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## Potassium Hexahydroperoxostannate: Synthesis and Structure

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**Abstract**—Polycrystalline potassium hexahydroperoxostannate was prepared by replacement of hydroxo groups in potassium hexahydroxostannate upon its dissolution in hydrogen peroxide. A comparative study of the product and the starting hydroxostannate by powder X-ray diffraction analysis, thermogravimetry, and IR,  $^2\text{H}$ ,  $^{39}\text{K}$ , and  $^{119}\text{Sn}$  NMR, and Mössbauer spectroscopy was carried out. The peroxy compound  $\text{K}_2\text{Sn}(\text{OOH})_6$  crystallizes in the hexagonal system with  $a = 7.264(7)$  Å,  $c = 10.168(4)$  Å. IR, NMR, and Mössbauer spectroscopy data show that the tin coordination polyhedron in the peroxy compound is an octahedron formed by the coordinated hydroperoxy groups.

Previously, sodium hexahydroperoxostannate was prepared and characterized by powder X-ray diffraction analysis, thermogravimetry, IR [1],  $^1\text{H}$  NMR, and Mössbauer spectroscopy [2], and by thermodynamic [3] and kinetic [4] methods. The tin atoms in this compound were found to occur in the octahedral environment of hydroperoxy groups [2]. It appeared pertinent to confirm the possibility of formation of this type of tin compound by preparing a new hydroperoxy complex. To this end, we performed the first synthesis of potassium hexahydroperoxostannate. Comparative study of potassium hexahydroxostannate (**1**) and hexahydroperoxostannate (**2**) and their deuterated analogues (**1a** and **2a**, respectively) was carried out by powder X-ray diffraction analysis, thermogravimetry, and IR, NMR ( $^2\text{H}$ ,  $^{39}\text{K}$ , and  $^{119}\text{Sn}$ ), and Mössbauer spectroscopy.

### EXPERIMENTAL

The initial potassium hexahydroxostannate  $\text{K}_2\text{Sn}(\text{OH})_6$  (**1**) was synthesized from tin tetrachloride and potassium hydroxide using a procedure similar to that used to prepare  $\text{Na}_2\text{Sn}(\text{OH})_6$  [5, 6]. The resulting compound is stable against hydrolysis; therefore, it can be recrystallized from aqueous solution to remove potassium chloride and carbonate impurities. Deuterium-substituted potassium hexahydroxostannate (**1a**) was prepared by recrystallizing compound **1** from  $\text{D}_2\text{O}$ .

The results of chemical analysis of **1** are given below.

For  $\text{K}_2\text{Sn}(\text{OH})_6$ , anal. calcd. (%): K, 26.16; Sn, 39.70. Found (%): K, 25.89; Sn, 39.57.

Potassium hexahydroperoxostannate  $\text{K}_2\text{Sn}(\text{OOH})_6$  (**2**) was synthesized by the following procedure. Com-

pound **1** (1.7 g) was dissolved in 3 ml of 96%  $\text{H}_2\text{O}_2$  upon stirring for 2 h at  $0^\circ\text{C}$ . The solution was allowed to stand in a desiccator over  $\text{P}_2\text{O}_5$  at  $-5^\circ\text{C}$  for 24 h. The colorless product that crystallized was treated with 2 ml of 96%  $\text{H}_2\text{O}_2$  without separation from the liquid and again kept in a desiccator over  $\text{P}_2\text{O}_5$  for 24 h at  $-5^\circ\text{C}$ . The resulting polycrystalline product was separated from the mother liquor by filtration, washed five times with ethanol and five times with ether, and dried in a vacuum desiccator over  $\text{P}_2\text{O}_5$  for 4 h. The deuterated analogue of potassium hexahydroperoxostannate (**2a**) was prepared by the reaction of **1a** with deuterated hydrogen peroxide. Deuteration of hydrogen peroxide was performed by diluting it with heavy water to reach the 1 : 2 volume ratio and subsequently concentrating it in a desiccator over  $\text{P}_2\text{O}_5$ .

The results of chemical analysis of **2** are given below.

