172. Cob(I)alamin as Catalyst

8th Communication

Cob(I)alamin and Heptamethyl Cob(I)yrinate During the Reduction of α,β-Unsaturated Carbonyl Derivatives[1])

by **Albert Fischli** and **John J. Daly**

Pharmaceutical Research Department and Central Research Units, *F. Hoffmann-La Roche & Co Ltd.*, CH-4002 Basle, Switzerland

Dedicated to Dr. *Otto Isler* on the occasion of his 70th birthday

(12.V.80)

Summary

Hydrogen bonds as presented in *Figure 2* cannot account for the enantioselective attack of cob(I)alamin (**4**(**I**)) or heptamethyl cob(I)yrinate (**5**(**I**)) on one of the two enantiotopic faces of the substrates. The attack of the strongly nucleophilic $3d_{z^2}$ orbital is preferentially directed to the *re*-side of the starting materials with (*Z*)-configuration and leads, after the highly stereoselective reductive cleavage of the Co,C bond, to saturated products with (*S*)-configuration in varying enantiomeric excesses (see *Schemes 1, 3* and *Table 1*).

1. Introduction. – The enantioselective reduction of the α,β-unsaturated ester **1** using cob(I)alamin (**4**(**I**); see *Schemes 1* and *2*) has been published in two earlier communications in these series [2] [3]. The product was shown to be the corresponding saturated ester **3** with (*S*)-configuration at the chiral center showing enantiomeric excesses of 16.2–23.8% depending on the reaction conditions applied. The formation of alkylcobalamins by a nucleophilic attack of cob(I)alamin on α,β-unsaturated carbonyl derivatives is well documented in the literature [4] [5]. It is therefore reasonable to expect intermediate alkylcobalamins during this overall reduction of a double bond. It has been shown in an earlier paper [1] that the reductive cleavage of a Co,C bond follows 97% retention of configuration at the C-atom using zinc as electron source in aqueous acetic acid. The mechanistic pathway followed in this enantioselective reduction can therefore be outlined as shown in *Scheme 1*. Cob(I)alamin (**4**(**I**)) attacks the electrophilic C-atom in position 3 of **1** with the lobe of the $3d_{z^2}$-orbital on the β-side of the catalyst[2]). This attack

[1]) For the 7th communication see [1].

[2]) The face of the corrin nucleus opposite to the ribonucleotide side chain is the β-side. It is known that cob(I)alamin (**4**(**I**)) is methylated almost exclusively on its β-side [7–9].

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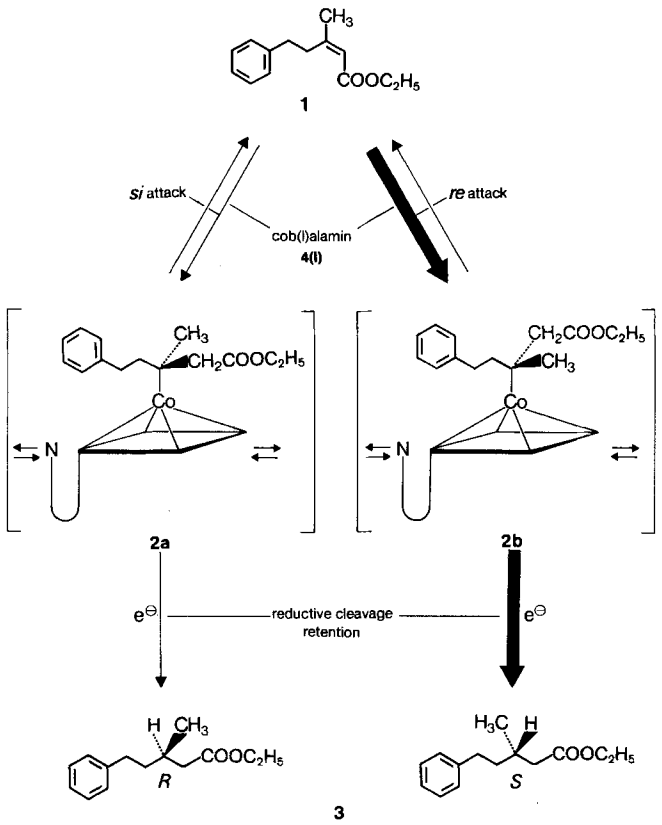
can be directed to the *si*- or the *re*-face of the double bond in the starting material, and accordingly leads to the two diastereomeric alkylcobalamins **2a** and **2b**.

