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The Crystal and Molecular Structure of $NaAgS_2O_3H_2O$

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$NaAgS_2O_3H_2O$ is monoclinic, Pc: a = *7.78(1)*, b = *9.07(1)*, c = *7.71(1) Å*, β = *96.3°(.2°)*, Z = *4. The crystal structure has been determined at room temperature from three-dimensional X-ray photographic data and refined by differential methods using anisotropic thermal parameters; final* R = *10.8%. In the asymmetric unit there are two independent silver atoms both tetrahedrally surrounded by three sulphur atoms from three thiosulphate groups and by one oxygen atom from the water molecule. Each thiosulphate group behaves as a monodentate ligand through the external sulphur which coordinates to three adjacent silver atoms (Ag(1)–S = 2.48, 2.54, 2.60 Å; Ag(2)–S = 2.52, 2.52, 2.65 Å) so that the coordination polyhedra result linked in layers running parallel to (010). These layers are joined together by sodium atoms which interact, in a distorted octahedral environment, with the oxygen atoms.*

Introduction

As a part of a study concerning the crystal structure of silver thiosulphate complexes, which are important in photographic process, the compounds appearing in the $Ag_2S_2O_3$–$Na_2S_2O_3$–H_2O system have been considered. As found by Bassett and Lemon[1] the salts formed in that system at 25°C are: $Na_3Ag(S_2O_3)_2 \cdot 2H_2O$, $Na_5Ag_3(S_2O_3)_4 \cdot 2H_2O$, $NaAgS_2O_3 \cdot H_2O$, $NaAg_3(S_2O_3)_2 \cdot H_2O$. Among these the compound corresponding to the simplest stoichiometric formula ($NaAgS_2O_3H_2O$) was considered for a structural analysis being the easiest one to prepare in good crystals suitable for an X-ray single crystal work.

The aim of this research is to define the nature of coordination around silver atoms and the role played by the thiosulphate groups.

Experimental Section

The crystals prepared according to Baines[2] were obtained as thick colourless triangular plates flattened along (010).

Cell parameters, determined from rotation and Weissenberg photographs (CuKα, λ = 1.5418 Å) are as follows (the e.s.d.'s given in parentheses are in units of the last decimal figure):

$NaAgS_2O_3H_2O$ $M = 261.0$

$a = 7.78(1)$; $b = 9.07(1)$; $c = 7.71(1)$ Å; $\beta = 96.3°(.2°)$
$V = 541.0$ Å^3; $Z = 4$; $D_x = 3.20$; $D_m = 3.12$ g cm^{-3};
$\mu = 376.3$ cm^{-1} (CuKα); $F(000) = 490$.

Space group: *Pc* (from systematic absences and strong piezoelectric behaviour).

No chemical analysis was carried out and the formula $NaAgS_2O_3H_2O$ given by Baines was assumed, being the morfological data quoted in his paper in agreement with the present X-ray crystal data.

Two series of equi-inclination integrated Weissenberg photographs (Ni-filtered Cu radiation, multiple film technique) were taken at room temperature around [100] with levels $h = 0,1 \ldots 6$ and around [001] with levels $l = 0,1 \ldots 6$. 1024 independent non zero reflexions were observed out of a possible 1254 within the CuKα sphere. The shape of the spots of non-equatorial layers was taken into account using the formula $I_{corr.} = I(1 \pm K \cos\theta)$ in which K was an empirical constant determined by comparison of corresponding expanded and contracted spots on the same photograph. To give an approximate correction for the absorption effects the samples were considered spheres with mean radii of 0.013 cm and 0.008 cm for the photographs taken around [100] and [001] respectively.

The structure amplitudes were obtained from the photometrically measured intensities after correction for Lorentz and polarization factors. All the data were put on the same scale by the least-squares cross correlation procedure of Rollett and Sparks[3] and a starting absolute scale was then established by Wilson's[4] method.

Structure analysis and refinement

The unit cell contains four formula units $NaAgS_2O_3H_2O$ which must occupy two independent positions as required by the symmetry of the space group (*Pc*). Bearing this in mind it was possible to deduce the coordinates of silver and sulphur atoms from a threedimensional Patterson synthesis. These coordinates were valuable to locate all the other non hydrogen atoms by standard Fourier methods. The refinement was carried out by means of several cycles of Booth's differential synthesis with anisotropic ther-

(1) H. Bassett and J. T. Lemon, *J. Chem. Soc.*, 1423 (1933).
(2) H. Baines, *J. Chem. Soc.*, 2763 (1929).
(3) J. S. Rollett and R. A. Sparks, *Acta Cryst.*, *13*, 273 (1960).
(4) A. J. C. Wilson, *Nature*, *150*, 152 (1942).

Table I. Final atomic fractional coordinates ($\times 10^4$), and thermal parameters ($\times 10^2 Å^2$)* with e.s.d.'s.

	x/a(σ)	y/b(σ)	z/c(σ)	$B_{11}(\sigma)$	$B_{22}(\sigma)$	$B_{33}(\sigma)$	$B_{12}(\sigma)$	$B_{13}(\sigma)$	$B_{23}(\sigma)$
Ag(1)	20(5)	455(3)	5(4)	210(14)	123(7)	431(18)	−18(16)	−6(21)	51(16)
Ag(2)	5103(5)	−607(3)	3082(4)	227(17)	92(6)	302(14)	3(15)	54(18)	18(13)
S(1)	3202(12)	774(6)	520(9)	154(4)	13(4)	163(47)	−3(0)	25(22)	11(11)
S(2)	3283(10)	2978(6)	1099(7)	48(5)	10(4)	81(35)	3(0)	3(6)	13(8)
S(3)	8103(12)	−790(6)	2144(9)	95(39)	9(14)	223(35)	0(37)	27(47)	−26(32)
S(4)	8249(10)	−2962(6)	1439(8)	38(1)	5(1)	92(35)	3(0)	16(3)	−18(4)
Na(1)	386(21)	4453(13)	3325(15)	163(81)	76(34)	173(56)	18(78)	26(9)	2(63)
Na(2)	5329(19)	−4891(13)	3423(14)	122(67)	37(26)	126(43)	−10(62)	−11(69)	−48(47)
O(1)	2889(42)	3250(29)	2893(50)	258(200)	114(64)	296(137)	33(176)	64(213)	−15(141)
O(2)	5022(31)	3493(20)	897(25)	19(17)	69(74)	114(89)	−40(0)	34(19)	−5(26)
O(3)	2029(45)	3708(22)	−134(34)	91(5)	28(6)	263(154)	38(0)	−25(13)	66(13)
O(4)	7956(43)	−3816(23)	2929(26)	128(22)	2(19)	202(140)	8(0)	23(22)	37(27)
O(5)	6871(70)	−3194(21)	−34(32)	113(107)	186(66)	174(81)	−65(116)	−19(126)	−87(92)
O(6)	15(34)	−3229(20)	969(32)	51(115)	152(59)	160(80)	−12(115)	58(129)	131(86)
O(7)	−1341(39)	2881(25)	1505(29)	198(139)	65(53)	211(99)	−19(129)	−25(149)	−14(104)
O(8)	3733(33)	−3023(16)	1679(19)	107(122)	130(66)	174(108)	−25(132)	55(155)	2(115)

* Anisotropic thermal factors in the form: $\exp[-b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)]$ in which $b_{11} = \frac{1}{4}a^{*2}B_{11}$, $b_{12} = \frac{1}{2}a^*b^*B_{12}$.