For  $\text{K}_2\text{Sn}(\text{OOH})_6$ , anal. calcd. (%): K, 19.80; O(act.), 24.31; Sn, 30.05. Found (%): K, 19.62; O(act.), 24.16; Sn, 30.27.

The resulting potassium hexahydroperoxostannate is a colorless polycrystalline solid poorly soluble in water and insoluble in standard organic solvents. Compound **2** is relatively stable. For example, during storage in a desiccator over  $\text{P}_2\text{O}_5$  at  $4^\circ\text{C}$ , it does not decompose for at least one month.

The tin content in the samples studied was determined by weight as  $\text{SnO}_2$  using a known procedure [7, p. 936]. Quantitative analysis for potassium was performed by precipitating the tetraphenylborate salt from an alkaline solution [7]. The amount of active oxygen was determined by permanganometric titration [8].

**Table 1.** Indexing of the powder X-ray diffraction pattern of potassium hexahydroxostannate

$d, \text{\AA}$	$I/I_0, \%$	$1/d_{\text{exp}}^2 \times 10^4$	$hkl$	$1/d_{\text{calcd}}^2 \times 10^4$	$\delta$
5.1752	100	373.40	0 1 1	372.0	1.4
4.2667	29	549.30	0 0 3	547.9	1.4
4.2667	29	549.30	0 1 2	554.6	-5.3
3.2743	23	932.70	1 1 0	933.2	-0.5
2.7865	5	1287.90	0 1 4	1285.1	2.8
2.7674	8	1305.70	0 2 1	1305.2	0.5
2.5977	29	1481.90	1 1 3	1481.1	0.8
2.5977	29	1481.90	0 2 2	1487.8	-5.9
2.1255	11	2213.50	0 2 4	2218.3	-4.8
2.0321	3	2421.60	1 2 2	2421.0	0.6
1.8909	4	2796.80	0 3 0	2799.7	-2.9
1.7878	8	3128.70	1 1 6	3124.8	3.9
1.7426	3	3293.10	0 1 7	3294.0	-0.9
1.7277	18	3350.10	0 3 3	3347.6	2.5
1.6371	7	3731.20	2 2 0	3732.9	-1.7
1.5613	3	4102.30	1 3 1	4104.9	-2.6
1.5384	4	4225.30	0 2 7	4227.2	-1.9
1.5283	2	4281.40	1 3 2	4287.5	-6.1
1.5283	2	4281.40	2 2 3	4280.8	0.6
1.4114	4	5020.00	1 3 4	5018.0	2.0
1.3928	2	5154.90	1 2 7	5160.5	-5.6
1.2955	6	5958.30	0 4 4	5951.2	7.1
1.2747	1	6154.40	2 3 2	6154.0	0.4
1.2504	1	6395.90	0 1 10	6398.7	-2.8
1.2369	2	6536.30	1 4 0	6532.6	3.7
1.2045	1	6892.70	2 3 4	6884.5	8.2
1.1928	1	7028.50	1 3 7	7026.9	1.6
1.1878	3	7087.80	1 4 3	7080.5	7.3
1.1676	1	7335.20	0 2 10	7331.9	3.3
1.1409	15	7682.50	0 1 11	7677.1	5.4
1.1228	1	7932.20	1 3 8	7940.1	-7.9
1.1000	3	8264.50	1 2 10	8265.1	-0.6
1.0708	2	8721.30	1 4 6	8724.1	-2.8
1.0617	1	8871.50	0 4 8	8873.3	-1.8
1.0572	1	8947.20	3 3 3	8946.9	0.3
1.0572	1	8947.20	2 4 2	8953.6	-6.4

The powder X-ray diffraction patterns of the compounds synthesized were recorded on a DRON-3 diffractometer ( $\text{CuK}\alpha$ , Ni filter). The crystal lattice parameters were calculated by the least-squares method. The thermal analysis of the samples was performed on a Q-1500D derivatograph (Hungary) in air in the temperature range from 20 to 150°C (heating rate 2 K/min, sample size 5–20 mg). IR spectra were measured as

KBr pellets on a Specord M 80 spectrophotometer in the region of 400–4000  $\text{cm}^{-1}$ .

