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The first structurally characterized coordination compounds with homocysteine

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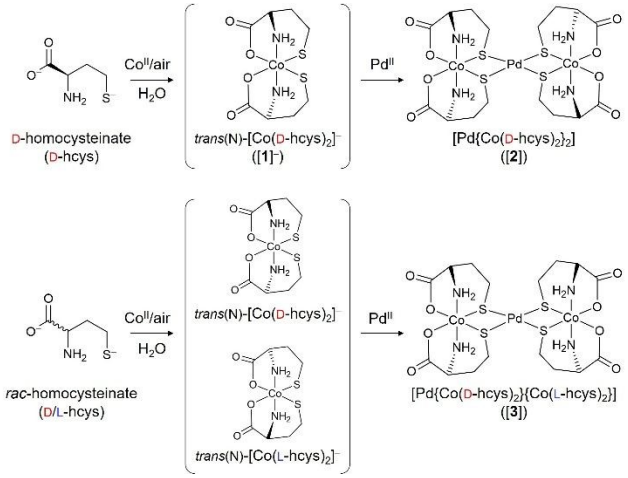
Masahiro Kouno,*[a,b] Takumi Konno,*[a,c] Naoto Kuwamura,[d] Tatsuhiro Kojima,[e] Shota Takamuku,[f] Soichiro Nishio[f] and Nobuto Yoshinari*[a]

D-Homocysteine (D-H_2hcys) coordinates to Co^{III} center in a tridentate-N,O,S mode to form *trans*(N)-[Co(D-hcys)$_2$]$^-$, which binds to Pd^{II} center to produce an S-bridged $Co^{III}_2Pd^{II}$ complex with two *trans*(N)-[Co(D-hcys)$_2$]$^-$ units. The use of racemic D/L-H_2hcys leads to the selective isolation of an analogous $Co^{III}_2Pd^{II}$ complex with *trans*(N)-[Co(D-hcys)$_2$]$^-$ and *trans*(N)-[Co(L-hcys)$_2$]$^-$ units.

Homocysteine (H_2hcys) is a key intermediate in methionine metabolism and is reverted back to methionine using methionine synthase that requires vitamin B_{12} (cobalamin) as a co-factor.[1-3] In vitamin B_{12}, Co^{III} exists as a metal center and plays an essential role in homocysteine metabolism in vivo.[4] Thus, the binding of homocysteine to a Co^{III} center, along with the structure of the resulting cobalt(III) complex, has attracted considerable interest in biochemistry as well as in coordination chemsity.[5-8] The deprotonated form of H_2hcys (hcys^{2-}) possesses three different Lewis base sites, amino, carboxylate and thiolate groups, which makes it to be a heterotopic chelating ligand exhibiting diverse coordination modes, as in the case of cysteine (H_2cys) and penicillamine (H_2pen).[8–13] While studies on the chemical reactivity[14–20] and biological activity of H_2hcys[21-25] have been more active than those of H_2cys and H_2pen, to our knowledge, any structurally characterized coordination compounds with hcys^{2-} have not been reported to date, despite the presence of a large number of crystal structures for coordination compounds with cys^{2-} or pen^{2-} in the literature.[8] This is most likely due to the flexible nature of large chelate rings of hcys^{2-} bound to a metal center, together with the high reactivity of thiolato group of hcys^{2-}. Herein, we report the first structurally characterized coordination compounds with D-hcys^{2-}, *trans*(N)-[Co(D-hcys)$_2$]$^-$ ([**1**]$^-$), in which a Co^{III} center is coordinated by two tridentate-N,O,S D-hcys^{2-} ligands. This complex was found to react with Pd^{II} to form an S-bridged $Co^{III}_2Pd^{II}$ trinuclear structure in [Pd{Co(D-hcys)$_2$}$_2$] ([**2**]), in which two [**1**]$^-$ units chelate to a Pd^{II} center through thiolato groups. The use of racemic D/L-H_2hcys instead of D-H_2hcys, which selectively produced a related $Co^{III}_2Pd^{II}$ complex with *trans*(N)-[Co(D-hcys)$_2$]$^-$ and *trans*(N)-[Co(L-hcys)$_2$]$^-$ units, [Pd{Co(D-hcys)$_2$}{Co(L-hcys)$_2$}] ([**3**]), is also reported (Scheme 1).



