - C4_2 - F7_2	-39.4(17)
C2_2 - C1_2 - C4_2 - F7_2	-161.2(13)
C3_2 - C1_2 - C4_2 - F7_2	79.1(14)
C1_7 - O1_7 - Al1 - O1_8	-135(4)
C1_7 - O1_7 - Al1 - O1_1	112(4)
C1_7 - O1_7 - Al1 - O1_9	-22(4)
C1_8 - O1_8 - Al1 - O1_7	8(4)
C1_8 - O1_8 - Al1 - O1_1	134(4)
C1_8 - O1_8 - Al1 - O1_9	-109(4)
C1_1 - O1_1 - Al1 - O1_7	-8(3)
C1_1 - O1_1 - Al1 - O1_8	-128(2)
C1_1 - O1_1 - Al1 - O1_18	104(2)
C1_1 - O1_1 - Al1 - O1_19	-129(2)
C1_1 - O1_1 - Al1 - O1_21	-7(3)
C1_1 - O1_1 - Al1 - O1_9	125(2)
C1_1 - O1_1 - Al1 - O1_22	-3(3)
C1_9 - O1_9 - Al1 - O1_7	158(3)
C1_9 - O1_9 - Al1 - O1_8	-83(3)
C1_9 - O1_9 - Al1 - O1_1	22(3)
C1_12 - O1_12 - Al2 - O1_2	25(4)
C1_12 - O1_12 - Al2 - O1_3	-95(3)
C1_12 - O1_12 - Al2 - O1_4	153(3)
C1_2 - O1_2 - Al2 - O1_12	-160(4)
C1_2 - O1_2 - Al2 - O1_3	-37(5)
C1_2 - O1_2 - Al2 - O1_4	75(5)
C1_11 - O1_11 - Al2 - O1_15	33(3)
C1_11 - O1_11 - Al2 - O1_20	-83(3)
C1_11 - O1_11 - Al2 - O1_10	162(2)
C1_15 - O1_15 - Al2 - O1_11	120(3)
C1_15 - O1_15 - Al2 - O1_20	-129(3)
C1_15 - O1_15 - Al2 - O1_10	-6(4)
C1_3 - O1_3 - Al2 - O1_12	-72(4)
C1_3 - O1_3 - Al2 - O1_2	162(4)
C1_3 - O1_3 - Al2 - O1_4	43(4)
C1_4 - O1_4 - Al2 - O1_12	-48(4)
C1_4 - O1_4 - Al2 - O1_2	81(4)
C1_4 - O1_4 - Al2 - O1_3	-166(3)
C1_10 - O1_10 - Al2 - O1_11	22(3)
C1_10 - O1_10 - Al2 - O1_15	150(3)
C1_10 - O1_10 - Al2 - O1_20	-87(3)
F1_16 - C1_16 - C2_16 - F2_16	0(2)
C6_16 - C1_16 - C2_16 - F2_16	-179.1(13)
F1_16 - C1_16 - C2_16 - C3_16	179.4(13)
C6_16 - C1_16 - C2_16 - C3_16	0(2)
F2_16 - C2_16 - C3_16 - F3_16	-1(2)
C1_16 - C2_16 - C3_16 - F3_16	179.9(13)
F2_16 - C2_16 - C3_16 - C4_16	179.9(13)
C1_16 - C2_16 - C3_16 - C4_16	1(2)
F3_16 - C3_16 - C4_16 - F4_16	0(2)
C2_16 - C3_16 - C4_16 - F4_16	179.2(15)
F3_16 - C3_16 - C4_16 - C5_16	179.9(13)
C2_16 - C3_16 - C4_16 - C5_16	-1(2)
F4_16 - C4_16 - C5_16 - C6_16	-179.8(15)
C3_16 - C4_16 - C5_16 - C6_16	0(2)
F1_16 - C1_16 - C6_16 - C5_16	-179.9(14)
C2_16 - C1_16 - C6_16 - C5_16	-1(2)
C4_16 - C5_16 - C6_16 - C1_16	0(2)
F1_17 - C1_17 - C2_17 - F2_17	0(2)
C6_17 - C1_17 - C2_17 - F2_17	179.9(14)
F1_17 - C1_17 - C2_17 - C3_17	-179.8(14)
C6_17 - C1_17 - C2_17 - C3_17	0(3)
F2_17 - C2_17 - C3_17 - F3_17	0(2)
C1_17 - C2_17 - C3_17 - F3_17	179.9(14)
F2_17 - C2_17 - C3_17 - C4_17	-179.7(14)
C1_17 - C2_17 - C3_17 - C4_17	0(3)
F3_17 - C3_17 - C4_17 - F4_17	0(2)
C2_17 - C3_17 - C4_17 - F4_17	-179.8(16)
F3_17 - C3_17 - C4_17 - C5_17	-180.0(14)
C2_17 - C3_17 - C4_17 - C5_17	0(3)
F4_17 - C4_17 - C5_17 - C6_17	179.7(16)
C3_17 - C4_17 - C5_17 - C6_17	0(3)
C4_17 - C5_17 - C6_17 - C1_17	0(3)
F1_17 - C1_17 - C6_17 - C5_17	179.7(14)
C2_17 - C1_17 - C6_17 - C5_17	0(3)
O1_1 - Al1 - O1_18 - C1_18	96(2)
O1_19 - Al1 - O1_18 - C1_18	-34(3)
O1_21 - Al1 - O1_18 - C1_18	-156(2)
Al1 - O1_18 - C1_18 - C3_18	-47(3)
Al1 - O1_18 - C1_18 - C4_18	75(3)
Al1 - O1_18 - C1_18 - C2_18	-165(2)
O1_18 - C1_18 - C2_18 - F2_18	178.1(16)
C3_18 - C1_18 - C2_18 - F2_18	58.0(18)
C4_18 - C1_18 - C2_18 - F2_18	-61.4(18)
O1_18 - C1_18 - C2_18 - F1_18	-59.3(19)
C3_18 - C1_18 - C2_18 - F1_18	-179.4(17)
C4_18 - C1_18 - C2_18 - F1_18	61.2(19)
O1_18 - C1_18 - C2_18 - F3_18	56.9(19)
C3_18 - C1_18 - C2_18 - F3_18	-63.2(19)
C4_18 - C1_18 - C2_18 - F3_18	177.4(17)
O1_18 - C1_18 - C3_18 - F4_18	47(2)
C4_18 - C1_18 - C3_18 - F4_18	-75.5(19)
C2_18 - C1_18 - C3_18 - F4_18	164.5(18)