Table II. Atomic peak heights ($e.Å^{-3}$), curvatures ($e.Å^{-5}$) and e.s.d.'s.

		ρ	$-A_{hh}$	$-A_{kk}$	$-A_{ll}$	A_{kl}	A_{hl}	A_{hk}
Ag(1)	obs.	121.3	1146	1470	953	86	27	−72
	calcd.	121.5	1139	1461	988	75	38	−67
Ag(2)	obs.	132.4	1171	1600	1250	40	136	−36
	calcd.	132.7	1170	1593	1258	34	127	−40
S(1)	obs.	50.3	447	673	486	11	32	−14
	calcd.	49.6	451	665	487	10	30	−14
S(2)	obs.	54.2	545	660	583	−28	47	−46
	calcd.	53.2	541	659	577	−28	45	−49
S(3)	obs.	47.1	444	606	454	−15	41	−31
	calcd.	46.9	440	601	453	−13	40	−32
S(4)	obs.	54.3	550	698	566	−25	64	−11
	calcd.	53.6	546	697	562	−22	63	−14
Na(1)	obs.	27.8	252	287	263	−12	17	−14
	calcd.	28.2	253	287	262	−12	20	−16
Na(2)	obs.	29.7	269	326	291	−3	20	4
	calcd.	29.4	269	323	289	−2	21	6
O(1)	obs.	15.4	126	176	84	8	1	13
	calcd.	15.0	127	175	81	8	2	13
O(2)	obs.	19.4	180	191	173	−11	25	−7
	calcd.	19.2	173	196	172	−8	22	−6
O(3)	obs.	17.0	138	179	137	11	17	−29
	calcd.	16.9	138	179	139	10	18	−30
O(4)	obs.	17.0	127	202	128	−19	0	22
	calcd.	16.8	125	204	129	−21	1	21
O(5)	obs.	14.9	96	133	163	−21	35	−29
	calcd.	15.2	96	136	164	−18	37	−30
O(6)	obs.	19.6	175	197	145	1	27	−11
	calcd.	19.2	165	201	147	5	23	−13
O(7)	obs.	15.6	136	159	131	−19	12	6
	calcd.	15.3	137	155	130	−20	13	6
O(8)	obs.	17.6	168	203	189	−30	11	−24
	calcd.	17.5	168	209	192	−32	13	−24
	e.s.d.	1.3	17	18	13	8	8	11

mal parameters. The final residual error indices are (R, for observed reflexions only, R' including $F_o = \frac{1}{2}F_{min}$ when $F_c \geqslant F_{min}$ for unobserved reflexions; multiplicities not considered): $R = 10.8\%$, $R' = 11.0\%$.

In Table I the final positional and thermal parameters with their e.s.d.'s, are given. The B_{ij} were determined by the method of Nardelli and Fava[5] using the second derivatives of the electron density from differential synthesis. The comparison between observed and calculated peak shapes is shown in Table II. Observed and calculated structure factors are shown in Table III. The atomic scattering factors are those of Thomas and Umeda[6] for Ag^+, of Dawson[7] for S and of Berghuis *et al.*[8] for Na^+, O.

All the calculations were performed on the Olivetti Elea 6001/S computer of the *Centro di Calcolo Elettronico dell'Università di Parma*, using the programmes of Nardelli, Musatti, Domiano and Andreetti.[9]

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Table III. Observed and calculated structure factors. A minus sign for F_o means « less than »