Scheme 1. Synthetic scheme of [**1**]$^-$, [**2**] and [**3**].

At first, we prepared D-homocysteine thiolactone via the optical resolution of DL-Homocysteine thiolactone using D-mandelic acid as a co-crystallization agent;[26] the crystal structure of the resulting D-homocysteine thiolactone·D-mandelic acid was confirmed by single-crystal X-ray

[a] The University of Osaka, 1-1 Machikaneyama, Toyonaka, Osaka, Japan 560-0043
[b] Hyogo Prefectural Institute of Technology, 3-1-12 Yukihira-cho, Suma, Hyogo, Japan 654-0037.
[c] Department of Chemistry, College of Science, National Taiwan Normal University, Taipei 11677, Taiwan
[d] Kogakuin University, 2665-1 Nakano-cho, Hachioji, Tokyo, Japan 192-0015.
[e] Kobe City College of Technology, 8-3 Gakuenhigashimachi, Nishi-ku, Kobe, Hyogo, Japan 651-2102
[f] QunaSys Inc., Aqua Hakusan Building 9F, 1-13-7 Hakusan, Bunkyo-ku, Tokyo, Japan 113-0001

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crystallography (Table S1, Fig. S1†). Subsequently, D-homocysteine thiolactone was converted to D-homocysteine by a ring-opening reaction, according to the procedure for synthesizing L-homocysteine.[27] All the products were characterized by the IR (Fig. S2†) and NMR (Fig. S3†) spectroscopies, as well as elemental analysis.

Next, D-H_2hcys was treated with $CoCl_2$ in water by adding NaOH under aerobic conditions, which gave a brown reaction solution. The absorption spectrum of the brown solution exhibited a broad visible band at around 560 nm, together with two intense near-UV bands at 268 and 302 nm (Fig. 1). Similar absorption spectral features have been observed for mononuclear cobalt(III) complexes with cys or pen ligands; visible and near-UV bands have been assigned to Co^{III} d–d and sulfur-to-Co charge-transfer transitions, respectively.[13,28] Compatible with the use of optically active D-H_2hcys in the reaction, the brown solution was CD active, giving positive and negative CD bands at 561 nm and 648 nm, respectively (Fig. 1). The reaction solution was concentrated to dryness to give a brown solid, which could not be recrystallized to isolate an analytically pure sample due to its very high solubility in water. However, several dark brown microcrystals appeared from a solution obtained by washing the brown solid with ethanol. Single-crystal X-ray analysis of one of the crystals revealed that this is a 1:1 complex salt consisting of sodium cations and complex anions ([**1**]$^-$) (Table S2, Fig. S4†). In [**1**]$^-$, two D-hcys^{2-} ligands each coordinate to an octahedral Co^{III} center in a tridentate-N,O,S mode, forming 5-membered N,O-, 6-membered N,S- and 7-membered O,S-chelate rings (Fig. 2). The coordination mode of D-hcys^{2-} to a Co^{III} center in [**1**]$^-$ differs from that of L-cys^{2-}, which coordinates in a bidentate-N,S mode to form [Co(L-cys)$_3$]$^{3-}$,[11] while D-pen^{2-} has been shown to adopt both tridentate-N,O,S and bidentate-N,S mode to form [Co(D-pen)$_2$]$^-$ and [Co(D-pen)$_3$]$^{3-}$, respectively, dependent on the reaction conditions. [12,13] The bond distances about the Co^{III} center in [**1**]$^-$ (Table S3†), Co-N (av. 1.93 Å), Co-O(av. 2.00 Å) and Co-S (av. 2.22 Å), are within the values normally observed for octahedral cobalt(III) complexes with cys^{2-} or pen^{2-}.[11,29-31] However, the Co-O bonds in [**1**]$^-$ are appreciably longer than those in the related cobalt(III) complex with tridentate-N,O,S pen^{2-} ligands, all-cis-[Co(D-pen)(L-pen)]$^-$ (av. Co-N = 1.95 Å, Co-O = 1.96 Å, Co-S = 2.23 Å), although the Co-N and Co-S bonds are similar.[29] Of three possible geometrical configurations, trans(N), trans(O) and trans(S),[32] [**1**]$^-$ adopts a trans(N) configuration, in which two N donors are at a trans position and two O donors and two S donors are each at a cis position (Fig. 2). Here, it should be noted that only a single brown band, which showed the same absorption spectrum of the reaction solution (Fig. S5†), was eluted with 0.05 M aqueous NaCl in an anion-exchange column chromatography (QAE-Sephadex A-25). This implies that [**1**]$^-$ with a trans(N) configuration was exclusively formed in the reaction of Co^{2+} and D-hcys^{2-}.

