RECEIVED
LAWRENCE
RADIATION LABORATORY
DEC 1 1970
LIBRARY AND
DOCUMENTS SECTION

UCRL-19985
UC-4 Chemistry
TID-4500 (56th Ed.)

c.2

THE CRYSTAL AND MOLECULAR STRUCTURE OF SODIUM GOLD(I) THIOSULFATE DIHYDRATE

Helena Ruben, Allan Zalkin, M. O. Faltens
and David H. Templeton

October 1970

AEC Contract No. W-7405-eng-48

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 5545

LAWRENCE RADIATION LABORATORY
UNIVERSITY of CALIFORNIA BERKELEY

UCRL-19985 c.2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

CONTRIBUTION FROM THE LAWRENCE RADIATION LABORATORY AND DEPARTMENT OF CHEMISTRY, UNIVERSITY OF CALIFORNIA, BERKELEY, CALIFORNIA 94720

The Crystal and Molecular Structure of Sodium Gold(I) Thiosulfate Dihydrate[1]

BY HELENA RUBEN, ALLAN ZALKIN, M. O. FALTENS, AND DAVID H. TEMPLETON

X-ray diffraction study of a single crystal of $Na_3Au(S_2O_3)_2 \cdot 2H_2O$ shows that it is monoclinic with $\underline{a}$ = 18.206 ± 0.006, $\underline{b}$ = 11.355 ± 0.006, $\underline{c}$ = 5.436 ± 0.004Å and $\underline{\beta}$ = 97.87 ± 0.05°. The space group is $P2_1/a$ with four formula units per unit cell. The X-ray density is 3.14g/cm^3. The gold is located between the two thiosulfate groups in a near linear arrangement (S-Au-S, 176.5°). The average Au-S bond distance is 2.28 ± .01Å, the S-S distance is 2.06 ± .01Å while the S-O distance is 1.46 ± .01Å. The three sodium atoms are surrounded by irregular polyhedra of oxygen neighbors.

Introduction

One of the authors, Faltens, had been studying aurous (Au^{I}) and auric (Au^{III}) compounds to elucidate their internal bonding.[2] Auric and aurous compounds are textbook examples of dsp^2 (square-planar) and sp (linear) hybridization respectively. Similar electric field gradients about the gold atoms might be expected as well as similar electric quadrapole splittings as observed via the Mossbauer effect. Instead the quadrapole splittings for the aurous chloride was observed to be an order of magnitude larger than that for the auric chloride. In addition to the gold halides (AuCl and $AuCl_4$) other gold compounds including sodium gold(I) thiosulfate dihydrate[3] were investigated, and the quadrapole splitting was observed to be consistently larger for the aurous compounds. This crystal structure investigation of $Na_3Au(S_2O_3)_2 \cdot 2H_2O$ was undertakes to remove any doubt of its identity and to establish the nature of the environment of the gold atom.

Experimental

Sodium gold(I) thiosulfate[3,4] was prepared by adding 21 grams of $HAuCl_4 \cdot 4H_2O$ to about 75cc of water. A 40% (by weight) solution of NaOH was added by drops until a vivid red-orange precipitate started to form. This solution was poured into a mechanically stirred solution of 50 grams. $Na_2(S_2O_3) \cdot 5H_2O$ in 100cc of water, causing no visible change. The order of pouring is important because if the solutions are mixed in the reverse order, the black precipitate of gold sulfide results. While still stirring vigorously, 4 molal HNO_3 drops were added at a rate that allowed the disappearance of any red coloration before the next drop was added. The acid was added until the red-orange precipitate was dissolved and the red coloration no longer formed. This solution, approximately 200cc, was filtered through a "fine" sintered glass funnel and 800cc of ethyl alcohol added to the filtrate. The white flocculent precipitate which formed was collected on a similar glass funnel and washed with ethanol (about 100cc) then recrystallized twice by dissolving the sodium gold(I) thiosulfate in a minimum of water and precipitating with four volumes of ethanol. The specimen for this study was prepared by dissolving a small amount in a minimum of water, adding two volumes of ethanol and allowing the crystals to grow overnight in the dark, as most gold compounds are photosensitive.

A clear thin crystal plate approximately .17 x .07 x .02mm was mounted along the c axis on the end of a thin pyrex glass fiber. A second crystal was mounted on its b axis, but since it was fractured, it was not suitable for taking data, but was useful in obtaining the

monoclinic $\underline{\beta}$ angle.

The crystals were aligned on our G.E. XRD-5 hand-operated diffractometer equipped with a quarter-circle Eulerian cradle, scintillation counter and pulse height discriminator. A molybdenum anode tube ($\lambda_{K\alpha 1}$ = 0.70926Å, $\lambda_{K\alpha 2}$ = 0.71354Å and $\lambda_{K\beta}$ = 0.632253Å) operated at 45 kilovolts, 20 milliamperes was used. The X-rays were filtered by a 3.0 mil zirconium filter. Cell dimensions were determined from a series of measurements along the h00, 0k0 and 00ℓ directions using peaks where the Kα1, Kα2 and Kβ X-rays were resolved. All measurements were made at room temperature. The intensities were measured with a take-off angle of 4°. 1965 independent reflections were observed and counted for ten seconds each using the stationary-crystal stationary-count technique. These are all of the data in a quarter of the sphere of reflection where $2\theta < 50^{\circ}$ or $\sin\theta/\lambda < 0.596$. Background was plotted as a function of 2θ and applied routinely to the reflections with the exception of a minority of intensities where they were measured individually because of streaking from lower orders. The most intense reflection (511) was about 2303 counts per second.

The absorption parameter μ was calculated to be $145 cm^{-1}$ for MoKα X-rays. An absorption correction using the program HORSE[5] was applied to the data, and resulted in substantial improvement of the final agreement.

The standard deviation of the intensities and the structure factors were estimated as follows. The standard deviation of the intensity, I, is $\sigma(I) = [C + B + (qI)^2]^{\frac{1}{2}}$, where C is total count,

B the background and q (taken here as 0.07) is an arbitrary fraction of the intensity which has been included to account for such non-random errors in the data as extinction, and the lack of stability of the electronic circuits of the instrument. The standard deviation of the structure factor, by the method of finite difference, is taken as $\sigma(F) = F_o - [F_o^2 - s\sigma(I)/Lp]^{\frac{1}{2}}$. s is the scaling factor in the equation $F_o = (sI/Lp)^{\frac{1}{2}}$. For the reflections where $I \leq \sigma(I)$, $\sigma(F) = [s\sigma(I)/Lp]^{\frac{1}{2}}$. Lp is the Lorentz-polarization correction.

Our unpublished full-matrix least-squares program minimizes the function R_2^2, where $R_2^2 = \Sigma \underline{w}(\Delta F)^2/\Sigma \underline{w}\underline{F}_o^2$. $\underline{F}_o$ and $\underline{F}_c$ are observed and calculated structure factors, and $\Delta \underline{F}$ is the difference of their magnitudes. The weighting factor $\underline{w}$ is $1/\sigma^2(F)$. The program accommodates both the real and imaginary parts of the dispersion correction.

Scattering factors for neutral gold, Na^+, neutral sulfur and oxygen[6] were used and modified for dispersion by adding -2.36, 0.0, 0.1 and 0.0 electrons[7] respectively. The imaginary dispersion terms were modified by adding 8.89, 0.04, 0.16 and 0.0 to gold, sodium, sulfur and oxygen respectively.

The anisotropic temperature factor has the form $\exp(-\underline{\beta}_{11}\underline{h}^2 - \underline{\beta}_{22}\underline{k}^2 - \underline{\beta}_{33}\underline{\ell}^2 - 2\underline{\beta}_{12}\underline{hk} - 2\underline{\beta}_{13}\underline{h\ell} - 2\underline{\beta}_{23}\underline{k\ell})$. $\underline{B}_{ij}$ values in Å^2 units are reported for the thermal parameters: $\underline{B}_{ij} = 4\underline{\beta}_{ij}/\underline{a}_i^*\underline{a}_j^*$, where $\underline{a}_i^*$ is the $\underline{i}$th reciprocal cell length.