h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$
0	0	2	300	250	86	1	0	6	157	153	12	1	6	5	206	166	225	2	2	5	547	600	92	2	8	6	298	302	146	3	4	6	111	59	257
0	0	4	863	943	74	1	0	6	332	437	67	1	6	5	257	214	38	2	2	6	773	821	348	2	8	6	358	318	135	3	4	6	127-	57	224
0	0	6	730	798	329	1	0	8	317	318	9	1	6	6	217	218	280	2	2	6	560	624	301	2	9	0	452	464	159	3	4	7	251	310	119
0	0	8	70-	66	246	1	1	0	75-	71	305	1	6	6	222	181	239	2	2	7	283	306	23	2	9	1	341	333	122	3	4	7	271	282	115
0	1	0	1056	1083	0	1	1	1	934	906	230	1	6	7	153	178	72	2	2	7	304	276	318	2	9	1	213	182	58	3	4	8	153	130	310
0	1	1	699	588	49	1	1	1	658	580	43	1	6	7	406	447	100	2	2	8	84	117	315	2	9	2	418	410	121	3	4	9	49-	63	61
0	1	2	420	360	329	1	1	2	1134	1315	35	1	6	8	234	234	162	2	2	9	131	123	57	2	9	2	399	376	62	3	5	0	239	182	34
0	1	3	479	423	152	1	1	2	1042	1219	8	1	7	0	504	446	1	2	3	0	643	520	297	2	9	3	358	331	160	3	5	1	899	720	146
0	1	4	815	912	16	1	1	3	522	472	65	1	7	1	419	329	151	2	3	1	681	562	55	2	9	3	475	473	81	3	5	1	1207	1054	136
0	1	5	185	160	171	1	1	3	782	803	47	1	7	1	375	335	131	2	3	1	750	715	67	2	9	4	403	403	230	3	5	2	452	355	227
0	1	6	205	218	17	1	1	4	591	648	288	1	7	2	792	700	239	2	3	2	864	693	23	2	9	4	380	351	206	3	5	2	600	543	199
0	1	7	237	196	330	1	1	4	694	817	319	1	7	2	602	547	188	2	3	2	318	222	289	2	9	5	237	229	279	3	5	3	962	907	104
0	1	8	203	186	143	1	1	5	312	309	36	1	7	3	654	583	70	2	3	3	113	68	119	2	9	5	242	235	190	3	5	3	769	851	69
0	1	9	76	77	87	1	1	5	151	152	93	1	7	3	711	741	76	2	3	3	344	301	237	2	9	6	275	312	165	3	5	4	353	288	229
0	2	0	920	978	0	1	1	6	262	303	79	1	7	4	513	487	112	2	3	4	608	527	53	2	10	0	734	827	204	3	5	4	285	235	328
0	2	1	910	1022	48	1	1	6	286	317	74	1	7	4	511	517	119	2	3	4	364	369	324	2	10	1	151	172	144	3	5	5	223	162	36
0	2	2	1091	1122	275	1	1	7	344	387	144	1	7	5	304	324	59	2	3	5	554	551	104	2	10	1	84-	66	124	3	5	5	188	140	242
0	2	3	447	406	183	1	1	7	117	134	155	1	7	5	104-	37	98	2	3	5	445	498	95	2	10	2	156	168	10	3	5	6	286	288	356
0	2	4	890	945	40	1	1	8	470	518	351	1	7	6	272	278	297	2	3	6	162	120	211	2	10	2	292	295	196	3	5	6	203	225	349
0	2	5	522	506	106	1	1	9	159	130	7	1	7	6	191	176	324	2	3	6	127	139	12	2	10	3	232	241	115	3	5	7	219	238	160
0	2	6	487	465	24	1	2	0	93-	63	335	1	7	7	265	310	147	2	3	7	220	254	17	2	10	3	521	541	82	3	5	7	260	240	126
0	2	7	121-	116	94	1	2	1	688	588	141	1	7	7	111	135	136	2	3	7	306	288	311	2	10	4	117	115	206	3	5	8	79-	76	93
0	2	8	289	238	202	1	2	1	589	628	152	1	8	0	124-	54	322	2	3	8	59-	41	257	2	10	4	392	421	255	3	6	0	251	226	346
0	2	9	255	249	217	1	2	2	1014	1027	36	1	8	1	422	415	91	2	3	8	84	81	161	2	10	5	22-	55	241	3	6	1	347	245	142
0	3	0	1788	1810	0	1	2	2	905	1041	2	1	8	1	337	318	95	2	3	9	156-	148	46	2	11	0	445	506	192	3	6	1	324	250	110
0	3	1	1138	1321	54	1	2	3	611	556	69	1	8	2	505	465	209	2	4	0	738	543	46	2	11	1	168	226	198	3	6	2	628	512	180
0	3	2	737	688	56	1	2	3	557	600	111	1	8	2	476	421	197	2	4	1	1170	1104	48	2	11	1	96	134	203	3	6	2	560	470	211
0	3	3	672	612	159	1	2	4	668	632	319	1	8	3	156	157	41	2	4	1	956	911	52	2	11	2	102	139	152	3	6	3	806	761	57
0	3	4	294	250	33	1	2	4	537	609	319	1	8	3	357	340	106	2	4	2	560	528	309	2	11	2	182	181	165	3	6	3	704	749	74
0	3	5	649	627	97	1	2	5	493	509	254	1	8	4	389	396	57	2	4	2	338	248	248	3	0	0	79-	67	276	3	6	4	134-	76	338
0	3	6	514	449	296	1	2	5	251	236	339	1	8	4	386	359	148	2	4	3	366	259	358	3	0	2	1200	1379	17	3	6	4	157	125	341
0	3	7	116-	57	73	1	2	6	283	280	86	1	8	5	343	360	79	2	4	3	596	628	226	3	0	2	1463	1721	18	3	6	5	288	283	117
0	3	8	122	153	31	1	2	6	99-	74	42	1	8	5	245	236	171	2	4	4	329	267	47	3	0	4	559	540	356	3	6	5	229	244	133
0	3	9	257	232	203	1	2	7	243	281	27	1	8	6	154	135	233	2	4	4	418	446	357	3	0	4	237	227	322	3	6	6	208	201	282
0	4	0	300	221	0	1	2	7	459	477	124	1	8	6	373	357	262	2	4	5	910	965	107	3	0	6	272	259	119	3	6	6	265	235	268
0	4	1	1155	1247	49	1	2	8	107	114	316	1	8	7	148	153	334	2	4	5	785	820	76	3	0	6	274	258	95	3	6	7	280	307	154
0	4	2	127	137	330	1	2	8	387	434	349	1	9	0	213	179	33	2	4	6	117	110	21	3	0	8	337	282	340	3	6	7	240	233	145
0	4	3	591	561	164	1	2	9	75	78	51	1	9	1	570	622	69	2	4	6	327	365	15	3	1	0	180	138	330	3	6	8	56-	53	325
0	4	4	262	175	195	1	3	0	281	217	11	1	9	1	323	281	172	2	4	7	150	156	22	3	1	1	510	433	142	3	7	0	468	408	22
0	4	5	547	525	132	1	3	1	840	779	191	1	9	2	711	732	229	2	4	7	217	228	21	3	1	1	822	819	191	3	7	1	311	240	138
0	4	6	337	278	342	1	3	1	678	723	139	1	9	2	608	606	193	2	4	8	93	65	136	3	1	2	1068	1227	20	3	7	1	522	399	130
0	4	7	338	275	358	1	3	2	695	592	13	1	9	3	330	320	138	2	4	9	203	255	153	3	1	2	1221	1411	13	3	7	2	640	551	218
0	4	8	113	114	347	1	3	2	614	563	5	1	9	3	95-	71	306	2	5	0	809	553	77	3	1	3	229	183	104	3	7	2	897	797	208
0	4	9	99	112	175	1	3	3	1091	1190	91	1	9	4	367	386	125	2	5	1	910	783	55	3	1	3	317	299	56	3	7	3	553	456	103
0	5	0	1138	1109	180	1	3	3	832	955	66	1	9	4	487	499	124	2	5	1	813	716	63	3	1	4	524	487	342	3	7	3	475	434	67
0	5	1	960	963	57	1	3	4	358	264	296	1	9	5	168	192	96	2	5	2	649	511	132	3	1	4	318	305	297	3	7	4	311	284	137
0	5	2	640	553	303	1	3	4	410	387	322	1	9	5	130	117	49	2	5	2	830	860	31	3	1	5	265	247	296	3	7	4	332	308	78
0	5	3	459	429	154	1	3	5	456	429	282	1	9	6	104	104	317	2	5	3	121	114	75	3	1	5	252	202	278	3	7	5	240	218	7
0	5	4	424	400	333	1	3	5	412	416	358	1	9	6	217	226	255	2	5	3	223	163	208	3	1	6	199	200	76	3	7	5	186	194	353
0	5	5	551	550	101	1	3	6	194	179	355	1	10	0	133	118	207	2	5	4	501	445	284	3	1	6	340	344	61	3	7	6	117	97	275