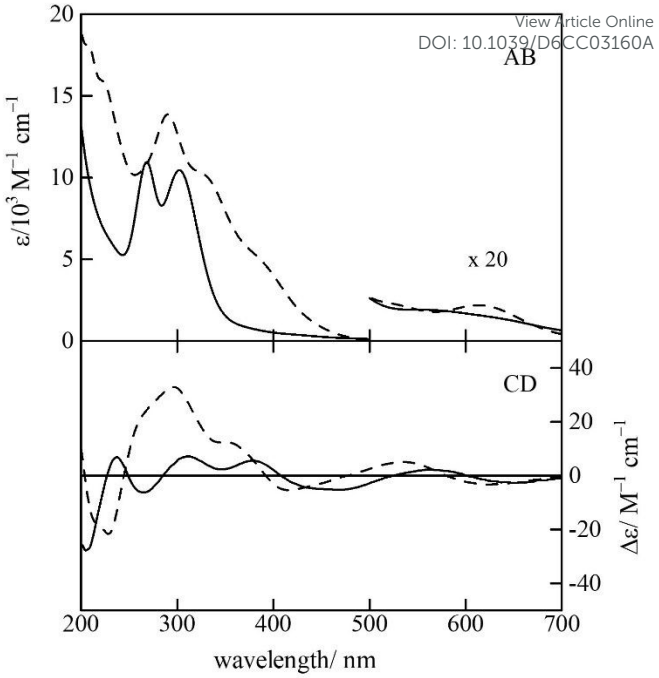

Fig. 1. Absorption and CD spectra of the reaction solution containing [**1**]$^-$ (Solid line) and those of [**2**] in water (dashed line).

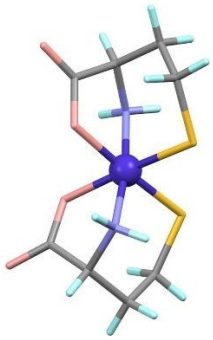

Fig. 2. The structure of one of four independent [**1**]$^-$ anions in the asymmetric unit. Color codes: Co, purple blue; S, yellow; O, pink; N, pale blue; C, gray; H, light blue.

Since [**1**]$^-$ possesses thiolato groups that can bind to another heavy metal center,[8,9,32] we carried out the reaction of the brown solution, which was in situ prepared from Co^{2+} and D-hcys^{2-} in water, with $Na_2[PdCl_4]$ at room temperature. As expected, the reaction proceeded smoothly to give a clear greenish yellow solution. When the reaction solution was successively chromatographed on cation-exchange (SP-Sephadex C-25) and anion-exchange (QAE-Sephadex A-25) columns, only a greenish yellow band was eluted with water, while no detectable bands, except for that of unreacted [**1**]$^-$, were adsorbed on the top of the columns. This is suggestive of the selective formation a single neutral species in the reaction. The greenish yellow eluate passing through the cation-exchange and anion-exchange columns was concentrated to