Scheme 1



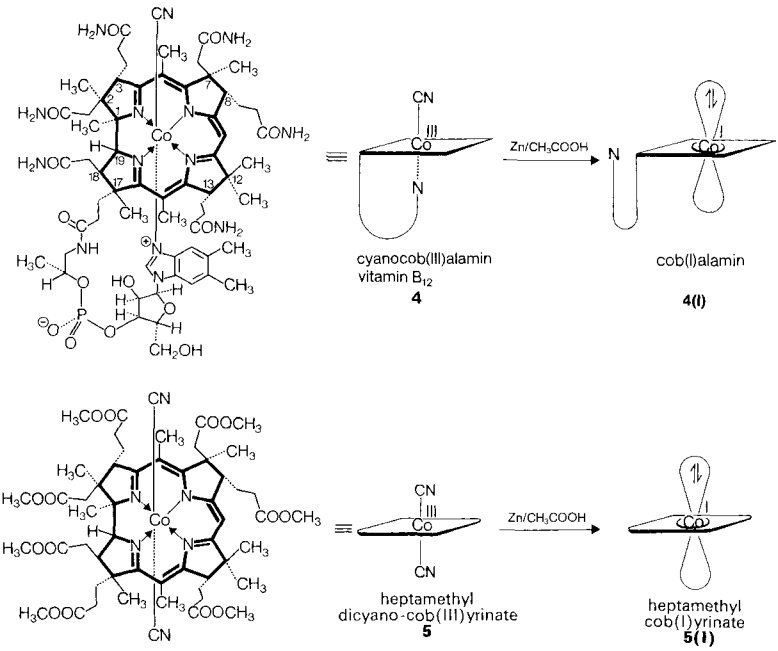
A fragmentation[3]) back to the α,β-unsaturated ester and cob(I)alamin (**4(I)**) with or without isomerization of the double bond has been observed *(vide infra)*. As the product displays the (*S*)-configuration a major amount of the starting material follows the path **1** → **2b** → **3**. One of the questions arising was, why does the catalyst prefer to attack on the *re*-face of the starting material? The chiral centers of the cobalamin molecule are arranged at the periphery of the corrin nucleus and cannot interfere in close proximity of the $3d_{z^2}$-orbital. It is also difficult to see how the helical chirality of the corrin system, based upon the direct link between C(1) and C(19), could influence the preferential attack of cob(I)alamin on the *re*-face of the substrate. One possibility for the transfer of chirality from the periphery of the catalyst to the substrate (α,β-unsaturated ester or amide) might be the formation of a H-bond between an amide N–H from the periphery of the

[3]) Experiments revealing such a reductive fragmentation have been published in an earlier communication within this series [6].

catalyst and the carbonyl moiety from the substrate or *vice versa* (for the latter case see *Fig. 2*). To test this hypothesis reductions using cob(I)alamin (**4(I)**) or heptamethyl cob(I)yrinate (**5(I)**[4]) as catalysts and α,β-unsaturated esters or amides have been carried out.

A deduction from such a set of experiments is only admissible if the two catalytic species may be correlated. Therefore, to enable a direct comparison with data obtained for cyanocobalamin (**4**) [11] and cobyric acid [12], an X-ray analysis of heptamethyl dicyanocob(III)yrinate (**5**) has been carried out.

Scheme 2



2. X-Ray Analysis of 5. – *Crystal Data.* Beautiful dark red crystals of **5** were obtained by slow growth from benzene/hexane. They apparently contain a little water. $C_{54}H_{73}CoN_6O_{14} \cdot xH_2O$ ($x \approx 1.0$), M = 1089.1, monoclinic, space group $P2_1$ with $a = 16.386$ (6) Å, $b = 13.220$ (5) Å, $c = 14.482$ (5) Å, $\beta = 109.84$ (5)°, $U = 2950.9$ Å^3, $D_{calc} = 1226$ kg · m^{-3} (without water), $Z = 2$, MoK_α radiation $\lambda = 0.71069$ Å.