The  $^2\text{H}$ ,  $^{39}\text{K}$ , and  $^{119}\text{Sn}$  NMR spectra of polycrystalline samples were recorded on a Bruker MSL-300 radiospectrometer in a 7.04 T field at 298 K. The  $^2\text{H}$  and  $^{119}\text{Sn}$  NMR spectra were run using a one-pulse sequence with variable dead time. The exciting pulse duration was 1–2  $\mu\text{s}$ , repetition time  $5T_1$ . In recording

the  $^{39}\text{K}$  NMR spectra (14.004 MHz), the spin system was excited using a spin echo sequence ( $\theta_x-\tau-2\theta_y-\tau-ACQ$ ). The first pulse width was 12  $\mu\text{s}$ ; it was selected from the condition  $\gamma B_1 \theta(I + 1/2) = \pi/2$ , where  $\gamma$  is the gyromagnetic ratio for  $^{39}\text{K}$ ,  $B_1$  is the radiofrequency field amplitude, and  $I$  is the nuclear spin (3/2). Chemical shifts for  $^{119}\text{Sn}$  were referred to  $\text{SnCl}_4$ .

The Mössbauer spectra were recorded on a MS1101E spectrometer (manufactured by MosTec, Rostov-on-Don). The  $\gamma$ -radiation sources used were standard calcium stannate  $^{119}\text{Sn}$  sources with an activity of 0.3 mCi. The chemical shifts were referred to  $\text{BaSnO}_3$ . The Mössbauer spectra were measured both at room temperature and at the liquid-nitrogen temperature. The sample size was taken to contain 20  $\text{mg}/\text{cm}^2$  tin. The spectra were processed using relevant software, by the least-squares fit.

## RESULTS AND DISCUSSION

According to the powder X-ray diffraction data obtained in this study, compounds **1** and **2** are individual compounds; the X-ray diffraction patterns contain no additional unindexed reflections.

The X-ray diffraction pattern of **1** was indexed under the assumption of a hexagonal lattice (space group  $R3$ ) with  $a = 6.546(7)$  Å,  $c = 12.816(7)$  Å (Table 1). Note that the X-ray diffraction patterns of the compound synthesized contain extra lines, which were not reported for  $\text{K}_2\text{Sn}(\text{OH})_6$  [9]. Therefore, our indexing was different.

The X-ray diffraction pattern of **2** displays a substantial number of fairly strong reflections, which are indexed satisfactorily in terms of a hexagonal unit cell with  $a = 7.264(7)$  Å,  $c = 10.168(4)$  Å (Table 2). Attention is attracted by the low intensity of lines with odd values of  $l$ , which might indicate the presence of a subcell with the parameter  $c_{\text{sub}} = c/2$ .

Compound **2** is thermally unstable and decomposes at 105°C, producing a significant exotherm. Decomposition is explosive; it is accompanied by matter emission, which stops the thermogravimetric study. In the case of the starting hydroxo complex **1**, weight loss with an endotherm occurs only at 285°C. Nevertheless, the decomposition temperature of compound **2** is far higher than that of the known sodium hexahydroperoxostannate (80°C [10]), indicating a higher stability of **2**.

The IR spectra of **1** exhibit an absorption band at 980  $\text{cm}^{-1}$  due to the  $\delta(\text{Sn}-\text{O}-\text{H})$  bending vibrations [11]; for the deuterated compound **1a**, this band shifts to 725  $\text{cm}^{-1}$ . The spectra of compound **2** (Table 3) do not contain this band. Instead, bands at 856 and 1432  $\text{cm}^{-1}$  due to the  $\nu(\text{O}-\text{O})$  and  $\delta(\text{O}-\text{O}-\text{H})$  modes and bands at 2800 and 3096  $\text{cm}^{-1}$  due to the O-H stretching vibrations of the hydroperoxo group appear [12–14]. In the spectrum of the deuterated derivative **2a**, the bands associated with the bending and stretching