dryness, and the resulting residue was recrystallized from water/ethanol to produce dark green microcrystals ([**2**]), which are well soluble in water. The elemental analytical data of [**2**] agreed well with the formula for a 1:2 adduct of Pd^{2+} and [Co(D-hcys)$_2$]$^-$, and its absorption and CD spectral features (Fig. 1) are reminiscent of those of the S-bridged $Co^{III}_2Pd^{II}$ trinuclear complex, [Pd{Co(D-pen)$_2$}$_2$].[33] The structure of [**2**] was established by single-crystal X-ray analysis (Tables S2 and S4†). As shown in Fig 3a, [**2**] has a $Co^{III}_2Pd^{II}$ structure in [Pd{Co(D-hcys)$_2$}$_2$], in which two trans(N)-[Co(D-hcys)$_2$]$^-$ octahedral units bind to a square-planar Pd^{II} center through thiolato groups in a boat-like fashion so as to have a D_2 molecular symmetry. Consistent with the molecular symmetry, the ^{1}H and ^{13}C NMR spectra of [**2**] exhibited only a single set of signals due to D-hcys^{2-} ligands (Fig. S6†). In crystal, each trinuclear molecule of [**2**] forms intermolecular NH···O hydrogen bonds with two adjacent molecules (av. N···O = 2.86 Å) in a 1D zigzag chain structure. The 1D chains are parallel arranged to construct a 3D packing structure with a cell volume of 3467 Å^3 (Fig. S7†).

To further investigate the coordination behavior of homocysteine, the aforementioned reactions were performed using the racemic homocysteine (D/L-H$_2$hcys) instead of D-H$_2$hcys. As in the case of the reaction using D-H$_2$hcys, the reaction of $CoCl_2$ with D/L-H$_2$hcys in water in the presence of NaOH gave a brown solution, which contained a single anionic species eluted with 0.05 M aqueous NaCl through an anion-exchange column. The absorption spectrum of the brown solution was nearly the same as that of [**1**]$^-$ (Fig. S8†), while its CD spectrum was silent. Thus, it is considered that a pair of enantiomers with a trans(N) octahedral geometry, trans(N)-[Co(D-hcys)$_2$]$^-$ and trans(N)-[Co(L-hcys)$_2$]$^-$, was selectively formed in the reaction using D/L-H$_2$hcys. Subsequent reaction of the brown solution with $Na_2[PdCl_4]$ at room temperature resulted in the precipitation of dark green microcrystals ([**3**]), which are insoluble in water. As in the case of [**2**], the elemental analytical data of [**3**] were consistent with the formula for a 2:1 adduct of [Co(hcys)$_2$]$^-$ and Pd^{II}. In addition, the IR and diffuse reflectance spectra of [**3**] were similar to those of [**2**] (Figs. S9 and S10†). Single-crystal X-ray analysis indicated that [**3**] is an S-bridged $Co^{III}_2Pd^{II}$ complex, the structure of which is comparable well to that of [**2**] (Tables S2 and S5†). In [**3**], however, a pair of enantiomeric octahedral units, trans(N)-[Co(D-hcys)$_2$]$^-$ and trans(N)-[Co(L-hcys)$_2$]$^-$, binds to a square-planar Pd^{II} center in a chair-like fashion (Fig. 3b). The coordination bonds about Co^{III} and Pd^{II} centers in [**3**] (av. Co-N = 1.95 Å, Co-O = 1.95 Å, Co-S = 2.24 Å, Pd-S = 2.32 Å) are slightly longer than those in [**2**] (av. Co-N = 1.92 Å, Co-O = 1.92 Å, Co-S = 2.22 Å, Pd-S = 2.29 Å).‡ In crystal, each trinuclear molecule of [**3**] is hydrogen-bonded with four adjacent molecules (av. N···O = 3.02 Å) in a 2D sheet structure (Fig. S11†). The 2D sheets are stacked to form a dense packing structure with a cell volume of 3028 Å^3, which appears to be responsible for the sparing solubility of [**3**] in water.

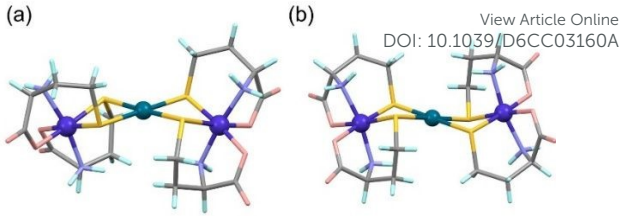

Fig. 3. The structures of (a) [**2**] and (b) [**3**]. Color codes: Pd, blue green; Co, purple blue; S, yellow; O, pink; N, pale blue; C, gray; H, light blue.