Results

Unit Cell and Space Group. The space group is $P2_1/a$ (C_{2h}^5) and contains four formula units per monoclinic unit cell. The cell dimensions at 23° are a = 18.206 ± .006, b = 11.355 ± .006, c = 5.436 ± .004Å and β = 97.87 ± .05°. The errors are subjective estimates. The volume is 1113.19Å^3. With four formula units per unit cell, the density calculated from the X-ray data is 3.14 g/cc which is to be compared with the literature value of 3.09 g/cc.[8]

Determination of the Structure. The gold atom location was deduced from a three dimensional Patterson function. A Fourier phased by the gold atom revealed the locations of the sodium and sulfur atoms. A least square refinement of this partial structure using isotropic temperature factors resulted in $R = \Sigma||F_o| - |F_c||/\Sigma|F_o| = 0.21$. With anisotropic thermal parameters on the gold atom the R factor went to 0.19. A difference Fourier revealed the oxygen atom locations. Final full-matrix, all atoms anisotropic, refinement brought R to 0.078 after several cycles. After making the absorption correction the final agreement was R = 0.055.

The final results are shown in Tables I, II, and III. Table I lists the observed and calculated structure factors. The final positional parameters with their standard deviations are listed in Table II, where the standard deviations are estimated by the least squares procedure assuming that the discrepancies represent random errors. The anisotropic thermal parameters are listed in Table III.

Attempts at locating the hydrogen atoms were unsuccessful. The difference Fourier showed many more peaks than the four hydrogen atoms present in the structure. Attempts to refine four of the peaks that were near the water oxygen atoms resulted in positions that gave unacceptable hydrogen-oxygen bond distances. The data are apparently inadequate to detect the hydrogen atoms. This is not surprising considering the big absorption correction and the presence of such a heavy atom as gold.

Description of the Structure. The most significant structural feature in this compound is the $Au(S_2O_3)_2^{-3}$ anion. A schematic drawing is shown in Fig. 1. The S - Au - S angle is short of linearity by about 3.5°. The variation of the Au - S(3) and Au - S(4) bond distances are less than 3σ, Table IV, and is not considered to be significant. The Au - S - S bond angles are somewhat intermediate between a right and a tetrahedral angle, being somewhat closer to the latter. Each terminal sulfur atom has a tetrahedral configuration of a sulfur and three oxygen atoms and is consistent with thiosulfate in sodium thiosulfate pentahydrate.[9] The two S - S distances in the anion are different by 3 to 4σ from each other, but this difference is not considered by the authors to be significant. The average S - O bond distance of all six such bonds is 1.458Å, and no individual value is greater than one σ from this average.

The dihedral angle between the two planes defined by atoms Au - S(3) - S(2) and Au - S(4) - S(1) is 67° (see Fig. 4).

The three sodium ions are well encapsulated in irregular coordination spheres of oxygen atoms. Na(1) is coordinated by six oxygen atoms ranging in distances of 2.36 to 2.63Å. Two of these

oxygen atoms come from the two waters of hydration. Na(2) is also coordinated by six oxygen atoms at distances from 2.35 to 2.54Å only one of which comes from a water of hydration. Na(3) is coordinated to five oxygen atoms ranging in distance from 2.34 to 2.53Å, with one water of hydration involved.

Of the four hydrogen atoms only one appears to be involved in a "conventional" O - H.....O hydrogen bond within this sturcture; that would be the donor water oxygen O(8) to O(5) at a distance of 2.75Å.

Hydrogen bonding to sulfur is not particularly a well documented effect, and if it does exist must certainly be fairly weak. Bonds of this type have been suggested[10] in S - H.....S at 3.86Å and N - H.....S at 3.35Å. In this context water O(7) in this structure offers a possibility of O - H.....S hydrogen bonding. O(7) is centered in an irregular tetrahedron consisting of Na(1), Na(2), S(3), and S(4). The S(3) - O(7) - S(4) angle is approximately 104° and the O - S distances are 3.24 and 3.33Å respectively.

TABLE I

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR SODIUM GOLD(I) THIOSULFATE DIHYDRATE