O1_18 - C1_18 - C3_18 - F6_18	170.1(17)
C4_18 - C1_18 - C3_18 - F6_18	47.5(19)
C2_18 - C1_18 - C3_18 - F6_18	-72.5(19)
O1_18 - C1_18 - C3_18 - F5_18	-70(2)
C4_18 - C1_18 - C3_18 - F5_18	167.7(18)
C2_18 - C1_18 - C3_18 - F5_18	48(2)
O1_18 - C1_18 - C4_18 - F9_18	43.8(19)
C3_18 - C1_18 - C4_18 - F9_18	166.8(17)
C2_18 - C1_18 - C4_18 - F9_18	-74.5(19)
O1_18 - C1_18 - C4_18 - F8_18	162.5(17)
C3_18 - C1_18 - C4_18 - F8_18	-74.5(19)
C2_18 - C1_18 - C4_18 - F8_18	44(2)
O1_18 - C1_18 - C4_18 - F7_18	-78.3(17)
C3_18 - C1_18 - C4_18 - F7_18	44.7(17)
C2_18 - C1_18 - C4_18 - F7_18	163.5(15)
O1_18 - Al1 - O1_19 - C1_19	150(3)
O1_1 - Al1 - O1_19 - C1_19	29(3)
O1_21 - Al1 - O1_19 - C1_19	-89(3)
Al1 - O1_19 - C1_19 - C4_19	-93(3)
Al1 - O1_19 - C1_19 - C3_19	148(3)
Al1 - O1_19 - C1_19 - C2_19	30(3)
O1_19 - C1_19 - C2_19 - F2_19	155.2(17)
C4_19 - C1_19 - C2_19 - F2_19	-80.3(18)
C3_19 - C1_19 - C2_19 - F2_19	38.6(19)
O1_19 - C1_19 - C2_19 - F3_19	36(2)
C4_19 - C1_19 - C2_19 - F3_19	160.5(18)
C3_19 - C1_19 - C2_19 - F3_19	-80.6(19)
O1_19 - C1_19 - C2_19 - F1_19	-80.4(18)
C4_19 - C1_19 - C2_19 - F1_19	44.1(18)
C3_19 - C1_19 - C2_19 - F1_19	163.1(15)
O1_19 - C1_19 - C3_19 - F4_19	43.7(19)
C4_19 - C1_19 - C3_19 - F4_19	-76.8(17)
C2_19 - C1_19 - C3_19 - F4_19	165.9(15)
O1_19 - C1_19 - C3_19 - F6_19	164.7(18)
C4_19 - C1_19 - C3_19 - F6_19	44.1(19)
C2_19 - C1_19 - C3_19 - F6_19	-73.2(18)
O1_19 - C1_19 - C3_19 - F5_19	-76.2(19)
C4_19 - C1_19 - C3_19 - F5_19	163.3(17)
C2_19 - C1_19 - C3_19 - F5_19	46.0(19)
O1_19 - C1_19 - C4_19 - F8_19	166.3(18)
C3_19 - C1_19 - C4_19 - F8_19	-77.4(19)
C2_19 - C1_19 - C4_19 - F8_19	41(2)
O1_19 - C1_19 - C4_19 - F7_19	-73.7(18)
C3_19 - C1_19 - C4_19 - F7_19	42.6(18)
C2_19 - C1_19 - C4_19 - F7_19	160.6(16)
O1_19 - C1_19 - C4_19 - F9_19	43.8(18)
C3_19 - C1_19 - C4_19 - F9_19	160.1(15)
C2_19 - C1_19 - C4_19 - F9_19	-81.9(16)
O1_11 - Al2 - O1_20 - C1_20	161(4)
O1_15 - Al2 - O1_20 - C1_20	42(5)
O1_10 - Al2 - O1_20 - C1_20	-84(4)
Al2 - O1_20 - C1_20 - C4_20	61(5)
Al2 - O1_20 - C1_20 - C2_20	-179(4)
Al2 - O1_20 - C1_20 - C3_20	-59(5)
O1_20 - C1_20 - C2_20 - F3_20	71(2)
C4_20 - C1_20 - C2_20 - F3_20	-167.6(16)