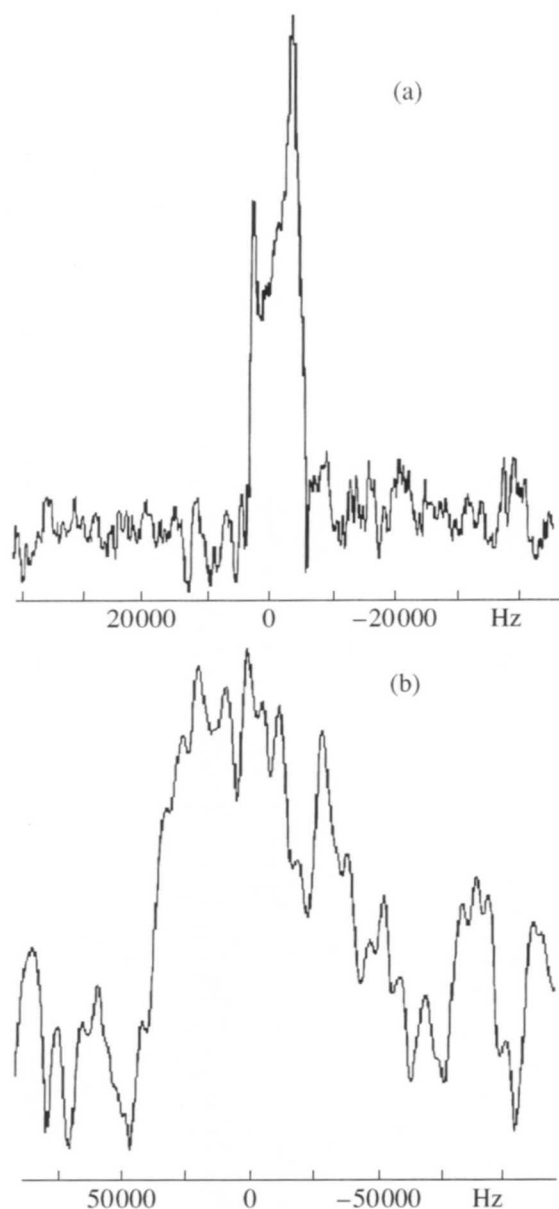


Fig. 1.  $^{29}\text{K}$  NMR spectra of (a)  $\text{K}_2\text{Sn}(\text{OH})_6$  and (b)  $\text{K}_2\text{Sn}(\text{OOH})_6$ .

vibrations of the hydroperoxo group shift to 1048 [ $\delta(\text{O}-\text{O}-\text{D})$ ], 2072, and 2288  $\text{cm}^{-1}$  [ $\nu(\text{O}-\text{O}-\text{D})$ ], in accordance with the expectations. The IR spectrum of potassium hexahydroperoxostannate also contains a band at 760  $\text{cm}^{-1}$ , which shifts to 570  $\text{cm}^{-1}$  in the spectrum of the deuterated derivative **2a**. This complies with the shift expected for the vibrations of the hexahydroperoxo group. These data, together with the fact that the band at 448  $\text{cm}^{-1}$ , belonging to the Sn-O stretching vibrations, in the tin hexahydroperoxo complex is not split, indicate apparently that the hydroxo groups have been completely replaced by hydroperoxo groups in **2** and **2a**.