FCA(0,0,0) = 1896

H FOB FCA	5 131 135	8 64 60	-14 115 126	-15 87 73	-11 310 313	13 280 269	13 115 99	9 144 140	5 119 119	3 97 104	-13 135 147	0 51 65	-8 141 150
K,L= 0, 0	6 35 41	9 72 69	-13 65 71	-14 30 33	-10 183 194	14 85 77	14 73 75	10 44 38	6 91 91	4 28 32	-12 0 5*	1 124 106	-7 0 10*
2 354 324	7 310 322	10 55 61	-12 154 166	-13 29 34	-9 186 185	15 156 156	15 40 38	11 56 52	7 23 24	5 115 126	-11 288 300	2 58 67	-6 183 197
4 113 113	8 64 65	11 328 318	-11 23 39	-12 144 135	-8 131 136	16 26 21	K,L= 9, 2	12 48 41	8 95 94	6 84 97	-10 0 11*	3 0 14*	-5 61 70
6 365 360	9 123 141	12 109 104	-10 23 35	-11 152 141	-7 48 41	17 38 46	-15 62 51	13 74 78	9 94 98	7 28 39	-9 105 105	4 40 28	-4 0 12*
8 225 210	10 22 11	13 205 201	-9 247 241	-10 92 84	-6 111 114	18 28 34	-14 100 98	14 0 9*	10 207 202	8 40 53	-8 96 89	5 90 98	-3 97 94
10 18 20	11 121 134	14 153 150	-8 142 139	-9 269 246	-5 365 375	K,L= 5, 2	-13 66 58	15 165 155	11 25 25	9 116 129	-7 94 89	6 0 4*	-2 78 76
12 524 491	12 33 22	15 23 3	-7 22 35	-8 151 138	-4 119 116	-19 29 39	-12 41 50	16 76 79	12 222 234	K,L= 11, 3	-6 70 72	7 71 68	-1 0 10*
14 414 387	13 279 291	16 152 149	-6 470 495	-7 144 169	-3 279 275	-18 29 43	-11 161 163	17 56 58	13 82 81	-8 173 163	-5 229 238	K,L= 10, 4	0 136 130
16 177 164	14 141 137	17 202 187	-5 77 80	-6 108 109	-2 123 128	-17 73 81	-10 28 12	K,L= 2, 3	14 38 51	-7 0 13*	-4 27 17	-7 90 85	1 27 30
18 25 40	15 150 159	18 78 64	-4 376 390	-5 26 9	-1 278 293	-16 94 106	-9 87 83	-20 99 91	15 91 93	-6 0 9*	-3 72 70	-6 110 102	2 93 101
20 149 137	16 26 32	19 85 80	-3 266 271	-4 130 120	0 192 190	-15 74 82	-8 201 194	-19 79 82	K,L= 6, 3	-5 31 30	-2 45 37	-5 139 134	3 71 83
K,L= 1, 0	17 0 10*	20 0 9*	-2 78 74	-3 125 115	1 230 226	-14 240 255	-7 81 80	-18 101 100	-17 67 61	-4 140 137	-1 35 18	-4 32 24	4 27 24
1 309 292	18 0 19*	K,L= 2, 1	-1 274 265	-2 50 41	2 159 146	-13 86 92	-6 107 99	-17 164 165	-16 0 14*	-3 86 88	0 34 22	-3 189 174	5 76 82
2 200 191	K,L= 8, 0	-21 103 100	0 166 158	-1 171 170	3 405 402	-12 138 142	-5 321 320	-16 0 7*	-15 76 82	-2 166 154	1 351 360	-2 89 87	6 195 189
3 74 73	0 373 368	-20 0 16*	1 156 145	0 97 81	4 188 181	-11 109 121	-4 59 62	-15 240 248	-14 102 116	-1 0 7*	2 73 73	-1 31 28	7 28 30
4 206 208	1 54 46	-19 187 186	2 242 236	1 24 16	5 354 344	-10 166 162	-3 132 115	-14 194 194	-13 0 7*	0 30 21	3 307 316	0 53 58	8 63 64
5 365 350	2 203 217	-18 89 91	3 162 165	2 230 240	6 194 191	-9 129 129	-2 134 125	-13 93 91	-12 210 203	1 0 12*	4 74 67	1 43 47	K,L= 6, 5
6 91 90	3 138 137	-17 171 184	4 98 100	3 243 231	7 308 307	-8 181 169	-1 99 92	-12 137 136	-11 136 128	2 125 107	5 135 137	2 60 57	-11 96 94
6 90 90	4 22 18	-16 174 186	5 221 218	4 58 54	8 72 75	-7 40 30	0 80 76	-11 138 130	-10 131 131	3 59 59	6 0 5*	3 104 114	-10 78 80
7 213 228	5 72 71	-15 23 28	6 245 249	5 206 219	9 238 230	-6 259 255	1 222 217	-10 83 83	-9 139 133	4 186 204	7 123 123	K,L= 0, 5	-9 63 71
8 246 253	6 227 235	-14 77 87	7 105 118	6 59 68	10 20 8	-5 22 25	2 138 144	-9 237 231	-8 123 123	5 0 13*	8 25 20	-14 0 11*	-8 64 70
9 382 381	7 86 84	-13 115 124	8 427 417	7 87 90	11 264 254	-4 0 10*	3 145 143	-8 68 64	-7 45 43	6 135 139	9 140 148	-12 167 152	-7 114 108
10 225 239	8 175 158	-12 123 128	9 121 118	8 155 163	12 154 147	-3 230 226	4 142 154	-7 20 18	-6 212 217	K,L= 0, 4	10 0 11*	-10 298 285	-6 70 76
11 170 171	9 52 49	-11 229 253	10 248 255	9 25 19	13 39 40	-2 258 252	5 96 104	-6 266 271	-5 57 56	-18 0 5*	11 79 72	-8 125 117	-5 94 95
12 123 123	10 0 11*	-10 300 302	11 170 166	10 67 76	14 24 26	-1 135 129	6 160 159	-5 246 247	-4 84 78	-16 182 158	12 27 27	-6 96 93	-4 160 159
13 284 283	11 0 10*	-9 18 14	12 39 37	11 181 191	15 150 141	0 490 503	7 127 134	-4 111 123	-3 137 123	-14 245 224	13 78 85	-4 184 184	-3 69 80
14 0 22*	12 185 182	-8 214 222	13 80 75	12 26 34	16 0 16*	1 54 64	8 51 60	-3 283 296	-2 34 25	-12 0 11*	K,L= 5, 4	-2 157 155	-2 168 168
15 176 179	13 72 61	-7 124 133	14 63 64	13 108 111	17 238 226	2 27 34	9 140 150	-2 134 134	-1 208 204	-10 281 265	-16 89 91	0 48 24	-1 41 45
16 114 116	14 206 219	-6 31 46	15 25 22	14 149 150	18 61 50	3 245 243	10 53 56	-1 295 305	0 252 238	-8 113 114	-15 29 32	2 239 245	0 64 63
17 59 53	15 76 57	-5 587 623	16 142 149	15 0 18*	19 0 12*	4 72 73	11 121 129	0 231 229	1 112 104	-6 261 250	-14 50 48	4 192 190	1 141 135
18 36 40	16 95 101	-4 185 198	17 26 32	K,L= 10, 1	K,L= 2, 2	5 78 79	12 39 37	1 27 21	2 208 200	-4 190 186	-13 80 82	6 127 122	2 74 78
19 74 76	17 0 9*	-3 109 114	18 27 17	-14 69 58	-21 153 148	6 233 232	13 0 6*	2 148 144	3 133 131	-2 169 172	-12 115 121	8 124 115	3 0 26*
20 0 12*	K,L= 9, 0	-2 207 210	19 84 86	-13 163 149	-20 97 93	7 20 12	K,L= 10, 2	3 56 54	4 85 83	0 302 294	-11 39 24	10 129 119	4 130 146
21 207 192	1 279 264	-1 122 123	K,L= 6, 1	-12 30 7	-19 66 75	8 198 202	-13 96 86	4 157 159	5 191 182	2 99 93	-10 185 178	K,L= 1, 5	5 56 67
K,L= 2, 0	2 138 141	0 449 441	-19 60 67	-11 162 149	-18 136 133	9 184 185	-12 67 59	5 188 183	6 142 145	4 61 57	-9 82 80	-15 105 104	6 0 13*