C3_20 - C1_20 - C2_20 - F3_20	-49.0(19)
O1_20 - C1_20 - C2_20 - F2_20	-167.9(19)
C4_20 - C1_20 - C2_20 - F2_20	-46.4(18)
C3_20 - C1_20 - C2_20 - F2_20	72.3(18)
O1_20 - C1_20 - C2_20 - F1_20	-45(2)
C4_20 - C1_20 - C2_20 - F1_20	76.0(17)
C3_20 - C1_20 - C2_20 - F1_20	-165.3(15)
O1_20 - C1_20 - C3_20 - F6_20	-158(2)
C4_20 - C1_20 - C3_20 - F6_20	81.4(19)
C2_20 - C1_20 - C3_20 - F6_20	-38(2)
O1_20 - C1_20 - C3_20 - F5_20	-37(2)
C4_20 - C1_20 - C3_20 - F5_20	-158.3(18)
C2_20 - C1_20 - C3_20 - F5_20	82.6(19)
O1_20 - C1_20 - C3_20 - F4_20	80(2)
C4_20 - C1_20 - C3_20 - F4_20	-40.6(18)
C2_20 - C1_20 - C3_20 - F4_20	-159.8(16)
O1_20 - C1_20 - C4_20 - F9_20	75(3)
C2_20 - C1_20 - C4_20 - F9_20	-46(2)
C3_20 - C1_20 - C4_20 - F9_20	-165(2)
O1_20 - C1_20 - C4_20 - F7_20	-43(2)
C2_20 - C1_20 - C4_20 - F7_20	-163.8(18)
C3_20 - C1_20 - C4_20 - F7_20	76.8(19)
O1_20 - C1_20 - C4_20 - F8_20	-164(2)
C2_20 - C1_20 - C4_20 - F8_20	76(2)
C3_20 - C1_20 - C4_20 - F8_20	-44(2)
O1_18 - Al1 - O1_21 - C1_21	63(4)
O1_1 - Al1 - O1_21 - C1_21	171(4)
O1_19 - Al1 - O1_21 - C1_21	-62(4)
Al1 - O1_21 - C1_21 - C3_21	-13(5)
Al1 - O1_21 - C1_21 - C4_21	109(4)
Al1 - O1_21 - C1_21 - C2_21	-132(4)
O1_21 - C1_21 - C2_21 - F1_21	-78(2)
C3_21 - C1_21 - C2_21 - F1_21	162.2(16)
C4_21 - C1_21 - C2_21 - F1_21	43.7(19)
O1_21 - C1_21 - C2_21 - F2_21	161(2)
C3_21 - C1_21 - C2_21 - F2_21	42(2)
C4_21 - C1_21 - C2_21 - F2_21	-76.9(19)
O1_21 - C1_21 - C2_21 - F3_21	40(2)
C3_21 - C1_21 - C2_21 - F3_21	-80.1(18)
C4_21 - C1_21 - C2_21 - F3_21	161.5(16)
O1_21 - C1_21 - C3_21 - F6_21	163.2(19)
C4_21 - C1_21 - C3_21 - F6_21	39.3(19)
C2_21 - C1_21 - C3_21 - F6_21	-78.0(19)
O1_21 - C1_21 - C3_21 - F5_21	-78(2)
C4_21 - C1_21 - C3_21 - F5_21	158.3(16)
C2_21 - C1_21 - C3_21 - F5_21	41.0(19)
O1_21 - C1_21 - C3_21 - F4_21	40(2)
C4_21 - C1_21 - C3_21 - F4_21	-83.5(19)
C2_21 - C1_21 - C3_21 - F4_21	159.2(18)
O1_21 - C1_21 - C4_21 - F7_21	41(2)
C3_21 - C1_21 - C4_21 - F7_21	164.1(16)
C2_21 - C1_21 - C4_21 - F7_21	-77.8(18)
O1_21 - C1_21 - C4_21 - F8_21	-77.5(19)
C3_21 - C1_21 - C4_21 - F8_21	45.2(18)
C2_21 - C1_21 - C4_21 - F8_21	163.3(16)
O1_21 - C1_21 - C4_21 - F9_21	162.0(19)