0	5	6	139	114	124	1	3	6	257	280	53	1	10	1	432	509	51	2	5	4	150	106	208	3	1	7	127-	118	85	3	7	6	344	305	262
0	5	7	99-	101	41	1	3	7	102	134	94	1	10	1	95-	26	49	2	5	5	616	650	97	3	1	7	219	211	130	3	7	7	285	289	110
0	5	8	70-	6	80	1	3	7	545	610	126	1	10	2	419	456	178	2	5	5	530	625	81	3	1	8	237	189	2	3	8	0	218	165	192
0	6	0	504	413	180	1	3	8	219	284	306	1	10	2	436	431	198	2	5	6	95-	24	73	3	1	9	44-	93	132	3	8	1	393	372	96
0	6	1	953	982	60	1	3	8	96	83	0	1	10	3	119	90	238	2	5	6	145	122	157	3	1	9	79-	61	107	3	8	1	370	334	81
0	6	2	311	269	28	1	3	9	91	110	67	1	10	3	186	139	241	2	5	7	180	208	29	3	2	0	113-	65	223	3	8	2	671	650	199
0	6	3	260	199	161	1	4	0	234	176	343	1	10	4	243	268	164	2	5	7	170	173	4	3	2	1	747	688	135	3	8	2	755	688	195
0	6	4	435	385	218	1	4	1	847	724	195	1	10	4	145	152	106	2	5	8	136	161	342	3	2	1	865	828	115	3	8	3	252	221	139
0	6	5	677	694	93	1	4	1	743	665	73	1	10	5	105	165	128	2	6	0	315	231	131	3	2	2	848	879	22	3	8	3	136	135	147
0	6	6	162	135	251	1	4	2	513	384	1	1	11	0	61-	28	186	2	6	1	795	658	73	3	2	2	1081	1029	21	3	8	4	218	203	190
0	6	7	151	153	64	1	4	2	527	499	49	1	11	1	170	209	21	2	6	1	758	676	54	3	2	3	678	643	91	3	8	4	130	88	287
0	6	8	211	230	339	1	4	3	822	848	58	1	11	1	252	308	23	2	6	2	493	403	78	3	2	3	562	577	73	3	8	5	173	152	318
0	7	0	707	723	180	1	4	3	907	1077	66	1	11	2	330	402	182	2	6	2	365	333	44	3	2	4	473	425	322	3	8	5	257	238	13
0	7	1	407	347	73	1	4	4	194	178	354	1	11	2	471	588	217	2	6	3	291	210	168	3	2	4	513	449	300	3	8	6	183	224	295
0	7	2	452	436	81	1	4	4	246	218	334	2	0	0	1450	1344	327	2	6	3	151	163	149	3	2	5	332	264	119	3	8	6	136	95	258
0	7	3	196	195	77	1	4	5	176	127	37	2	0	2	1063	1176	330	2	6	4	151	125	207	3	2	5	337	290	162	3	9	0	251	262	26
0	7	4	729	707	222	1	4	5	191	209	90	2	0	2	1242	1302	235	2	6	4	386	351	253	3	2	6	196	190	30	3	9	1	378	365	321
0	7	5	252	248	113	1	4	6	154	110	283	2	0	4	859	947	86	2	6	5	317	308	113	3	2	6	309	286	56	3	9	1	459	424	321
0	7	6	242	213	240	1	4	6	110-	62	62	2	0	4	570	629	53	2	6	5	421	467	116	3	2	7	295	297	177	3	9	2	609	582	209
0	7	7	190	162	20	1	4	7	375	493	119	2	0	6	406	434	351	2	6	6	439	441	150	3	2	7	137-	22	192	3	9	2	796	746	203
0	8	0	1035	1160	180	1	4	7	366	410	123	2	0	6	539	644	329	2	6	6	315	333	94	3	2	8	252	227	42	3	9	3	295	274	49
0	8	1	265	255	89	1	4	8	70-	116	32	2	0	8	67-	131	267	2	6	7	240	260	34	3	2	9	167	144	2	3	9	3	260	252	71
0	8	2	199	159	300	1	4	8	84	72	104	2	0	8	271	247	197	2	6	7	246	239	320	3	3	0	364	267	358	3	9	4	303	302	152
0	8	3	159	160	51	1	4	9	208	192	10	2	1	0	1123	1102	351	2	6	8	128	103	263	3	3	1	796	671	171	3	9	4	274	279	114
0	8	4	403	358	255	1	5	0	585	467	5	2	1	1	461	352	29	2	7	0	670	576	195	3	3	1	1011	968	156	3	9	5	173	210	82
0	8	5	243	238	85	1	5	1	894	771	168	2	1	1	317	301	80	2	7	1	721	640	63	3	3	2	681	557	13	3	9	5	223	227	64
0	8	6	292	286	145	1	5	1	879	809	149	2	1	2	666	580	296	2	7	1	631	556	56	3	3	2	711	646	8	3	10	0	87-	77	172
0	8	7	140	134	16	1	5	2	444	393	267	2	1	2	482	428	320	2	7	2	280	289	34	3	3	3	947	907	74	3	10	1	258	294	352
0	9	0	779	867	180	1	5	2	268	217	262	2	1	3	248	192	28	2	7	2	119-	100	114	3	3	3	989	1086	66	3	10	1	473	476	0
0	9	1	223	233	134	1	5	3	862	907	77	2	1	3	395	358	241	2	7	3	197	147	101	3	3	4	335	274	348	3	10	2	288	284	200
0	9	2	110	67	90	1	5	3	859	1066	86	2	1	4	611	674	11	2	7	3	304	309	129	3	3	4	176	151	353	3	10	2	266	221	182
0	9	3	334	290	4	1	5	4	539	503	42	2	1	4	635	746	35	2	7	4	105-	68	342	3	3	5	309	235	93	3	10	3	76	84	304
0	9	4	314	298	238	1	5	4	378	367	138	2	1	5	456	460	105	2	7	4	655	653	287	3	3	5	338	286	206	3	10	3	98	81	249
0	9	5	292	297	63	1	5	5	337	314	307	2	1	5	324	323	51	2	7	5	442	466	96	3	3	6	160	134	101	3	10	4	260	300	134
0	9	6	283	331	153	1	5	5	265	253	329	2	1	6	642	766	327	2	7	5	383	415	82	3	3	6	128-	92	45	3	11	0	150	194	152
0	10	0	250	230	180	1	5	6	165	144	52	2	1	6	484	521	289	2	7	6	507	515	156	3	3	7	401	407	182	3	11	1	134	180	22
0	10	1	364	418	211	1	5	6	335	327	300	2	1	7	85-	55	227	2	7	6	475	467	81	3	3	7	361	351	164	4	0	0	1405	1722	40
0	10	2	441	457	109	1	5	7	142	199	106	2	1	7	124	130	68	2	7	7	38-	61	55	3	3	8	242	247	321	4	0	2	922	1046	267
0	10	3	401	395	22	1	5	7	376	468	137	2	1	8	216	198	43	2	7	7	160	187	81	3	3	9	222	204	6	4	0	2	427	377	330
0	10	4	436	497	212	1	5	8	58-	66	171	2	1	9	208	175	162	2	8	0	570	533	147	3	4	0	332	248	346	4	0	4	367	364	65
0	10	5	134	168	330	1	5	8	145	143	250	2	2	0	1380	1598	18	2	8	1	386	325	89	3	4	1	1025	944	129	4	0	4	1100	1297	50
0	11	0	294	294	180	1	6	0	163	93	44	2	2	1	809	794	51	2	8	1	334	279	72	3	4	1	1077	914	159	4	0	6	412	412	345
0	11	1	174	181	210	1	6	1	680	565	108	2	2	1	703	669	49	2	8	2	580	512	124	3	4	2	298	240	47	4	0	6	300	389	313
0	11	2	203	213	138	1	6	1	597	526	128	2	2	2	789	748	261	2	8	2	563	512	46	3	4	2	349	281	342	4	0	8	219	140	192
0	11	3	211	204	17	1	6	2	535	444	253	2	2	2	501	398	309	2	8	3	246	230	114	3	4	3	631	556	88	4	1	0	749	854	11
1	0	0	70-	59	235	1	6	2	337	286	126	2	2	3	242	171	314	2	8	3	350	334	80	3	4	3	579	583	70	4	1	1	308	294	80
1	0	2	1216	1436	43	1	6	3	761	747	98	2	2	3	406	368	235	2	8	4	482	495	246	3	4	4	375	302	358	4	1	1	353	308	21
1	0	2	1028	1156	43	1	6	3	459	440	55	2	2	4	186	168	15	2	8	4	448	421	214	3	4	4	300	263	333	4	1	2	127-	24	292
1	0	4	660	735	282	1	6	4	349	319	49	2	2	4	827	901	75	2	8	5	111	139	75	3	4	5	176	115	280	4	1	2	531	457	312
1	0	4	940	1053	320	1	6	4	243	214	130	2	2	5	510	510	105	2	8	5	168	163	73	3	4	5	177	95	206	4	1	3	303	233	233