0 450 473	3 40 40	1 432 447	-18 107 116	-10 170 150	-17 56 52	10 50 58	-11 29 22	6 227 223	7 0 15*	6 338 327	-8 62 67	-14 62 60	7 99 105
1 170 174	4 132 136	2 240 223	-17 91 85	-9 28 33	-16 122 122	11 108 105	-10 132 130	7 41 37	8 224 226	8 118 106	-7 242 252	-13 27 30	K,L= 7, 5
2 15 26	5 208 216	3 155 144	-16 143 154	-8 104 94	-15 81 87	12 260 259	-9 148 138	8 174 169	9 24 21	10 86 90	-6 203 201	-12 70 68	-10 0 4*
3 339 333	6 74 79	4 396 375	-15 102 121	-7 188 177	-14 39 44	13 0 6*	-8 28 11	9 157 156	10 50 48	12 195 180	-5 62 58	-11 149 156	-9 161 151
4 176 176	7 217 236	5 25 25	-14 168 192	-6 0 5*	-13 109 116	14 133 134	-7 325 315	10 84 93	11 147 149	14 39 48	-4 226 231	-10 57 50	-8 0 8*
5 358 339	8 99 104	6 65 66	-13 133 146	-5 221 204	-12 125 127	15 68 78	-6 28 14	11 269 261	12 58 61	K,L= 1, 4	-3 48 57	-9 107 112	-7 56 59
6 492 473	9 138 138	7 253 246	-12 25 28	-4 148 135	-11 29 28	16 38 41	-5 89 82	12 137 136	13 27 38	-18 49 42	-2 121 115	-8 86 81	-6 46 18
7 88 94	10 132 142	8 125 124	-11 169 158	-3 115 106	-10 224 228	17 78 82	-4 79 73	13 102 99	14 187 180	-17 72 70	-1 105 102	-7 0 5*	-5 97 99
8 299 297	11 67 76	9 224 220	-10 115 106	-2 96 89	-9 259 264	K,L= 6, 2	-3 96 88	14 76 79	15 0 24*	-16 27 14	0 99 99	-6 95 99	-4 55 56
9 100 103	12 107 112	10 165 155	-9 41 38	-1 112 101	-8 135 132	-18 136 150	-2 55 48	15 26 29	K,L= 7, 3	-15 284 273	1 80 83	-5 172 176	-3 166 158
10 130 128	13 161 147	11 28 28	-8 242 239	0 173 158	-7 387 385	-17 0 10*	-1 118 118	16 130 124	-16 53 60	-14 44 51	2 194 198	-4 25 23	-2 0 5*
11 241 241	14 81 97	12 254 256	-7 72 66	1 291 273	-6 378 375	-16 110 116	0 27 14	17 97 92	-15 110 126	-13 116 119	3 110 116	-3 203 205	-1 42 38
12 136 144	15 130 131	13 143 138	-6 155 155	2 51 54	-5 321 318	-15 143 165	1 138 132	K,L= 3, 3	-14 30 29	-12 87 91	4 128 129	-2 46 54	0 29 45
13 90 92	K,L= 10, 0	14 100 104	-5 296 296	3 154 160	-4 289 302	-14 27 41	2 140 133	-19 28 23	-13 201 188	-11 71 75	5 136 141	-1 139 143	1 71 70
14 131 136	0 197 171	15 203 199	-4 206 211	4 124 132	-3 59 57	-13 127 144	3 64 66	-18 91 86	-12 29 15	-10 89 95	6 121 130	0 133 133	2 0 7*
15 22 21	1 124 114	16 108 113	-3 30 24	5 51 60	-2 114 121	-12 196 196	4 156 156	-17 0 6*	-11 164 154	-9 188 195	7 93 93	1 132 131	3 135 147
16 57 61	2 80 77	17 87 91	-2 327 328	6 114 125	-1 323 319	-11 44 41	5 185 203	-16 169 176	-10 175 168	-8 44 38	8 110 119	2 68 73	4 41 41
17 196 201	3 269 296	18 132 125	-1 125 121	7 134 118	0 32 23	-10 205 200	6 0 12*	-15 105 108	-9 28 25	-7 167 165	9 0 6*	3 114 107	5 145 151
18 107 102	4 50 57	19 54 57	0 135 129	8 37 39	1 242 234	-9 199 201	7 227 209	-14 82 83	-8 61 63	-6 43 50	10 179 179	4 0 14*	K,L= 8, 5
19 74 73	5 86 101	20 84 74	1 252 243	9 160 176	2 320 309	-8 34 35	8 38 35	-13 84 84	-7 225 217	-5 121 131	11 27 37	5 108 111	-7 56 50
20 125 125	6 50 46	K,L= 3, 1	2 62 64	10 54 51	3 61 62	-7 94 92	9 27 25	-12 78 71	-6 46 36	-4 75 82	12 28 36	6 80 79	-6 32 34
21 49 38	7 0 10*	-21 51 46	3 192 187	11 27 34	4 197 201	-6 267 263	10 48 63	-11 114 110	-5 213 203	-3 307 304	13 113 107	7 0 17*	-5 0 11*
K,L= 3, 0	8 26 28	-20 120 124	4 252 248	12 92 101	5 170 167	-5 125 118	11 28 38	-10 299 299	-4 84 88	-2 23 21	K,L= 6, 4	8 46 46	-4 133 137
1 264 271	9 177 195	-19 86 94	5 58 66	13 109 107	6 30 33	-4 371 374	K,L= 11, 2	-9 31 22	-3 26 22	-1 351 381	-15 53 45	9 114 107	-3 111 115
2 331 333	10 53 34	-18 154 164	6 203 217	K,L= 11, 1	7 424 411	-3 89 87	-11 31 34	-8 166 167	-2 51 53	0 55 53	-14 109 121	10 0 20*	-2 122 116
3 92 80	11 173 191	-17 77 85	7 219 211	-12 251 212	8 243 231	-2 226 223	-10 43 38	-7 43 37	-1 223 217	1 102 98	-13 30 32	11 201 196	-1 31 31
4 569 565	12 133 141	-16 49 61	8 41 37	-11 43 41	9 220 213	-1 299 293	-9 30 20	-6 71 70	0 60 49	2 156 149	-12 42 33	K,L= 2, 5	0 0 5*
5 148 138	13 39 42	-15 109 110	9 166 175	-10 186 163	10 228 221	0 140 132	-8 215 204	-5 110 111	1 314 296	3 64 57	-11 150 146	-15 143 149	1 30 20
6 192 185	14 90 91	-14 223 249	10 175 179	-9 0 10*	11 112 113	1 68 69	-7 0 23*	-4 211 225	2 130 141	4 30 22	-10 129 119	-14 40 46	2 127 146
7 108 107	K,L= 11, 0	-13 96 104	11 23 16	-8 41 35	12 126 124	2 206 204	-6 168 158	-3 126 130	3 180 187	5 200 198	-9 40 31	-13 119 119	K,L= 0, 6
8 299 321	1 61 58	-12 304 338	12 169 184	-7 29 22	13 228 217	3 132 129	-5 88 90	-2 380 389	4 0 19*	6 22 31	-8 197 199	-12 38 47	-10 122 106
9 70 75	2 203 198	-11 29 33	13 89 88	-6 165 154	14 24 13	4 120 117	-4 41 35	-1 114 121	5 127 125	7 164 163	-7 69 65	-11 112 116	-8 78 78
10 450 468	3 93 88	-10 63 73	14 134 133	-5 29 20	15 112 109	5 118 122	-3 41 30	0 225 225	6 24 29	8 33 40	-6 40 25	-10 152 158	-6 94 77
11 58 55	4 160 174	-9 93 87	15 125 122	-4 140 132	16 152 153	6 0 11*	-2 173 169	1 151 149	7 143 148	9 24 9	-5 131 125	-9 58 63	-4 150 152
12 156 146	5 27 25	-8 152 162	16 102 103	-3 0 5*	17 64 64	7 136 149	-1 0 1*	2 322 327	8 56 53	10 49 43	-4 0 9*	-8 36 46	-2 38 42
13 138 138	6 71 73	-7 56 57	17 90 93	-2 63 58	18 27 29	8 235 239	0 177 172	3 131 123	9 129 134	11 243 230	-3 0 16*	-7 62 59	0 142 135
14 73 75	7 27 22	-6 384 392	18 152 156	-1 48 47	19 119 110	9 50 58	1 28 30	4 323 324	10 0 16*	12 37 23	-2 224 219	-6 26 28	2 185 176