**Table 2.** Indexing of the powder X-ray diffraction pattern of potassium hexahydroperoxostannate

$d, \text{\AA}$	$I/I_0, \%$	$1/d_{\text{exp}}^2 \times 10^4$	$hkl$	$1/d_{\text{calcd}}^2 \times 10^4$	$\delta$
10.1128	2	97.8	0 0 1	96.7	1.1
6.2876	100	252.9	0 1 0	252.6	0.3
5.0787	19	387.7	0 0 2	386.9	0.8
3.9510	22	640.6	0 1 2	639.5	1.1
3.6325	39	757.9	1 1 0	757.9	-0.0
3.4201	6	854.9	1 1 1	854.6	0.3
3.1493	3	1008.3	0 2 0	1010.6	-2.3
3.0114	2	1102.7	0 2 1	1107.3	-4.6
2.9546	87	1145.5	1 1 2	1144.8	0.7
2.6756	9	1396.9	0 2 2	1397.4	-0.5
2.4764	3	1630.6	1 1 3	1628.4	2.2
2.3782	2	1768.1	1 2 0	1768.5	-0.4
2.3581	2	1798.4	0 1 4	1800.1	-1.7
2.1539	10	2155.5	1 2 2	2155.3	0.2
2.0971	29	2273.8	0 3 0	2273.8	0.0
2.0838	29	2303.0	1 1 4	2305.4	-2.4
1.9761	6	2560.8	0 2 4	2558.0	2.8
1.9391	14	2659.5	0 3 2	2660.6	-1.1
1.8164	10	3030.9	2 2 0	3031.7	-0.8
1.7882	1	3127.3	2 2 1	3128.4	-1.1
1.7377	7	3311.7	1 2 4	3315.9	-4.2
1.7112	14	3415.1	2 2 2	3418.5	-3.4
1.6945	3	3482.7	0 0 6	3481.7	1.0
1.6488	4	3678.4	1 3 2	3671.2	7.2
1.6360	1	3736.2	0 1 6	3734.4	1.8
1.6177	6	3821.2	0 3 4	3821.2	0.0
1.6005	2	3903.8	2 2 3	3902.1	1.7
1.5353	3	4242.4	1 1 6	4239.6	2.8
1.5014	2	4436.2	0 4 2	4429.1	7.1
1.4932	2	4485.0	0 2 6	4492.3	-7.3
1.4778	4	4579.0	2 2 4	4579.1	-0.1
1.4431	4	4801.8	2 3 0	4800.1	1.7
1.3737	3	5299.3	1 4 0	5305.4	-6.1
1.3368	2	5595.9	0 4 4	5589.7	6.2
1.3233	8	5710.6	1 3 5	5702.2	8.4
1.3175	4	5761.0	0 3 6	5755.5	5.5
1.2712	2	6188.3	0 0 8	6189.7	-1.4
1.2386	2	6518.4	2 2 6	6513.4	5.0
1.2080	7	6852.8	1 4 4	6852.9	-0.1
1.2025	3	6915.6	3 3 1	6918.0	-2.4
1.1887	1	7077.1	2 4 0	7073.9	3.2
1.1769	2	7219.7	2 3 5	7218.0	1.7
1.1279	1	7860.7	0 5 4	7863.4	-2.7
1.0674	1	8777.0	0 4 7	8781.2	-4.2
1.0485	1	9096.3	0 6 0	9095.0	1.3
1.0417	1	9215.4	2 2 8	9221.4	-6.0
1.0273	1	9475.6	1 3 8	9474.1	1.5
1.0273	1	9475.6	0 6 2	9481.9	-6.3