Table III. (continued)

h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$	h	k	l	$10F_o$	$10F_c$	$\alpha°$
$\bar{4}$	1	3	245	244	54	$\bar{4}$	6	5	392	389	120	5	2	7	340	336	110	5	9	0	154	162	93	$\bar{6}$	5	4	292	249	306	7	4	3	482	404	43
4	1	4	599	647	43	$\bar{4}$	6	5	381	365	81	$\bar{5}$	2	7	309	240	64	5	9	1	386	417	148	6	5	5	338	369	120	$\bar{7}$	4	3	435	524	74
$\bar{4}$	1	4	401	421	339	4	6	6	130	120	79	$\bar{5}$	2	8	254	218	305	$\bar{5}$	9	1	478	514	88	$\bar{6}$	5	5	352	350	87	7	4	4	176	154	12
4	1	5	200	169	55	$\bar{4}$	6	6	350	335	167	5	3	0	152	166	6	5	9	2	277	283	231	$\bar{6}$	5	6	225	210	72	$\bar{7}$	4	4	105-	113	314
$\bar{4}$	1	5	436	414	105	$\bar{4}$	6	7	249	257	15	5	3	1	265	224	178	$\bar{5}$	9	2	504	485	192	$\bar{6}$	5	7	65	48	5	7	4	5	153	141	62
4	1	6	318	285	300	4	7	0	749	706	187	5	3	1	678	546	138	5	9	3	156	173	251	6	6	0	323	280	156	$\bar{7}$	4	5	85-	44	123
$\bar{4}$	1	6	524	565	345	4	7	1	360	286	82	5	3	2	378	334	17	$\bar{5}$	9	3	117	145	148	6	6	1	514	480	80	7	5	0	176	182	61
$\bar{4}$	1	7	130	96	211	$\bar{4}$	7	1	548	450	66	5	3	2	390	300	14	$\bar{5}$	9	4	217	262	93	$\bar{6}$	6	1	507	430	52	7	5	1	271	258	172
$\bar{4}$	1	8	272	215	91	4	7	2	157	157	115	5	3	3	563	473	104	5	10	0	42-	20	247	6	6	2	136	154	77	$\bar{7}$	5	1	628	597	113
$\bar{4}$	1	9	90	81	269	$\bar{4}$	7	2	363	312	347	5	3	3	494	553	69	$\bar{5}$	10	1	219	246	60	$\bar{6}$	6	2	254	240	14	7	5	2	179	198	276
4	2	0	910	1163	11	4	7	3	234	196	108	5	3	4	353	296	321	6	0	0	1080	1509	8	6	6	3	191	142	123	$\bar{7}$	5	2	235	203	133
4	2	1	648	629	67	$\bar{4}$	7	3	140	104	45	5	3	4	314	269	280	$\bar{6}$	0	2	536	506	29	$\bar{6}$	6	3	121	110	159	7	5	3	453	358	102
$\bar{4}$	2	1	643	599	17	4	7	4	471	476	285	5	3	5	479	445	7	$\bar{6}$	0	2	242	233	117	6	6	4	144	137	218	7	5	3	390	415	65
4	2	2	531	489	329	$\bar{4}$	7	4	154	131	173	5	3	5	475	407	285	6	0	4	248	269	95	$\bar{6}$	6	4	401	356	217	7	5	4	165	161	10
$\bar{4}$	2	2	570	423	205	4	7	5	240	261	99	5	3	6	199	206	48	$\bar{6}$	0	4	516	550	65	6	6	5	281	310	105	7	5	4	140	141	188
4	2	3	318	278	230	$\bar{4}$	7	5	367	353	92	5	3	6	213	205	355	6	0	6	353	302	5	$\bar{6}$	6	5	419	443	77	7	5	5	60	50	188
$\bar{4}$	2	3	208	170	153	4	7	6	231	238	73	5	3	7	332	371	115	$\bar{6}$	0	6	582	557	287	$\bar{6}$	6	6	121	105	330	7	6	0	148	170	356
4	2	4	499	454	91	$\bar{4}$	7	6	530	517	160	5	3	7	412	362	86	$\bar{6}$	0	8	85	31	180	6	7	0	341	340	179	7	6	1	258	290	102
$\bar{4}$	2	4	395	364	358	$\bar{4}$	7	7	53-	37	34	5	3	8	213	179	358	6	1	0	531	708	349	6	7	1	355	376	77	7	6	1	352	316	174
4	2	5	312	281	108	4	8	0	678	609	227	5	4	0	130-	55	332	6	1	1	229	235	51	$\bar{6}$	7	1	228	188	45	7	6	2	288	316	235
$\bar{4}$	2	5	444	399	97	4	8	1	262	222	73	5	4	1	335	282	17	$\bar{6}$	1	1	274	288	48	6	7	2	231	221	113	7	6	2	285	234	165
4	2	6	208	203	338	$\bar{4}$	8	1	257	239	85	5	4	1	226	193	230	6	1	2	257	278	303	$\bar{6}$	7	2	320	312	59	7	6	3	574	503	109
$\bar{4}$	2	6	766	799	336	4	8	2	401	401	50	5	4	2	314	220	42	$\bar{6}$	1	2	228	192	284	6	7	3	85	37	14	$\bar{7}$	6	3	262	334	30
4	2	7	101-	78	339	$\bar{4}$	8	2	317	278	122	5	4	2	453	342	6	6	1	3	177	145	143	$\bar{6}$	7	3	183	185	112	7	6	5	140	181	56
$\bar{4}$	2	7	294	262	15	4	8	3	281	284	72	5	4	3	977	966	77	$\bar{6}$	1	3	283	278	174	6	7	4	286	278	219	7	7	0	176	233	38
$\bar{4}$	2	8	281	228	113	$\bar{4}$	8	3	107-	94	105	5	4	3	663	728	55	6	1	4	448	432	31	$\bar{6}$	7	4	553	553	220	7	7	1	84	80	173
$\bar{4}$	2	9	353	329	152	4	8	4	269	258	228	5	4	4	159	116	17	$\bar{6}$	1	4	565	591	22	$\bar{6}$	7	5	206	207	94	7	7	1	269	259	88
4	3	0	599	517	24	$\bar{4}$	8	4	536	497	231	5	4	4	130-	46	320	6	1	5	197	162	162	6	8	0	511	695	94	7	7	2	272	312	251
4	3	1	871	842	67	4	8	5	173	202	97	5	4	5	80	66	107	$\bar{6}$	1	5	101-	70	187	6	8	1	145	149	111	7	7	2	435	427	166
$\bar{4}$	3	1	755	633	36	$\bar{4}$	8	5	209	225	71	5	4	5	167	116	52	6	1	6	409	361	353	$\bar{6}$	8	1	124	132	66	7	8	0	52-	44	82
4	3	2	330	253	262	$\bar{4}$	8	6	194	184	133	5	4	6	85-	50	22	$\bar{6}$	1	6	93-	62	56	6	8	2	167	136	191	7	8	2	303	309	174
$\bar{4}$	3	2	694	597	2	4	9	0	524	491	213	5	4	6	107-	13	30	$\bar{6}$	1	7	185	178	310	$\bar{6}$	8	2	235	224	300	8	0	0	145	168	34
4	3	3	419	352	224	4	9	1	160	155	70	5	4	7	235	247	132	$\bar{6}$	1	8	119	69	105	6	8	3	42-	55	80	8	0	2	510	616	319
$\bar{4}$	3	3	386	358	133	$\bar{4}$	9	1	308	337	123	5	4	7	407	382	107	6	2	0	392	443	22	$\bar{6}$	8	3	205	225	51	8	0	4	271	240	87
4	3	4	409	339	6	4	9	2	297	322	78	5	4	8	127	125	32	6	2	1	421	467	61	$\bar{6}$	8	4	294	287	238	8	1	0	275	364	9
$\bar{4}$	3	4	634	561	45	$\bar{4}$	9	2	292	271	115	5	5	0	373	306	28	$\bar{6}$	2	1	424	398	44	6	9	0	444	519	184	8	1	1	128-	139	64
4	3	5	418	393	97	4	9	3	409	415	66	5	5	1	248	218	183	6	2	2	556	578	304	6	9	1	185	207	147	$\bar{8}$	1	1	134-	46	115
$\bar{4}$	3	5	519	457	96	$\bar{4}$	9	3	252	232	183	5	5	1	663	543	151	$\bar{6}$	2	2	413	380	238	$\bar{6}$	9	1	50-	37	143	8	1	2	183	229	286
4	3	6	306	271	326	4	9	4	219	244	214	5	5	2	209	222	328	6	2	3	156	116	77	$\bar{6}$	9	2	76	82	0	8	1	3	98	102	344
$\bar{4}$	3	6	168	160	190	$\bar{4}$	9	4	461	444	220	5	5	2	412	294	284	$\bar{6}$	2	3	373	396	103	7	0	0	136-	189	246	$\bar{8}$	1	3	104-	109	266
4	3	7	194	175	329	$\bar{4}$	9	5	160	147	314	5	5	3	717	628	98	6	2	4	280	261	22	7	0	2	500	634	50	8	1	4	309	249	45