15 88 88	8 81 92	-5 205 209	K,L= 7, 1	0 230 226	K,L= 3, 2	10 273 284	2 126 115	5 96 93	11 0 24*	13 117 120	-1 52 47	-5 88 87	4 39 44
16 256 267	9 47 56	-4 338 348	-18 0 13*	1 27 8	-20 149 149	11 146 156	3 0 4*	6 188 185	12 38 34	14 39 43	0 123 124	-4 169 178	K,L= 1, 6
17 35 27	10 215 187	-3 130 128	-17 142 154	2 315 286	-19 0 24*	12 142 148	4 112 120	7 76 63	13 135 138	K,L= 2, 4	1 166 162	-3 78 76	-10 80 80
18 163 168	11 28 27	-2 23 19	-16 0 4*	3 38 29	-18 89 74	13 79 81	5 28 25	8 22 13	14 57 61	-18 0 20*	2 66 72	-2 151 164	-9 0 8*
19 0 9*	12 146 153	-1 376 373	-15 228 244	4 108 129	-17 37 46	14 26 33	6 186 206	9 22 12	K,L= 8, 3	-17 144 139	3 75 80	-1 89 93	-8 88 88
20 0 14*	K,L= 12, 0	0 455 459	-14 126 117	5 27 17	-16 195 204	15 27 36	7 40 45	10 197 189	-15 0 19*	-16 118 127	4 142 142	0 0 19*	-7 83 90
K,L= 4, 0	0 145 128	1 68 66	-13 110 98	6 72 81	-15 100 96	16 91 85	8 137 134	11 115 117	-14 147 133	-15 26 31	5 25 37	1 196 203	-6 68 69
0 135 129	1 115 105	2 391 403	-12 85 74	7 55 57	-14 335 319	17 40 36	9 0 18*	12 238 229	-13 43 31	-14 129 119	6 146 149	2 124 122	-5 130 136
1 282 283	2 118 113	3 20 31	-11 138 132	8 135 140	-13 32 36	K,L= 7, 2	K,L= 12, 2	13 61 54	-12 205 189	-13 67 68	7 81 90	3 69 65	-4 28 15
2 363 363	3 183 204	4 305 303	-10 102 95	9 48 53	-12 137 143	-18 31 33	-8 53 48	14 0 17*	-11 66 61	-12 0 7*	8 78 84	4 86 95	-3 0 15*
3 422 419	4 40 44	5 161 156	-9 307 296	10 69 64	-11 202 198	-17 140 154	-7 165 155	15 130 124	-10 0 23*	-11 202 196	9 0 23*	5 71 68	-2 30 33
4 46 40	5 114 127	6 192 190	-8 120 117	11 29 31	-10 167 169	-16 30 21	-6 0 11*	16 109 116	-9 114 101	-10 132 130	10 77 78	6 26 33	-1 0 20*
5 436 428	6 0 17*	7 127 115	-7 157 155	K,L= 12, 1	-9 98 104	-15 51 56	-5 53 57	17 49 53	-8 157 152	-9 40 35	11 83 93	7 100 101	0 0 8*
6 139 130	7 0 8*	8 465 463	-6 24 23	-9 0 2*	-8 270 281	-14 29 16	-4 61 49	K,L= 4, 3	-7 125 116	-8 119 122	12 113 119	8 37 39	1 197 201
7 87 94	8 0 13*	9 0 6*	-5 115 105	-8 105 96	-7 70 66	-13 178 167	-3 92 89	-19 29 32	-6 292 277	-7 185 189	K,L= 7, 4	9 0 14*	2 39 32
8 35 44	9 164 171	10 298 290	-4 23 11	-7 213 196	-6 339 341	-12 27 26	-2 43 42	-18 0 5*	-5 0 1*	-6 172 174	-14 32 35	10 135 127	3 72 76
9 258 269	K,L= 13, 0	11 106 106	-3 391 394	-6 52 51	-5 101 101	-11 254 247	-1 183 176	-17 117 122	-4 154 156	-5 281 288	-13 109 99	K,L= 3, 5	4 39 39
10 130 124	1 102 86	12 149 138	-2 49 50	-5 170 165	-4 103 95	-10 91 89	0 79 77	-16 27 33	-3 47 36	-4 138 143	-12 44 41	-15 41 39	5 28 14
11 245 257	2 114 107	13 152 146	-1 343 342	-4 0 6*	-3 130 130	-9 218 211	1 130 132	-15 136 141	-2 66 59	-3 211 226	-11 74 75	-14 118 124	K,L= 2, 6
12 36 34	3 0 15*	14 150 152	0 305 298	-3 100 103	-2 282 286	-8 0 12*	2 79 87	-14 26 27	-1 155 150	-2 141 142	-10 84 85	-13 28 37	-10 41 50
13 116 120	4 136 148	15 33 36	1 143 124	-2 112 98	-1 138 131	-7 25 33	3 30 32	-13 36 39	0 233 224	-1 100 108	-9 171 166	-12 133 131	-9 95 95
14 105 107	5 91 115	16 221 217	2 20 26	-1 51 47	0 430 441	-6 155 150	4 30 49	-12 78 79	1 25 23	0 158 158	-8 41 43	-11 99 93	-8 64 64
15 125 122	K,L= 0, 1	17 72 72	3 223 222	0 41 24	1 53 53	-5 251 239	5 157 149	-11 327 322	2 168 175	1 165 165	-7 240 242	-10 0 20*	-7 76 74
16 64 64	-20 47 40	18 52 51	4 139 147	1 178 163	2 62 58	-4 25 16	6 84 89	-10 24 12	3 83 79	2 0 1*	-6 50 59	-9 54 60	-6 64 72
17 257 247	-18 71 60	19 27 29	5 342 346	2 29 8	3 198 193	-3 243 237	K,L= 0, 3	-9 355 371	4 0 5*	3 183 181	-5 91 86	-8 159 166	-5 0 11*
18 26 18	-16 329 293	20 101 97	6 21 5	3 126 146	4 251 240	-2 33 11	-20 166 144	-8 23 18	5 75 74	4 79 72	-4 0 24*	-7 54 53	-4 89 91
19 147 140	-14 71 69	K,L= 4, 1	7 162 161	4 50 51	5 80 83	-1 82 78	-18 185 153	-7 148 139	6 170 177	5 31 25	-3 116 114	-6 246 250	-3 144 155
20 0 16*	-12 85 82	-20 29 26	8 54 57	5 41 38	6 414 404	0 83 78	-16 25 15	-6 33 28	7 89 96	6 241 242	-2 0 16*	-5 0 18*	-2 0 26*
K,L= 5, 0	-10 408 390	-19 126 142	9 134 147	6 41 47	7 109 110	1 237 233	-14 194 176	-5 101 91	8 218 227	7 257 260	-1 198 198	-4 59 53	-1 101 105
1 17 43	-8 420 396	-18 27 30	10 23 16	7 136 165	8 99 92	2 62 56	-12 246 227	-4 68 64	9 65 65	8 24 20	0 38 24	-3 30 20	0 78 76
2 226 231	-6 221 202	-17 151 170	11 250 269	8 0 13*	9 0 16*	3 351 362	-10 136 131	-3 222 216	10 81 86	9 202 208	1 65 61	-2 139 143	1 28 38
3 47 41	-4 383 358	-16 0 10*	12 137 143	K,L= 13, 1	10 110 112	4 49 43	-8 184 177	-2 57 51	11 48 50	10 50 45	2 131 145	-1 83 86	2 134 124
4 393 425	-2 447 429	-15 129 130	13 134 141	-5 0 5*	11 53 53	5 141 145	-6 485 480	-1 192 192	12 63 73	11 178 170	3 108 112	0 204 202	3 93 89
5 38 22	0 428 423	-14 42 48	14 26 22	-4 167 152	12 238 238	6 125 126	-4 197 199	0 30 17	K,L= 9, 3	12 133 135	4 53 55	1 150 151	4 0 14*
6 129 143	2 263 252	-13 279 298	15 0 7*	-3 139 126	13 40 36	7 94 96	-2 105 101	1 129 124	-13 82 74	13 38 41	5 176 182	2 114 110	K,L= 3, 6
7 247 285	4 410 402	-12 39 55	16 104 101	-2 0 11*	14 127 130	8 87 92	0 134 130	2 20 11	-12 61 47	14 39 46	6 46 49	3 51 47	-9 42 33
8 126 129	6 350 345	-11 271 307	17 132 132	-1 70 73	15 61 57	9 213 226	2 317 317	3 340 340	-11 74 72	K,L= 3, 4	7 148 159	4 0 7*	-8 115 129