Intensity Measurements. Intensities were measured up to $0 \leq 28°$ with the help of a computer (PDP8) controlled four circle diffractometer (*Hilger & Watts* Y290) operating in the 10/20 scan mode and using zirconium filtered Mo*K* radiation. Independent data for 7453 planes were used to solve the structure and 4758 of these with $I \geq 4.50$ (I) were used in the refinement.

Structure Determination and Refinement. The structure was determined by MULTAN [13] and refined by full-matrix least-squares, with an anisotropic temperature factor for the cobalt atom in the later stages, to a final *R*-value of 0.106. During the refinement maps showed electron density which did not arise from **5**. After some trials the two largest peaks were given oxygen scattering factors and site occupation factors of 0.5 and were assumed to be a disordered water molecule. The SHELX-76 programming system [14] was used for this part of the work.

[4]) Prepared according to [10].

Results and Discussion. The principal results: final parameters, bond lengths, bond angles, some torsion angles, and the least squares plane are shown in *Tables 2–6*[5]), and *Figure 1* shows a stereoprojection of the molecule with the labeling used in the analysis.

The X-ray analysis confirms that the methanolysis of vitamin B_{12} giving **5** has not affected the configurations of any of the chiral centres common to both molecules. The bond lengths and angles in the cobalt-corrin system are very similar to those found in other corrins [11] [12] [15–18], cobyric acid [12] may be taken as an example. The local symmetry of the cobalt coordination octahedron is approximately *mm*2 (C_{2v}) with the two-fold axis passing through C(10) and the Co-atom. Delocalisation in the inner ring of atoms, from N(22) *via* C(10) to N(23), is interrupted by the C(1)–C(19) single bond of 1.53 Å. The fivemembered rings do not all have the same conformations as those in cobyric acid: rings A, B, and D are in approximate envelope forms (see *Table 5*) with C(2), C(8), and C(18) lying out of the planes while ring C has a roughly two-fold axis passing through N(20).

In **5** the conformations of the side chains, which will be also influenced by packing forces, show slight differences from those found in cobyric acid. In the former it may be seen from the *Tables* and the stereoscopic drawing in *Figure 1* that the C_3-side chains have all adopted the extended form and that those on C(8) and C(17) run approximately parallel to the Co–C(24)≡N(26) line while those on C(13) and C(3) point slightly from this line. In cobyric acid the C(3), C(8), and C(17) side chains adopt an at least approximately extended form and those on C(8) and C(17) are again roughly parallel to the Co–C≡N line: not only the C(3) but also the C(13) side chain points away from this line leaving the lower part of the molecule somewhat more exposed to attack compared to the α-face[6]) of **5**. The disordered water molecule makes a hydrogen bond (O(76)...N(26)=2.76 Å) to a cyanide group bonded to the Co-atom.

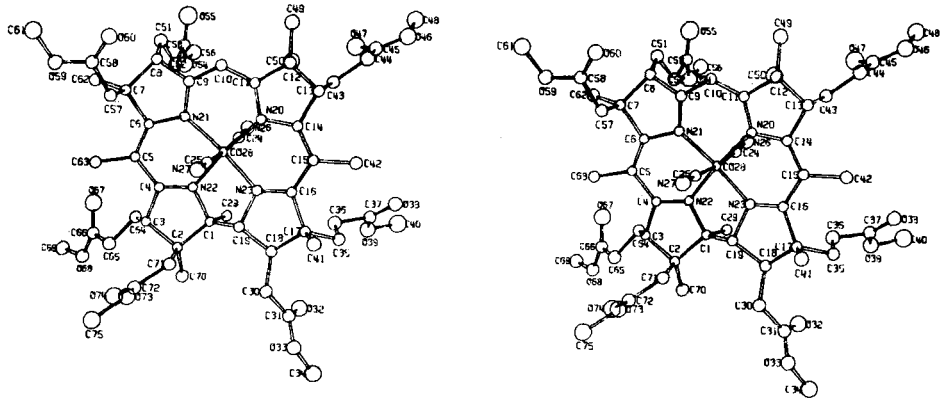


Fig. 1. *A stereoscopic view of heptamethyl dicyano-cob(III)yrinate* (**5**)

[5]) See exper. part.