$\bar{4}$	3	7	252	238	23	4	10	0	547	634	161	5	5	3	616	632	62	$\bar{6}$	2	4	747	803	24	7	0	4	186	201	281	8	2	0	412	468	43
$\bar{4}$	3	8	90-	100	317	4	10	1	219	252	231	5	5	4	306	271	117	6	2	5	260	268	129	7	0	6	147	99	309	8	2	1	209	240	83
$\bar{4}$	3	9	343	363	138	$\bar{4}$	10	1	277	333	147	5	5	4	525	501	52	$\bar{6}$	2	5	387	370	72	7	1	0	133-	95	317	$\bar{8}$	2	1	131-	153	10
4	4	0	318	154	56	4	10	2	304	349	183	5	5	5	196	179	352	6	2	6	369	357	36	7	1	1	500	568	226	8	2	2	170	201	316
$\bar{4}$	4	1	852	795	76	$\bar{4}$	10	2	186	194	352	5	5	5	380	351	274	$\bar{6}$	2	6	128	105	358	7	1	1	361	314	67	8	2	3	130	116	316
$\bar{4}$	4	1	963	795	24	$\bar{4}$	10	3	140	127	3	5	5	6	194	158	277	$\bar{6}$	2	7	111	76	183	7	1	2	480	553	40	8	2	4	70	47	263
4	4	2	239	180	325	5	0	0	157	149	308	5	5	6	147	100	300	$\bar{6}$	2	8	229	211	173	7	1	2	643	646	350	8	3	0	127	187	325
$\bar{4}$	4	2	455	361	294	5	0	2	511	494	33	5	5	7	347	331	103	6	3	0	669	742	358	7	1	3	294	237	2	$\bar{8}$	3	1	255	312	74
4	4	3	471	359	232	$\bar{5}$	0	2	617	647	31	5	6	0	130-	50	15	6	3	1	516	533	58	7	1	3	223	287	65	$\bar{8}$	3	1	168	144	33
$\bar{4}$	4	3	228	230	81	5	0	4	727	777	321	5	6	1	625	548	143	$\bar{6}$	3	1	706	626	56	7	1	4	223	200	319	8	3	2	196	198	325
4	4	4	219	188	324	$\bar{5}$	0	4	666	733	275	5	6	1	634	531	108	6	3	2	422	377	71	7	1	4	213	222	323	8	3	3	168	147	309
$\bar{4}$	4	4	312	241	52	5	0	6	337	297	54	5	6	2	90-	45	170	$\bar{6}$	3	2	341	314	20	7	1	5	203	188	64	8	3	4	257	242	66
4	4	5	355	357	88	$\bar{5}$	0	6	221	208	29	5	6	2	215	158	275	6	3	3	300	268	136	7	1	5	102-	125	228	8	4	0	127	132	10
$\bar{4}$	4	5	799	839	100	5	0	8	447	361	344	5	6	3	265	210	80	$\bar{6}$	3	3	308	337	187	7	1	6	49-	76	80	8	4	1	288	372	76
4	4	6	306	288	40	5	1	0	170	160	288	5	6	3	421	389	101	6	3	4	254	234	65	7	2	0	131-	51	267	8	4	1	203	162	38
$\bar{4}$	4	6	119-	67	307	5	1	1	517	501	346	5	6	4	321	304	118	$\bar{6}$	3	4	170	130	163	7	2	1	263	282	126	8	4	2	179	169	357
4	4	7	222	208	58	5	1	1	220	185	289	5	6	4	176	146	83	6	3	5	350	351	122	7	2	1	399	378	134	8	4	2	113	126	249
$\bar{4}$	4	7	133	99	341	5	1	2	547	544	30	5	6	5	278	277	15	$\bar{6}$	3	5	380	369	79	7	2	2	399	421	41	8	4	3	196	150	355
$\bar{4}$	4	8	159	135	255	$\bar{5}$	1	2	671	678	19	5	6	5	163	91	315	6	3	6	188	211	304	7	2	2	628	560	358	8	4	4	190	244	344
4	5	0	723	596	277	5	1	3	652	650	82	5	6	6	142	139	284	$\bar{6}$	3	6	291	275	294	7	2	3	432	352	106	8	5	0	214	225	25
4	5	1	779	676	66	$\bar{5}$	1	3	470	518	39	5	6	6	162	124	274	$\bar{6}$	3	7	81	43	197	7	2	3	200	195	64	8	5	1	275	348	74
$\bar{4}$	5	1	802	639	36	5	1	4	557	572	318	5	6	7	239	211	63	$\bar{6}$	3	8	121	127	349	7	2	4	265	242	341	8	5	1	255	243	42
4	5	2	681	601	36	$\bar{5}$	1	4	470	454	282	5	7	0	340	296	53	6	4	0	292	232	49	7	2	4	202	203	286	8	5	2	265	274	120
$\bar{4}$	5	2	364	261	131	5	1	5	234	179	112	5	7	1	124	75	99	6	4	1	652	672	64	7	2	5	171	179	255	$\bar{8}$	5	2	353	330	27
4	5	3	300	231	198	$\bar{5}$	1	5	194	177	78	5	7	1	364	291	132	$\bar{6}$	4	1	672	562	40	7	2	5	186	191	69	8	6	0	65-	27	299
$\bar{4}$	5	3	228	211	101	5	1	6	150	146	85	5	7	2	242	222	245	6	4	2	183	215	320	7	2	6	85-	68	18	8	6	1	248	322	86
4	5	4	131-	10	56	$\bar{5}$	1	6	344	318	74	5	7	2	436	352	200	$\bar{6}$	4	2	167	131	82	7	3	0	128-	78	333	$\bar{8}$	6	1	194	192	36
$\bar{4}$	5	4	504	455	257	5	1	7	79-	83	213	5	7	3	547	518	90	6	4	3	190	163	110	7	3	1	205	223	190	$\bar{8}$	6	2	145	116	65
4	5	5	409	423	95	$\bar{5}$	1	7	297	247	125	5	7	3	487	510	49	$\bar{6}$	4	3	574	611	171	7	3	1	545	487	139	9	0	0	125	80	342
$\bar{4}$	5	5	540	545	95	$\bar{5}$	1	8	383	336	309	5	7	4	406	395	139	6	4	4	114	94	214	7	3	2	272	267	29	9	0	2	363	346	12
4	5	6	95-	36	266	$\bar{5}$	1	9	39-	35	266	5	7	4	410	407	91	$\bar{6}$	4	4	107	75	339	7	3	2	335	240	344	9	1	0	137	86	331
$\bar{4}$	5	6	111-	70	340	5	2	0	180	172	302	5	7	5	144	152	105	6	4	5	350	365	146	7	3	3	574	492	110	9	1	1	255	276	94
4	5	7	153	147	27	5	2	1	421	421	166	5	7	5	163	158	101	$\bar{6}$	4	5	295	288	89	7	3	3	381	493	26	9	1	2	304	291	25
$\bar{4}$	5	7	136	133	26	$\bar{5}$	2	1	455	402	164	5	7	6	330	311	282	6	4	6	104	98	327	7	3	4	130	120	301	9	2	0	116	100	312
$\bar{4}$	5	8	133	160	33	5	2	2	488	483	29	5	8	0	156	101	16	$\bar{6}$	4	6	242	228	322	7	3	4	232	205	340	9	2	1	136	139	171
4	6	0	419	333	233	$\bar{5}$	2	2	666	614	9	5	8	1	249	264	101	$\bar{6}$	4	7	228	218	303	7	3	5	147	166	252	9	2	2	176	183	29
4	6	1	868	771	69	5	2	3	289	211	87	5	8	1	180	162	90	6	5	0	591	530	178	7	3	5	96	99	79	9	3	0	95	77	21
$\bar{4}$	6	1	669	543	53	$\bar{5}$	2	3	358	320	100	5	8	2	311	302	210	6	5	1	516	527	60	7	3	6	229	194	58	9	3	1	73-	27	64
4	6	2	335	284	34	$\bar{5}$	2	4	487	433	332	5	8	2	406	330	243	$\bar{6}$	5	1	660	553	54	7	4	0	176	199	350	9	3	2	174	209	13
$\bar{4}$	6	2	246	199	55	$\bar{5}$	2	4	442	395	310	5	8	3	311	289	88	6	5	2	269	225	258	7	4	1	565	636	202	$\bar{9}$	3	4	52-	33	25
4	6	3	128-	52	114	5	2	5	337	320	320	5	8	3	213	211	59	$\bar{6}$	5	2	501	429	302	7	4	1	499	460	84	9	4	0	61-	75	335
$\bar{4}$	6	3	461	425	162	$\bar{5}$	2	5	481	464	278	5	8	4	311	343	111	6	5	3	228	154	113	7	4	2	116-	72	276	9	4	1	298	387	114
4	6	4	320	303	257	5	2	6	101-	25	275	5	8	4	347	352	73	$\bar{6}$	5	3	338	327	164	7	4	2	209	158	18	9	5	0	36-	53	35
$\bar{4}$	6	4	183	175	156	$\bar{5}$	2	6	298	242	87	5	8	5	268	293	99	6	5	4	240	249	350												