9 0 14*	8 24 21	-10 37 47	K,L= 8, 1	0 62 69	16 36 38	10 103 111	4 110 113	4 29 17	-10 42 37	-17 29 32	8 27 39	5 77 75	-7 67 56
10 272 284	10 196 179	-9 94 98	-17 44 40	1 31 13	17 109 100	11 113 128	6 346 347	5 278 283	-9 78 66	-16 68 71	9 0 13*	6 194 195	-6 67 77
11 21 20	12 430 399	-8 28 35	-16 164 150	2 111 104	18 106 109	12 108 114	8 268 259	6 67 68	-8 137 126	-15 27 29	10 28 32	7 37 33	-5 54 52
12 75 81	14 163 145	-7 203 200	-15 0 16*	3 53 74	K,L= 4, 2	13 0 21*	10 165 163	7 108 110	-7 185 174	-14 75 75	K,L= 8, 4	8 131 130	-4 98 108
13 118 116	16 156 136	-6 19 30	-14 148 141	4 31 40	-20 0 6*	14 0 17*	12 227 209	8 89 94	-6 29 6	-13 69 67	-12 71 60	9 0 10*	-3 49 50
14 23 6	18 275 248	-5 473 519	-13 80 74	K,L= 0, 2	-19 29 38	15 157 163	14 155 143	9 75 67	-5 240 223	-12 165 159	-11 54 36	10 48 49	-2 74 87
15 79 84	20 134 111	-4 26 25	-12 28 27	-20 128 105	-18 0 11*	16 40 45	16 222 192	10 23 20	-4 115 112	-11 100 103	-10 97 98	K,L= 4, 5	-1 44 42
16 229 222	K,L= 1, 1	-3 278 279	-11 86 82	-18 214 183	-17 65 68	K,L= 8, 2	K,L= 1, 3	11 259 262	-3 57 49	-10 215 219	-9 68 67	-14 0 13*	0 103 97
17 26 1	-21 177 175	-2 131 132	-10 278 253	-16 198 170	-16 0 10*	-16 127 118	-20 0 3*	12 25 19	-2 226 221	-9 140 138	-8 177 170	-13 88 85	1 41 50
18 174 163	-20 27 30	-1 388 394	-9 186 178	-14 157 151	-15 264 286	-15 0 13*	-19 190 181	13 51 52	-1 72 60	-8 24 6	-7 30 21	-12 41 41	2 0 6*
19 95 90	-19 0 10*	0 32 33	-8 304 279	-12 247 223	-14 0 3*	-14 29 23	-18 46 41	14 64 70	0 38 35	-7 120 134	-6 125 121	-11 40 46	3 0 18*
K,L= 6, 0	-18 44 40	1 373 401	-7 138 135	-10 506 492	-13 262 259	-13 91 83	-17 109 104	15 66 77	1 117 111	-6 172 173	-5 0 11*	-10 28 22	K,L= 4, 6
0 184 183	-17 122 123	2 44 39	-6 106 97	-8 112 109	-12 83 85	-12 146 138	-16 86 94	16 28 22	2 0 17*	-5 105 99	-4 89 95	-9 106 113	-7 106 113
1 104 92	-16 41 48	3 207 211	-5 49 44	-6 452 433	-11 134 128	-11 91 88	-15 203 199	K,L= 5, 3	3 46 42	-4 214 223	-3 51 52	-8 110 105	-6 0 15*
2 218 215	-15 191 208	4 63 59	-4 144 142	-4 538 536	-10 93 93	-10 290 272	-14 23 21	-18 66 71	4 147 154	-3 27 14	-2 198 195	-7 210 218	-5 0 17*
3 219 220	-14 177 193	5 17 7	-3 93 85	-2 35 36	-9 200 213	-9 38 42	-13 156 161	-17 0 9*	5 75 79	-2 59 60	-1 94 95	-6 0 7*	-4 34 27
4 387 414	-13 148 165	6 30 30	-2 326 322	0 256 249	-8 52 56	-8 58 60	-12 22 20	-16 170 177	6 60 74	-1 34 14	0 202 191	-5 159 169	-3 146 145
5 302 318	-12 158 176	7 404 405	-1 86 83	2 563 574	-7 251 247	-7 82 74	-11 148 150	-15 77 76	7 207 229	0 131 127	1 48 42	-4 53 45	-2 0 15*
6 385 398	-11 285 317	8 18 21	0 202 201	4 467 476	-6 21 18	-6 126 117	-10 127 127	-14 93 92	8 27 35	1 71 68	2 28 17	-3 0 5*	-1 124 127
7 158 153	-10 171 199	9 332 320	1 86 85	6 17 7	-5 174 177	-5 51 49	-9 120 121	-13 171 174	9 130 136	2 235 238	3 150 149	-2 0 23*	0 0 2*
8 388 370	-9 441 472	10 28 6	2 131 144	8 141 139	-4 126 121	-4 295 296	-8 56 56	-12 58 66	10 115 119	3 78 70	4 122 132	-1 84 82	1 0 9*
9 183 176	-8 0 8*	11 72 75	3 80 83	10 236 230	-3 309 321	-3 79 66	-7 296 300	-11 68 72	11 29 36	4 124 125	5 47 59	0 0 11*	2 0 15*
10 120 124	-7 352 353	12 71 68	4 259 264	12 38 34	-2 53 43	-2 152 143	-6 141 131	-10 245 246	K,L= 10, 3	5 89 99	6 182 185	1 163 169	K,L= 5, 6
11 176 188	-6 128 125	13 174 172	5 128 135	14 192 170	-1 519 546	-1 105 100	-5 433 439	-9 25 21	-11 54 56	6 69 67	7 28 44	2 52 41	-3 48 53
12 81 87	-5 168 166	14 0 8*	6 283 281	16 344 310	0 212 205	0 79 74	-4 176 177	-8 155 153	-10 0 2*	7 120 114	8 56 61	3 0 18*	-2 122 123
13 23 21	-4 116 107	15 215 215	7 32 15	18 154 131	1 287 291	1 124 113	-3 19 8	-7 100 101	-9 149 129	8 96 98	9 81 75	4 52 45	
14 125 131	-3 251 242	16 0 19*	8 0 5*	K,L= 1, 2	2 53 52	2 229 241	-2 58 65	-6 35 26	-8 67 51	9 43 42	K,L= 9, 4	5 144 135	
15 43 56	-2 122 117	17 131 129	9 24 12	-21 29 7	3 109 106	3 84 75	-1 205 213	-5 131 128	-7 52 54	10 149 145	-10 45 42	6 27 25	
16 26 27	-1 468 533	18 38 40	10 123 128	-20 68 64	4 36 38	4 314 325	0 74 71	-4 253 251	-6 149 131	11 58 51	-9 76 77	7 207 213	
17 163 166	0 353 356	19 62 49	11 25 30	-19 171 170	5 270 276	5 23 22	1 389 391	-3 24 22	-5 111 118	12 53 52	-8 44 49	8 27 22	
18 119 120	1 49 51	K,L= 5, 1	12 223 237	-18 26 45	6 27 33	6 24 20	2 167 167	-2 325 324	-4 30 21	13 38 35	-7 53 58	9 68 65	
19 28 39	2 345 325	-20 141 137	13 58 53	-17 247 259	7 291 279	7 34 36	3 48 52	-1 220 226	-3 209 204	14 97 93	-6 106 103	K,L= 5, 5	
K,L= 7, 0	3 377 368	-19 41 33	14 75 82	-16 76 80	8 28 23	8 124 131	4 233 229	0 197 190	-2 50 58	K,L= 4, 4	-5 43 40	-13 0 16*	
1 398 386	4 404 387	-18 194 208	15 77 76	-15 56 53	9 163 157	9 25 36	5 79 77	1 215 214	-1 131 131	-17 110 105	-4 137 135	-12 90 100	
2 0 11*	5 664 679	-17 82 96	16 88 82	-14 121 128	10 0 5*	10 182 203	6 158 152	2 158 154	0 130 127	-16 0 9*	-3 185 178	-11 60 60	
3 34 52	6 141 119	-16 80 91	K,L= 9, 1	-13 30 35	11 251 239	11 0 18*	7 430 437	3 144 143	1 40 29	-15 0 3*	-2 67 65	-10 0 2*	
4 53 56	7 145 140	-15 166 185	-16 31 23	-12 94 98	12 46 54	12 70 76	8 21 26	4 200 206	2 69 62	-14 28 16	-1 162 155	-9 100 96	

