# The Absolute Configuration of the $(-)_{589}$-[Co(NCS)$_2$tn$_2$]-[Sb((+)-tart)]$\cdot$2H$_2$O Diastereoisomer

Keiji Matsumoto, Michitaka Yonezawa, Hisao Kuroya
Hiroshi Kawaguchi and Shinichi Kawaguchi

*Department of Chemistry, Faculty of Science, Osaka City University, Sugimoto-cho, Sumiyoshi-ku, Osaka*

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It has been shown by X-ray studies that the absolute configurations of $(+)_{589}$-[Co(CN)$_2$en$_2$]$^{+}$[1] and $(-)_{589}$-[Co ox en$_2$]$^{+}$[2] are of the $\Lambda$- and $\Delta$- types respectively.[3] These results are consistent with the empirical predictions derived from CD or ORD measurements. Few investigations have, though, been made of the cobalt(III) complexes involving trimethylenediamine (=tn); with regard to the absolute configuration particularly, only that of $(-)_{589}$-[Co tn$_3$]$^{3+}$[4] has been reported. We have now determined the crystal structure of $(-)_{589}$-[Co(NCS)$_2$tn$_2$][Sb((+)-tart)]$\cdot$2H$_2$O as well as the absolute configuration of the complex cation.

Crystal data: orthorhombic, space group $P2_12_12$; $a=12.14$, $b=19.51$, $c=9.13$ Å; $Z=4$. Three-dimensional Fourier methods were used, the absolute configuration of the (+)-tartrate ion being referred to. The $R$ value is 0.149 for 870 observed reflections.

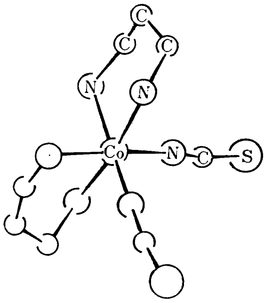

Fig. 1

Figure 1 is a perspective drawing of the complex cation, which has an approximately two-fold axis passing through the cobalt atom and bisecting the N(NCS)–Co–N(NCS) angle. Both of the two six-membered Co-tn rings are of the chair form. The absolute configuration of $(-)_{589}$-[Co(NCS)$_2$tn$_2$]$^{+}$ can be denoted as $\Lambda$, as is the case with $(-)_{589}$-[Co tn$_3$]$^{3+}$.

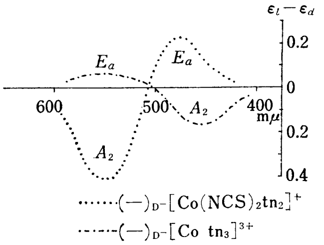

Fig. 2

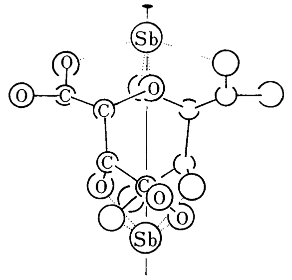

Fig. 3

The sign of the $E_a$ component of the CD peaks in the first absorption-band region is regarded as diagnostic of the absolute configuration of the trigonal cobalt(III) complex ion.[5] The CD curve of $(-)_{589}$-[Co tn$_3$]$^{3+}$[6,7] in this region shows a weak positive $E_a$ peak in the longer-wavelength region and a strong negative $A_2$ peak on the shorter-wavelength side (Fig. 2). Therefore, the assignments indicated in Fig. 2 were made for the two components in the CD diagram of $(-)_{589}$-[Co(NCS)$_2$tn$_2$]$^{+}$ obtained in the present work.

In Fig. 3 the geometry of the (+)-tartratoantimonate(III) ion is presented. A symmetric "dimerized" structure is built up of the two tetradentate tartrate ions bridging the two metal atoms lying on the two-fold axis of rotation.

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