C3_21 - C1_21 - C4_21 - F9_21	-75.2(19)
C2_21 - C1_21 - C4_21 - F9_21	42.9(19)
O1_1 - Al1 - O1_22 - C1_22	157(6)
Al1 - O1_22 - C1_22 - C4_22	61(7)
Al1 - O1_22 - C1_22 - C3_22	-61(6)
Al1 - O1_22 - C1_22 - C2_22	180(6)
O1_22 - C1_22 - C2_22 - F2_22	-161(3)
C4_22 - C1_22 - C2_22 - F2_22	-40(3)
C3_22 - C1_22 - C2_22 - F2_22	80(3)
O1_22 - C1_22 - C2_22 - F3_22	80(3)
C4_22 - C1_22 - C2_22 - F3_22	-160(3)
C3_22 - C1_22 - C2_22 - F3_22	-39(3)
O1_22 - C1_22 - C2_22 - F1_22	-40(3)
C4_22 - C1_22 - C2_22 - F1_22	80(3)
C3_22 - C1_22 - C2_22 - F1_22	-159(3)
O1_22 - C1_22 - C3_22 - F6_22	73(3)
C4_22 - C1_22 - C3_22 - F6_22	-49(3)
C2_22 - C1_22 - C3_22 - F6_22	-168(3)
O1_22 - C1_22 - C3_22 - F5_22	-164(3)
C4_22 - C1_22 - C3_22 - F5_22	74(3)
C2_22 - C1_22 - C3_22 - F5_22	-46(3)
O1_22 - C1_22 - C3_22 - F4_22	-46(3)
C4_22 - C1_22 - C3_22 - F4_22	-168(3)
C2_22 - C1_22 - C3_22 - F4_22	72(3)
O1_22 - C1_22 - C4_22 - F7_22	-44(3)
C3_22 - C1_22 - C4_22 - F7_22	78(3)
C2_22 - C1_22 - C4_22 - F7_22	-163(3)
O1_22 - C1_22 - C4_22 - F9_22	75(3)
C3_22 - C1_22 - C4_22 - F9_22	-164(3)
C2_22 - C1_22 - C4_22 - F9_22	-44(3)
O1_22 - C1_22 - C4_22 - F8_22	-166(3)
C3_22 - C1_22 - C4_22 - F8_22	-44(3)
C2_22 - C1_22 - C4_22 - F8_22	75(3)