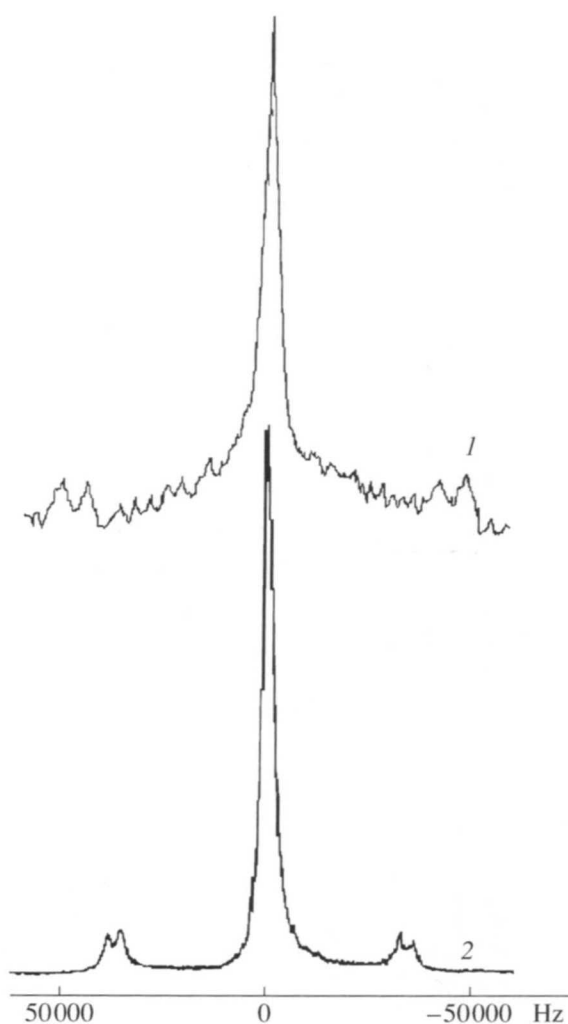


Fig. 2.  $^2\text{H}$  NMR spectra of (1)  $\text{K}_2\text{Sn}(\text{OOD})_6$  and (2)  $\text{K}_2\text{Sn}(\text{OD})_6$ .

The  $^{39}\text{K}$  NMR line shape in the spectrum of potassium hexahydroxostannate **1** shows second-order quadrupole coupling with a zero asymmetry parameter and the quadrupole coupling constant (QCC)  $C_Q(^{39}\text{K}) \approx 0.83$  MHz. In the case of tin hydroperoxo complex **2**, the  $^{39}\text{K}$  NMR spectrum is much more intricate (Fig. 1) due to a nonzero asymmetry parameter  $\eta$  in the potassium position. The  $^2\text{H}$  NMR spectral patterns of compounds **1a** and **2a** are similar (Fig. 2). The presence of an intense central component in these spectra suggests that, apart from immobile deuterons, which are responsible for quadrupole coupling with a nonzero asymmetry parameter and the QCC  $C_Q(^2\text{H}) \approx 96$  kHz (for **1a**) and  $C_Q(^2\text{H}) \approx 127$  kHz (for **2a**), there exist mobile deuterons, whose number is greater than that of immobile ones at a given temperature. The higher QCC value for compound **2a** points to a shorter O–D bond length compared to that in the initial hydroxo complex **1a** [15, 16]. The  $^{119}\text{Sn}$  NMR spectrum of compound **2** (chemical shift  $\delta = -439 \pm 5$  ppm) is similar to that for the initial

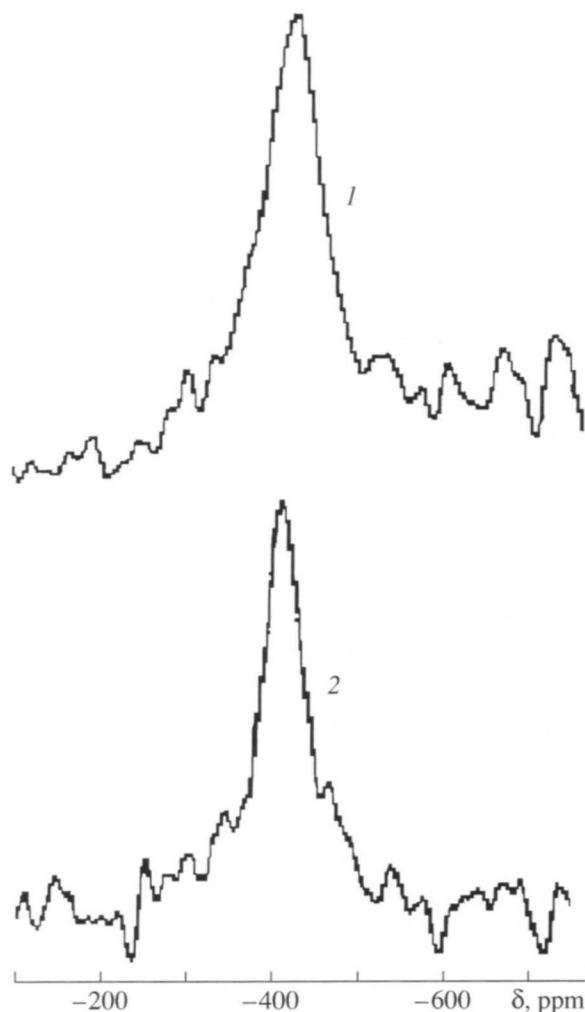


Fig. 3.  $^{119}\text{Sn}$  NMR spectra of (1)  $\text{K}_2\text{Sn}(\text{OOH})_6$  and (2)  $\text{K}_2\text{Sn}(\text{OH})_6$ .