Discussion

Both the independent stoichiometric units are practically equivalent from the chemical point of view, being Ag(1) and Ag(2) tetrahedrally surrounded by three sulphur atoms and one water molecule as shown in Figure 1.

Bond distances and angles in the coordination tetrahedra are quoted in Table IV. The Ag–S distances are near to the sum of covalent radii (2.57 Å) and are in the range of the values found in other tetrahedral Ag^I complexes: *e.g.* 2.47–2.74 Å in $NH_4Ag(SCN)_2$ [10]; 2.48–2.66 Å in $Ag(CH_2S)_3ClO_4 \cdot H_2O$ [11];

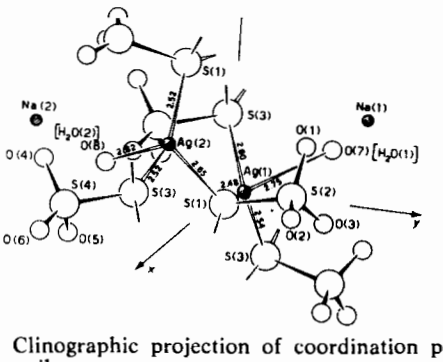

Figure 1. Clinographic projection of coordination polyhedra around the silver atoms.

(10) J. Lindqvist and B. Strandberg, *Acta Cryst.*, *10*, 173 (1957).

2.55–2.69 Å in $Ag(CH_2S)_3NO_3 . H_2O$ [11]; 2.46–2.60 Å in $Ag[(CH_2S)_3]_2NO_3$ [12]; 2.48–2.59 Å in $Ag[SC(NH_2)_2]Cl$ [13]; 2.48–2.49 Å in $Ag_2Br_2[SC(NH_2)NHNH_2]_3$ [14]; 2.43–2.48 Å in $AgNCS[SC(NH_2)NHNH_2]_2$ [15].

Table IV. Bond distances and angles in the coordination polyhedra

Ag(1)—S(1)	= 2.48(1) Å
Ag(1)—S(3″)	= 2.60(1)
Ag(1)—S(3‴)	= 2.54(1)
Ag(1)—O(7)	= 2.75(2)
S(1)—Ag(1)—S(3″)	= 125.5(.5)°
S(1)—Ag(1)—S(3‴)	= 126.9(.7)
S(1)—Ag(1)—O(7)	= 105.2(.5)
S(3″)—Ag(1)—O(7)	= 78.9(.8)
S(3″)—Ag(1)—S(3‴)	= 106.2(.5)
S(3‴)—Ag(1)—O(7)	= 93.0(.8)
Ag(2)—S(1)	= 2.65(1) Å
Ag(2)—S(3)	= 2.52(1)
Ag(2)—S(1′)	= 2.52(1)
Ag(2)—O(8)	= 2.62(2)
S(1)—Ag(2)—S(3)	= 106.0(.4)°
S(1)—Ag(2)—S(1′)	= 105.0(.4)
S(1)—Ag(2)—O(8)	= 85.3(.8)
S(1′)—Ag(2)—O(8)	= 90.6(.8)
S(3)—Ag(2)—S(1′)	= 122.2(.6)
S(3)—Ag(2)—O(8)	= 100.0(.8)

x, $\bar{y}$, z+½ ″ x−1, y, z ‴ x−1, $\bar{y}$, z−½

Nevertheless in the present compound one distance is significantly longer than the other two in both tetrahedra.

The Ag–O distances concern the water molecule and their values (2.62 and 2.75 Å) are consistent with the sum of the ionic radii (2.66 Å).

The two coordination polyhedra, even if of the same kind, show some relevant differences concerning bond lengths and angles, particularly when water molecules are implied. It is difficult to give a direct explanation of this fact, considering that the environments of the two crystallographically independent parts of the structure are similar.