[6]) Face substituted with the four propionate side chains = α-face.

The C_2-side chains in **5** on C(2), C(7) and C(18) occupy positions parallel to the ones of the corresponding C_2-side chains in cobyric acid [12] and vitamin B_{12} [11].

3. Enantioselective Reductions. – The X-ray analysis of heptamethyl dicyanocob(III)yrinate (**5**) shows the two acetate side chains on the rings A and B in a 'quasi axial' situation[7]). The remaining C_2-side chain on ring D occupies a 'quasi equatorial' position[7]). Such an arrangement of the side chains on the β-face[8]) of the cobyrinate parallels very closely the arrangement of the corresponding groupings in the molecule of cyanocob(III)alamin (**4**)[9]). An interference of the 'quasi equatorial' side chain on ring D with a molecular system approaching the central cobalt atom perpendicularly to the plane of the macrocyclic corrin nucleus is not very likely. The two 'quasi axial' C_2-side chains in **5** are much better situated to create a contact with a molecule attacking the $3d_{z^2}$-orbital of the Co-atom on the β-side of the catalyst. Model studies show clearly that a H-bond from an acrylic derivative such as **9** (see below), used as a substrate in our study, to a chain at the periphery of the catalyst or *vice versa* might possibly be produced involving the C_2-side chain from ring B (see *Fig. 2*). Such a H-bond would hold the acrylic

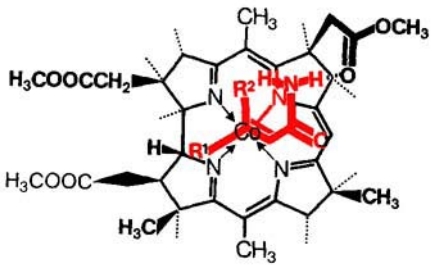


Fig. 2. *Formally possible hydrogen bond between an α,β-unsaturated amide and the C_2-side chain on ring B of* **5(I)**. The electrophilic β-carbon atom of the amide is just above the central cobalt atom, in an ideal position for a nucleophilic attack by the $3d_{z^2}$ orbital of **5(I)**.

derivative just above the macrocyclic system in a plane almost parallel to the corrin nucleus, and with the electrophilic center C(β) of the substrate in an ideal situation for an attack on the central Co-atom. When the C_2-side chain from ring A acts as a H-bond anchor for the substrate, it is not possible to reach a similar arrangement of the electrophilic β-carbon atom of the substrate and of the nucleophilic $3d_{z^2}$-orbital of the central Co-atom, as shown by model studies.

Therefore, a H-bond between the substrate and the C_2-side chain on ring B might account for the enantiomeric excess observed after cobalamin catalyzed reductions of acrylic derivatives.