compound **1** ( $\delta = -410 \pm 5$  ppm) (Fig. 3). The upfield shift of the  $^{119}\text{Sn}$  signal in hydroperoxo complex **2** implies an increase in the electron density on the tin atom relative to that in compound **1**.

Table 3. IR spectra of potassium hexahydroperoxostannate and its deuterated analogue

$\text{K}_2\text{Sn}(\text{OOH})_6$		$\text{K}_2\text{Sn}(\text{OOD})_6$	
Band, $\text{cm}^{-1}$	Assignment	Band, $\text{cm}^{-1}$	Assignment
488	$\nu(\text{Sn}-\text{O})$	488	$\nu(\text{Sn}-\text{O})$
760	—	570	—
856	$\nu(\text{O}-\text{O})$	856	$\nu(\text{O}-\text{O})$
1432	$\delta(\text{O}-\text{O}-\text{H})$	1048	$\delta(\text{O}-\text{O}-\text{D})$
2800	$\nu(\text{O}-\text{H})$	2072	$\nu(\text{O}-\text{D})$
3096	$\nu(\text{O}-\text{H})$	2288	$\nu(\text{O}-\text{D})$

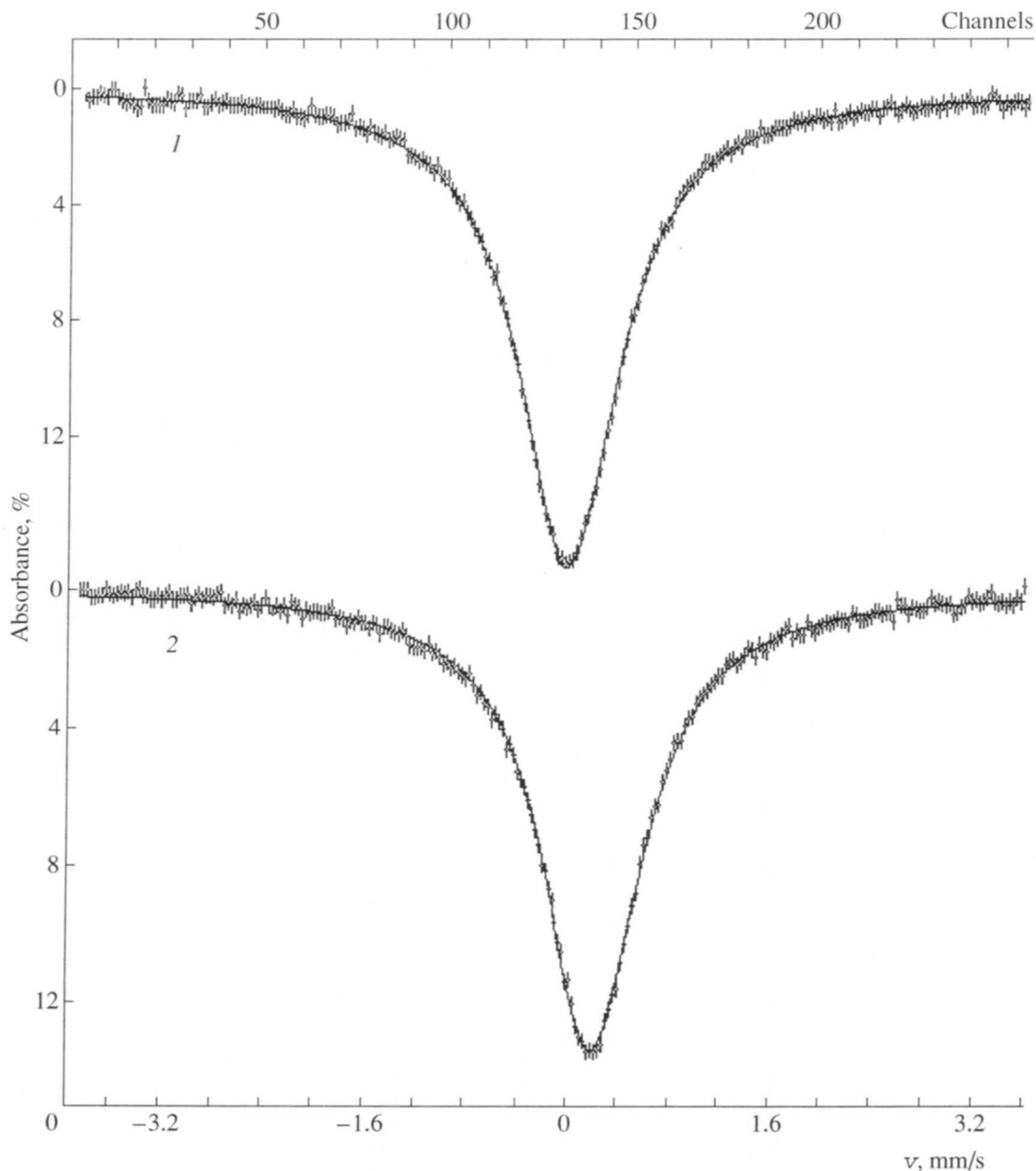


Fig. 4. Mössbauer spectra of (1)  $K_2Sn(OH)_6$  and (2)  $K_2Sn(OOH)_6$ .

The Mössbauer spectra of **1** (Fig. 4) at room temperature exhibit only one singlet, which confirms the octahedral environment of the tin atom ( $\delta = -0.03 \pm 0.01$  mm/s,  $\Gamma_{exp} = 0.96 \pm 0.01$  mm/s). In compound **2**, resonance absorption moves toward positive isomer shifts ( $\delta = 0.19 \pm 0.01$  mm/s,  $\Gamma_{exp} = 0.87 \pm 0.01$  mm/s) with respect to its position in hydroxo complex **1**. No quadrupole splitting is observed in the hydroperoxo complex at 293 K. These data are consistent with the results of a Mössbauer study of sodium hexahydroperoxostannate at room temperature, in which a positive isomer shift was also observed [2].