To rationalize the stereoselectivity of the coordination compounds derived from D- or D/L-homocysteine, we carried out the density functional theory (DFT) calculations for the three isomers (trans(N), trans(O) and trans(S)) possible for the homochiral [Co(D-hcys)$_2$]$^-$ and the two isomers (all-cis and all-trans) possible for the heterochiral [Co(D-hcys)(L-hcys)]$^-$,[32‡‡] at the ωB97X-D3/def2-TZVPD level using ORCA 6.0.1.[34†] The optimized structures of these isomers are shown in Fig. S12†, and their Gibbs free energies and selected bond distances and angles are summarized in Table S6†. The calculated Gibbs free energies indicate that the homochiral trans(N) isomer is the most thermodynamically favorable, being 4.3–9.4 kcal/mol lower in energy than the other isomers. This is compatible with the selective formation of [**2**] with two *trans*(N)-[Co(D-hcys)$_2$]$^-$ units and [**3**] with *trans*(N)-[Co(D-hcys)$_2$]$^-$ and *trans*(N)-[Co(L-hcys)$_2$]$^-$ units, as well as the formation of the mononuclear *trans*(N)-[Co(D- or L-hcys)$_2$]$^-$ rather than [Co(D-hcys)(L-hcys)]$^-$. The shortest Co-S and Co-N bonds for the trans(N) isomer among the possible isomers appear to reflect the stabilization of this isomer. The DFT calculations were carried out also for the trinuclear [**2**] and [**3**] (Table S7 and Fig. S13†). The difference in the calculated Gibbs free energies between [**2**] and [**3**] is less than 1 kcal mol^{-1}. In addition, no significant differences in the bond lengths and angles were observed between [**2**] and [**3**] in the optimized structures. Thus, the selective production of [**3**], rather than the racemic compound of [Pd{Co(D-hcys)$_2$}$_2$]/[Pd{Co(L-hcys)$_2$}$_2$], by using DL-H$_2$hcys is not explained by its intrinsic thermodynamic stability. Considering the sparing solubility of [**3**] with a 2D sheet structure versus the high solubility of [**2**] with a 1D chain structure in water, this selectivity is most likely ascribed to the equilibrium shift driven by the crystallization of [**3**].

In summary, we showed that D-hcys^{2-} coordinates to an octahedral Co^{III} center in a tridentate-N,O,S mode to form the mononuclear [Co(D-hcys)$_2$]$^-$ ([**1**]$^-$). Complex [**1**]$^-$ adopted a trans(N) configuration, rather than trans(O) or trans(S), which was rationalized by the DFT calculations. While only a few crystals were obtained for [**1**]$^-$, we were able to isolate the trinuclear [Pd{Co(D-hcys)$_2$}$_2$] ([**2**]) bearing [**1**]$^-$ as the constituent unit in a satisfactory yield, thanks to the binding ability of [**1**]$^-$ to a Pd^{II} center through thiolato groups. Note that the trinuclear [Pd{Co(D-hcys)$_2$}{Co(L-hcys)$_2$}] ([**3**]) was selectively produced when D/L-H$_2$hcys was used instead of D-H$_2$hcys. This result is explained by the sparing solubility of [**3**] in solution, together with the thermodynamic stability of the homochiral *trans*(N)-[Co(D- or L-hcys)$_2$]$^-$ compared with the heterochiral [Co(D-hcys)(L-hcys)]$^-$. The present study should provide insight into the interactions between homocysteine and transition metals in

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biological systems, as well as the structural chemistry of coordination compounds with homocysteine.

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Conflicts of interest

There are no conflicts to declare.

Data availability

The data supporting this article, including experimental procedures, characterization data, and computational details, have been included as part of the ESI. CCDC 2555928-2555931 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/

Notes and references

‡ The slight difference in the bond distances between [**2**] and [**3**] is most likely due to the differences in the packing environments and intermolecular contacts in crystal because no significant difference was observed in the optimized molecular structures obtained by the DFT calculations.

‡‡ The presence of two $hcys^{2-}$ ligands with opposite chirality in $[Co(D\text{-}hcys)(L\text{-}hcys)]^-$ prevents the formation of trans(N), trans(O) and trans(S) configurations.

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