*Zero weighted state

TABLE II

POSITIONAL PARAMETERS[a]

ATOM	X	Y	Z
AU	.07361(3)	.06692(5)	.1479(1)
S(1)	.0006(2)	.3396(3)	.2178(5)
S(2)	.2592(2)	.0358(3)	.1207(5)
S(3)	.1591(2)	-.0366(3)	-.0338(6)
S(4)	-.0063(2)	.1713(3)	.3497(6)
NA(1)	.2176(3)	.3252(5)	.3495(10)
NA(2)	.1254(3)	-.4095(4)	.3159(9)
NA(3)	.4129(3)	-.1027(5)	.2427(10)
O(1)	.0762(5)	.3809(8)	.2892(17)
O(2)	-.0521(5)	.4044(8)	.3419(16)
O(3)	-.0179(5)	.3425(10)	-.0505(15)
O(4)	.3108(5)	-.0169(9)	-.0319(16)
O(5)	.2543(5)	.1633(8)	.0916(16)
O(6)	.2783(5)	.0010(8)	.3803(15)
O(7)	.1652(5)	-.2179(9)	.4284(19)
O(8)	.3387(5)	-.2627(8)	.3212(17)

[a]Standard deviations appear in parenthesis.

TABLE III

ANISOTROPIC THERMAL PARAMETERS[a]

ATOM	B11	B22	B33	B12	B13	B23
AU	2.02(2)	1.84(3)	2.58(3)	.18(2)	.31(2)	-.23(2)
S(1)	1.82(12)	1.71(12)	1.41(11)	.02(10)	.15(9)	.03(10)
S(2)	1.99(12)	1.73(12)	1.05(11)	.03(10)	.14(9)	.04(9)
S(3)	2.10(13)	2.15(14)	2.03(13)	.38(11)	.11(10)	-.52(11)
S(4)	2.57(14)	1.88(14)	3.01(15)	.19(11)	.93(11)	.02(12)
NA(1)	4.33(28)	2.62(25)	2.47(22)	1.05(21)	.19(19)	.35(19)
NA(2)	2.70(22)	2.13(22)	1.97(20)	.07(17)	.19(17)	-.09(17)
NA(3)	2.65(23)	2.90(24)	2.57(23)	-.25(19)	.30(18)	-.22(19)
O(1)	2.13(38)	2.48(41)	3.12(43)	-.45(31)	-.17(31)	.44(34)
O(2)	2.53(38)	2.29(39)	2.71(40)	.41(31)	.98(31)	-.10(31)
O(3)	2.95(42)	4.46(52)	1.56(36)	.02(39)	-.64(30)	-.19(35)
O(4)	2.66(40)	3.00(42)	2.03(37)	.67(34)	.31(30)	-.30(33)
O(5)	3.12(41)	1.95(37)	2.15(35)	-.52(32)	-.47(30)	.40(31)
O(6)	3.20(40)	1.92(39)	1.52(34)	.08(31)	-.21(29)	.07(29)
O(7)	2.51(40)	3.25(46)	3.91(46)	-.01(35)	.85(35)	.31(39)
O(8)	4.30(50)	2.09(40)	2.40(39)	-.34(35)	-.05(35)	-.43(32)

[a]Standard deviations appear in parenthesis.

TABLE IV

INTERATOMIC DISTANCES (Å) IN SODIUM GOLD THIOSULFATE DIHYDRATE[a,b]

Atoms	Dist.	Atoms	Dist.	Atoms	Dist.
Au -S(3)	2.280(3)	S(4) -O(1)	2.858(10)	Na(2)-O(4)	2.390(11)
Au -S(4)	2.272(3)	S(4) -O(2)	2.774(10)	Na(2)-O(6)	2.459(10)
S(1)-O(1)	1.457(9)	S(4) -O(3)	2.904(10)	Na(2)-O(7)	2.348(11)
S(1)-O(2)	1.458(9)	Na(1)-O(1)	2.626(10)	Na(3)-O(1)	2.532(11)
S(1)-O(3)	1.451(9)	Na(1)-O(4)	2.494(11)	Na(3)-O(2)	2.381(11)
S(1)-S(4)	2.051(5)	Na(1)-O(5)	2.460(11)	Na(3)-O(3)	2.383(11)
S(2)-O(4)	1.463(9)	Na(1)-O(6)	2.473(10)	Na(3)-O(4)	2.423(10)
S(2)-O(5)	1.458(9)	Na(1)-O(7)	2.355(11)	Na(3)-O(8)	2.338(11)
S(2)-O(6)	1.461(9)	Na(1)-O(8)	2.399(11)	O(1) -O(4)	2.885(12)
S(2)-S(3)	2.069(5)	Na(2)-O(1)	2.540(10)	O(1) -O(8)	2.940(12)
S(3)-O(4)	2.770(10)	Na(2)-O(2)	2.433(10)	O(2) -O(8)	2.940(12)
S(3)-O(5)	2.881(9)	Na(2)-O(3)	2.392(10)	O(5) -O(8)	2.751(12)
S(3)-O(6)	2.936(9)				

[a]Table contains all interatomic distances 3.00Å or less.

[b]Estimated standard deviations are indicated in parentheses.

TABLE V

SELECTED ANGLES IN SODIUM GOLD THIOSULFATE DIHYDRATE[a]

S(3) - Au -S(4)	176.5(2)	O(2)-Na(2)-O(3)	88.0(4)
O(1) -S(1)-O(2)	112.0(7)	O(2)-Na(2)-O(4)	150.7(5)
O(1) -S(1)-O(3)	109.9(7)	O(3)-Na(2)-O(6)	170.6(5)
O(2) -S(1)-O(3)	112.3(7)	O(4)-Na(2)-O(6)	81.8(4)
O(4) -S(2)-O(5)	112.2(7)	O(4)-Na(2)-O(7)	118.8(5)
O(4) -S(2)-O(6)	110.5(7)	O(6)-Na(2)-O(7)	92.4(4)
O(5) -S(2)-O(6)	112.1(7)	O(1)-Na(3)-O(2)	82.0(4)
Au -S(3)-S(2)	103.6(1)	O(1)-Na(3)-O(3)	117.7(4)
Au -S(4)-S(1)	104.1(1)	O(1)-Na(3)-O(4)	126.6(5)
O(1)-Na(1)-O(4)	68.5(3)	O(1)-Na(3)-O(8)	74.1(4)
O(1)-Na(1)-O(5)	116.6(4)	O(2)-Na(3)-O(8)	146.8(5)
O(1)-Na(1)-O(6)	80.2(4)	O(3)-Na(3)-O(8)	113.3(5)
O(1)-Na(1)-O(7)	156.6(5)	S(3)- O(7)-S(4)	103.9(2)
O(1)-Na(1)-O(8)	71.5(4)	S(3)- O(7)-Na(1)	101.4(3)
O(4)-Na(1)-O(6)	79.5(4)	S(3)- O(7)-Na(2)	114.2(3)
O(5)-Na(1)-O(7)	80.7(4)	S(4)- O(7)-Na(1)	123.6(3)
O(5)-Na(1)-O(8)	107.0(4)	S(4)- O(7)-Na(2)	89.4(2)
O(7)-Na(1)-O(8)	88.9(4)	Na(1)-O(7)-Na(2)	123.5(4)
O(1)-Na(2)-O(2)	80.8(4)	Na(1)-O(8)-Na(3)	97.4(3)
O(1)-Na(2)-O(3)	90.6(4)	Na(1)-O(8)-O(5)	117.2(4)
O(1)-Na(2)-O(7)	167.7(5)	Na(3)-O(8)-O(5)	113.2(4)

[a]Standard deviation is in parentheses and refers to the least significant digit.

References

(1) Research performed under the auspices of the U. S. Atomic Energy Commission.

(2) M. O. Faltens, Mossbauer Resonance Studies of Gold Compounds, PhD Thesis, UCRL 18706.

(3) Gold sodium thiosulfate, long known clinically as Sanocrycin, has been and is presently being used in some medical circles for the treatment of illnesses including arthritis, tuberculosis and leprosy.

(4) H. Brown, J. Am. Chem. Soc. 49 (1927) 958.

(5) Walter C. Hamilton, private communication.

(6) D. T. Cromer and J. T. Waber, Acta Cryst. 18, 104 (1965)

(7) D. T. Cromer, Acta Cryst. 18, 17 (1965)

(8) Handbook of Chem. And Phys., 45th ed., R. C. Weast, Ed., The Chemical Rubber Co.. Cleveland, Ohio, B225.