Distances and angles in the thiosulphate groups agree fairly well with those generally observed in other thiosulphates as shown in Table V. The $S_2O_3^{2-}$ group coordinates as a monodentate ligand in agreement with the I.R. spectrum in which no splitting is observed for the ν_4 (1123 cm^{-1}) S–O asymmetric stretching vibration.

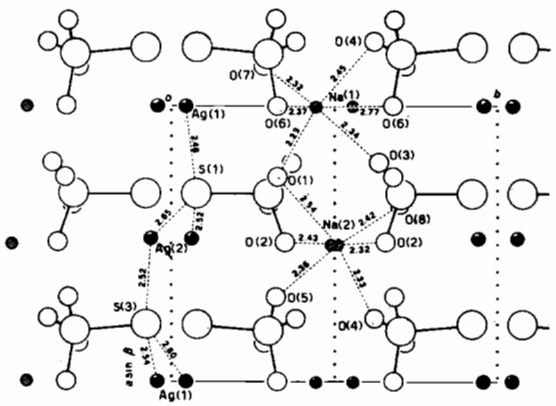

Figure 2. Diagrammatic projection of the structure along [001].

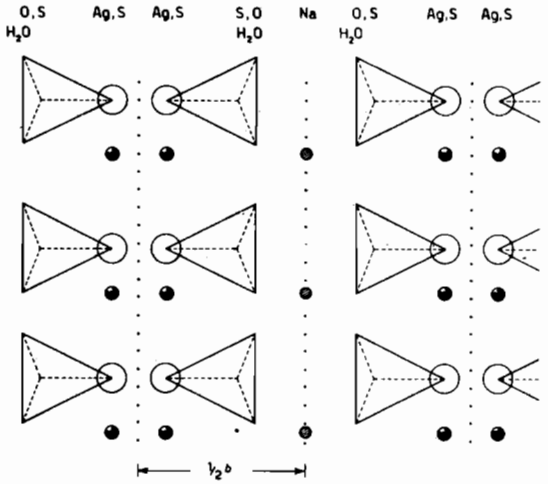

Figure 3. Diagrammatic sketching of the layers parallel to (010).

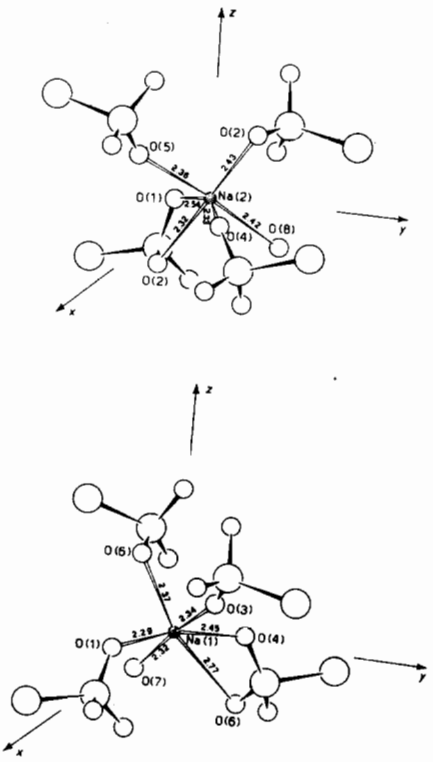

Figure 4. Clinographic projection of cordination polyhedra around the Na^+ ions.

(11) R. S. Ashworth, A. Domenicano, C. K. Prout, and A. Vaciago, *J. Chem. Soc.*, A93 (1968).
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(15) L. Calzolari Capacchi, G. Fava Gasparri, M. Ferrari, and M. Nardelli, *Chem. Comm.*, 910 (1968).

Table V. Bond distances and angles in $S_2O_3^{2-}$ group

	$NaAgS_2O_3H_2O$	$Zn[SC(NH_2)_2]_3S_2O_3 . H_2O$ [16]	$Ni[SC(NH_2)_2]_4S_2O_3 . H_2O$ [17]	$BaS_2O_3 . H_2O$ [18]	$Na_2S_2O_3$ [19]	$Mg(OH_2)_6S_2O_3$ [20]
S–S	2.05(1) Å	2.03(1) Å	2.01(1) Å	1.96(1) Å	2.01(2) Å	2.02(1) Å
	2.05(1)					
S–O	1.46(2)	1.46(1)	1.50(1)	1.57(4)	1.52(3)	1.48(1)
	1.45(3)	1.45(1)	1.46(1)	1.52(3)	1.46(3)	1.48(4)
	1.47(4)	1.45(1)	1.43(1)	1.44(3)	1.42(3)	
	1.49(4)					
	1.42(2)					
	1.48(3)					
O–S–O	110.4(1.7)°	111.0(.5)°	110.7(.6)°	105.3(2.3)°	109.4(3.6)°	110.9(1.1)°
	111.2(1.7)	111.0(.6)	110.4(.7)	104.3(1.9)	107.9(3.6)	111.0(1.1)
	109.1(1.9)	111.3(.6)	111.6(.7)	116.3(1.4)	114.4(3.6)	
	111.1(2.0)					
	110.1(1.8)					
	112.0(1.9)					
S–S–O	107.1(1.0)	108.3(.5)	104.8(.4)	109.7(1.3)	108.3(2.4)	107.6(.8)
	107.8(1.1)	106.8(.5)	108.6(.5)	112.0(.8)	109.2(2.4)	108.5(.8)
	111.3(1.2)	108.3(.4)	110.6(.5)	108.7(1.3)	107.6(2.4)	
	106.6(1.2)					
	106.4(1.0)					
	107.5(1.1)					

The structure is polymeric in nature as each coordinated sulphur atom belongs to three coordination polyhedra. This can be seen in Figure 1 and in Figure 2 which shows a projection along [001].

The whole crystal structure is characterized by layers running parallel to (010) as diagrammatically shown in Figure 3. Every two double layers of coordination polyhedra there is a layer of Na^+ ions which join together the double layers by means of Na–O interactions.

The coordination polyhedra around the Na^+ ions are distorted octahedra as shown in Figure 4. The Na–O distances are ranging around the sum of the ionic radii (2.44 Å) and agree with the values generally found in other structures with similar coordination [*e.g.* 2.42 Å (mean value) in $Na[C_{10}H_6 . NH_2 . SO_3] . 4H_2O$ [21], 2.35 Å (mean value) in $NaBr . 2CH_3CONH_3$ [22]; 2.41, 2.44, 2.45, 2.46, 2.49, 2.50 Å in $Na_2O . SiO_2 . 9H_2O$ [23]] excepting for the Na(1)–O(6) = 2.77 Å distance which is much longer than the others.

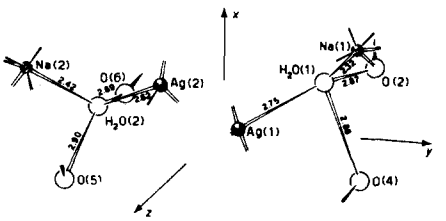

Figure 5. Clinographic projection of the environment of the water molecules.

The water molecules are both surrounded by a tetrahedral environment concerning silver and sodium atoms which are in the directions of the lone pairs and two oxygen atoms which form hydrogen bonds (O–H ... O = 2.87, 2.88, 2.89, 2.90 Å). These environments are shown in the clinographic projection of Figure 5.

No packing distances less than 3.5 Å are observed.

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