References

[1] a) S. C. Meier, A. Holz, A. Schmidt, D. Kratzert, D. Himmel, I. Krossing, *Chem. Eur. J.* **2017**, *23*, 14658; b) J. Bohnenberger, W. Feuerstein, D. Himmel, M. Daub, F. Breher, I. Krossing, *Nat. Commun.* **2019**, *10*, 624.

[2] I. Krossing, A. Reisinger, *Coord. Chem. Rev.* **2006**, *250*, 2721.

[3] a) I. Krossing, *Chem. Eur. J.* **2001**, *7*, 490; b) I. M. Riddlestone, A. Kraft, J. Schaefer, I. Krossing, *Angew. Chem. Int. Ed.* **2018**, *57*, 13982; c) W. A. Herrmann (Ed.) *Synthetic methods of organometallic and inorganic chemistry*. *Transition Metals*, Thieme, Stuttgart [u.a.], **2000**.

[4] L. Krause, R. Herbst-Irmer, G. M. Sheldrick, D. Stalke, *J. Appl. Cryst.* **2015**, *48*, 3.

[5] G. M. Sheldrick, *Acta Cryst.* **2008**, *64*, 112.

[6] G. M. Sheldrick, *Acta Cryst. A* **2015**, *71*, 3.

[7] a) D. Kratzert, J. J. Holstein, I. Krossing, *J. Appl. Cryst.* **2015**, *48*, 933; b) D. Kratzert, I. Krossing, *J. Appl. Cryst.* **2018**, *51*, 928.

[8] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339.

[9] a) R. Ahlrichs, M. Bär, M. Häser, H. Horn, C. Kölmel, *Chem. Phys. Lett.* **1989**, *162*, 165; b) O. Treutler, R. Ahlrichs, *J. Chem. Phys.* **1995**, *102*, 346; c) M. von Arnim, R. Ahlrichs, *J. Comput. Chem.* **1998**, *19*, 1746.

[10] a) Becke, *Phys. Rev. A Gen. Phys.* **1988**, *38*, 3098; b) Perdew, *Phys. Rev. , B Condens Matter* **1986**, *33*, 8822.

[11] a) R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2004**, *6*, 5119; b) M. Sierka, A. Hogekamp, R. Ahlrichs, *J. Chem. Phys.* **2003**, *118*, 9136; c) F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057.

[12] a) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297; b) F. Weigend, M. Häser, H. Patzelt, R. Ahlrichs, *Chem. Phys. Lett.* **1998**, *294*, 143.

[13] a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104; b) S. Grimme, S. Ehrlich, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456.

[14] a) P. Deglmann, F. Furche, *J. Chem. Phys.* **2002**, *117*, 9535; b) P. Deglmann, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2002**, *362*, 511; c) P. Deglmann, K. May, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2004**, *384*, 103.

[15] R. F. W. Bader, *Chem. Rev.* **1991**, *91*, 893.

[16] T. Lu, F. Chen, *J. Comput. Chem.* **2012**, *33*, 580.