(9) P. G. Taylor, C. A. Beevers, Acta Cryst. 5, 341 (1952)

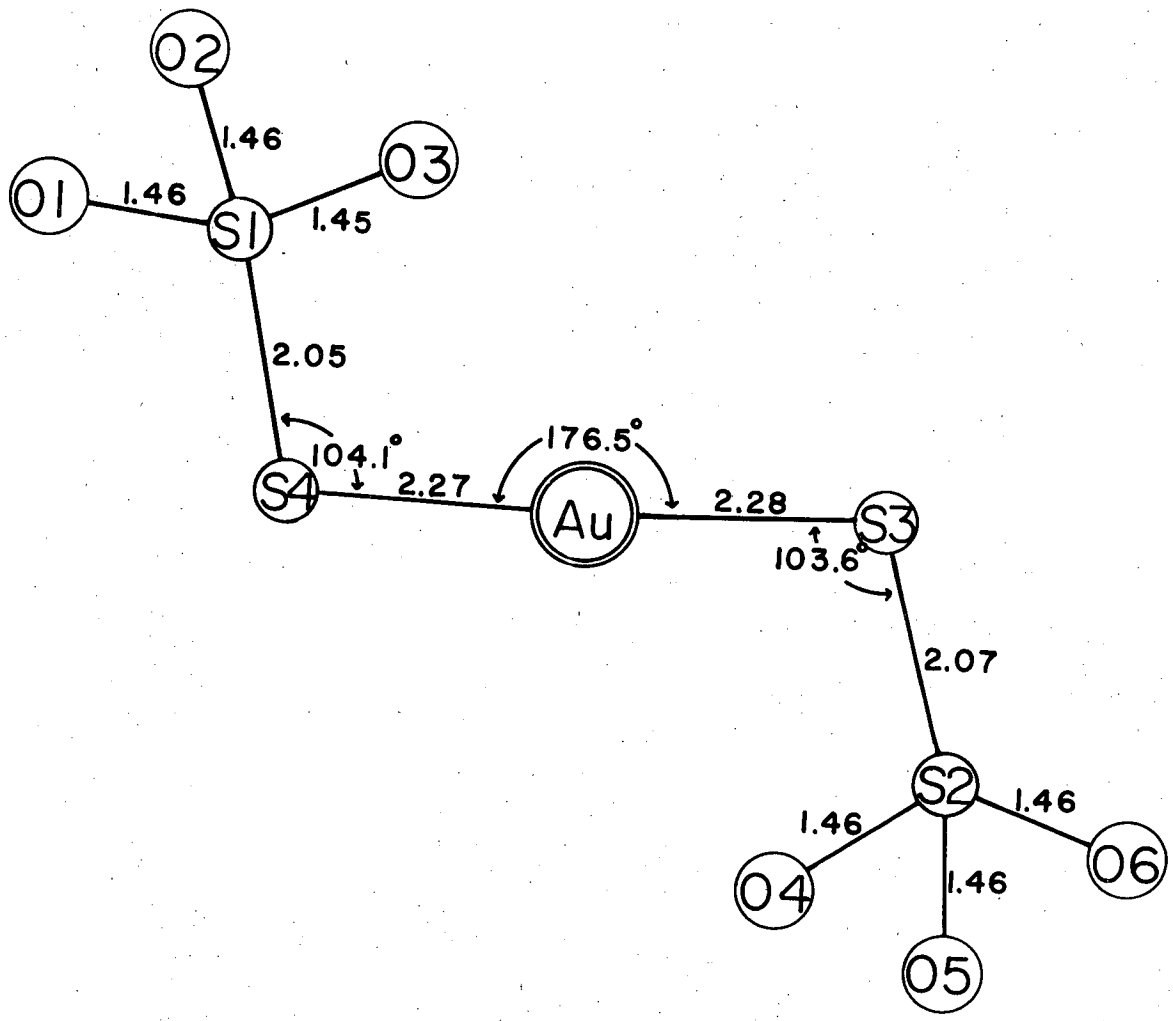
(10) "Hydrogen Bonding in Solids", W. C. Hamilton and J. A. Ibers, W. A. Benjamin Inc., New York, 1968, p167.

Figure Captions

Fig. 1 Schematic drawing of $Au(S_2O_3)_2^{-3}$ anion.

Fig. 2 Molecular packing in the unit cell of Sodium Gold(I) Thiosulfate Dihydrate.

Fig. 3 Stereo view of Sodium Gold(I) Thiosulfate Dihydrate showing examples of the bonding of the sodium atoms.



XBL 707-1307

Fig. 1

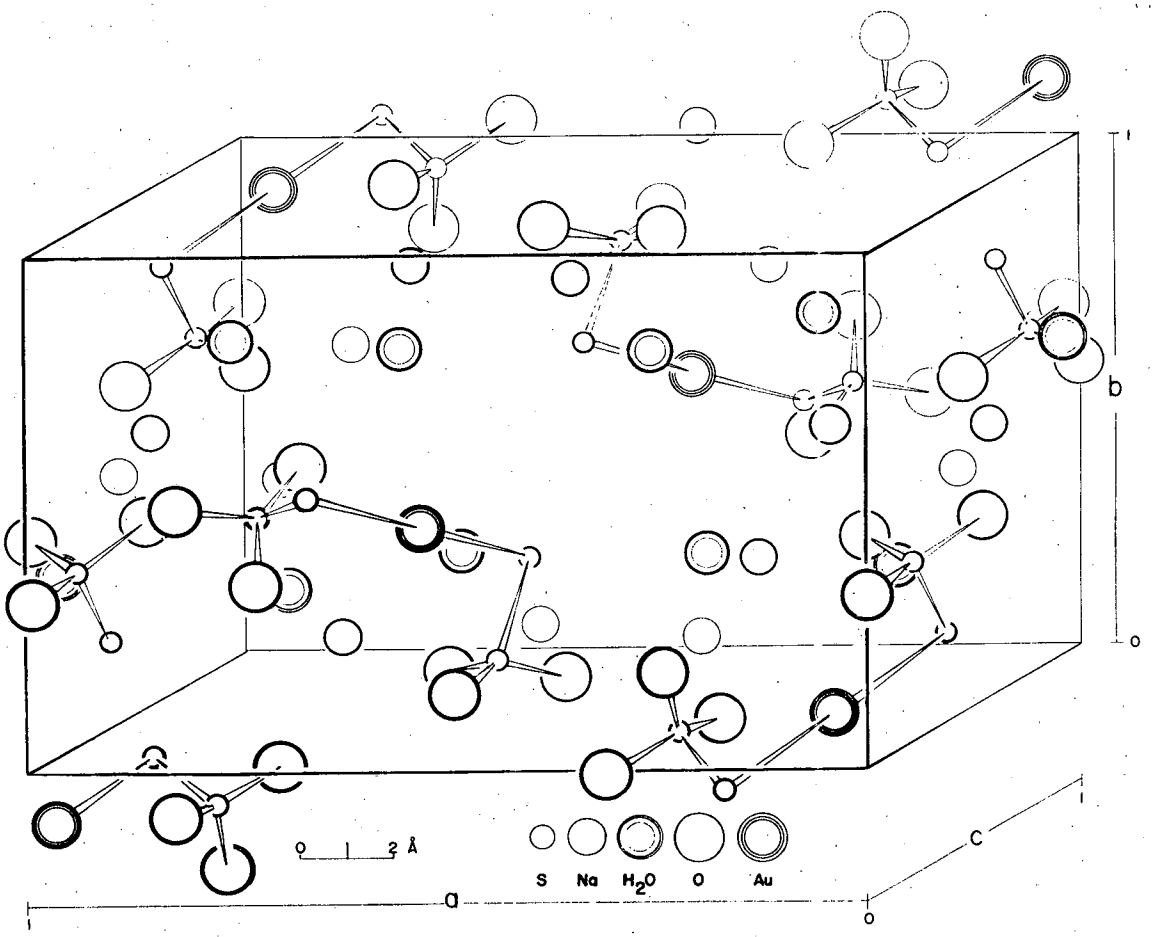


Fig. 2

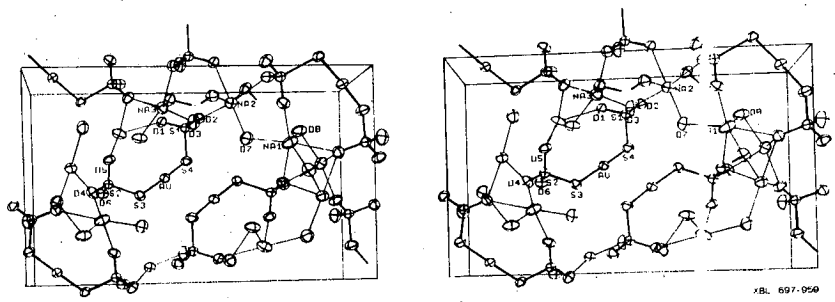


Fig. 3

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

TECHNICAL INFORMATION DIVISION
LAWRENCE RADIATION LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720