The upfield displacement of the isomer shift for the hydroperoxo-substituted tin complex attests to an

increase in the electron density on the tin atomic orbitals. Only the hydroperoxo ligands (more precisely, their antibonding orbitals) can serve as the electron-density donors. Apparently, in the case of compound **2**, the electron density transfer from the antibonding orbitals of the hydroperoxo groups is more pronounced than in  $Na_2Sn(OOH)_6$ ; obviously, this correlates with the higher stability of potassium hydroperoxostannate.

The absence of quadrupole splitting for compound **2** implies, on the one hand, that the octahedral environment of the central atom is retained and, on the other hand, that this environment is uniform, i.e., that the hydroxo ligands have been completely substituted by hydroperoxo ligands. The quadrupole splitting

observed in the Mössbauer spectra of potassium hydroxostannate (**1**) and hydroperoxostannate (**2**) ( $\delta = 0.07 \pm 0.01$  mm/s,  $\Delta = 0.59 \pm 0.01$  mm/s,  $\Gamma_{\text{exp}} = 1.16 \pm 0.02$  mm/s for **1**; and  $\delta = 0.21 \pm 0.01$  mm/s,  $\Delta = 0.47 \pm 0.02$  mm/s,  $\Gamma_{\text{exp}} = 1.17 \pm 0.02$  mm/s for **2**) might be related to the presence of both intra- and intermolecular hydrogen bonds in the crystal lattices of these compounds. These bonds insignificantly distort the tin coordination polyhedron, which is expressed upon heavy cooling.

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