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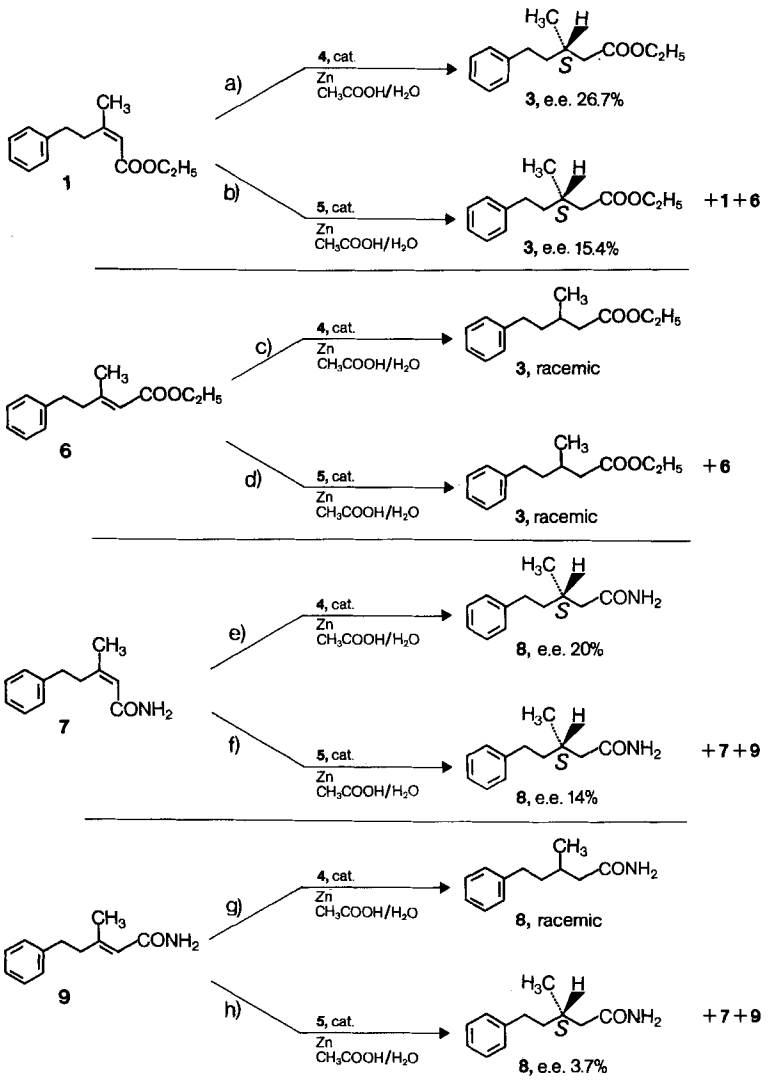
[7]) The term 'quasi axial' is used to denote the almost perpendicular orientation of the first C,C single bond of a side chain relative to the plane of the corrin nucleus. A side chain is specified 'quasi equatorial' if the first C,C single bond stretches out almost in plane of the corrin nucleus.

[8]) Face substituted with the tree acetate side chains = β-face.

[9]) Compare the results of the X-ray analysis of vitamin B_{12} [11].

The X-ray analysis of **5** reveals conformations of the C_2-side chains parallel to the ones of the corresponding groupings in cyanocob(III)alamin (**4**). As the ribonucleotide loop, blocking partially[10]) the α-face of **4** (**I**), is missing in **5** the almost exclusive attack of an electrophile on the β-side of **4** (**I**) could formally not be realized in **5**. However, experimental elucidation of the methylation of different Co(I)-corrinoids revealed the following behaviour. Cob(I)alamin is methylated to 93% on its β-face and the corresponding α-methylcobalamin is formed in

Scheme 3



[10]) The catalytic species **4** (**I**) exists in a 'base off' form [19].

Table 1. *Reductions using cob(I)alamin* (**4**(**I**)) *or heptamethyl cob(I)yrinate* (**5**(**I**)) *as catalyst*

Experiment	Starting material	Catalyst	Time[a]) in h	Products after chromatography in %					
				1	**3**	**6**	**7**	**8**	**9**
a)	**1**	**4**(**I**)	70	–	80, *S* e.e. 26.7	–			
b)	**1**	**5**(**I**)	90[b])	31	43, *S* e.e. 15.4	8			
c)	**6**	**4**(**I**)	70	–	78, rac.	–			
d)	**6**	**5**(**I**)	90[b])	–	52, rac.	36			
e)	**7**	**4**(**I**)	24				–	78, *S* e.e. 20	
f)	**7**	**5**(**I**)	46[b])				14	55, *S* e.e. 14	16
g)	**9**	**4**(**I**)	90				–	95, rac.	–
h)	**9**	**5**(**I**)	46[b])				6	56, *S*	21

[a]) All the reductions have been carried out using the following conditions: CH_3COOH/H_2O 6:1, +10°, in the dark, under argon, 20 mol-equiv. of activated zinc.

[b]) The excess of zinc has been exhausted after this time and the colour of the suspensions turned to red.

7% yield[11]). Co(I)-cobyric acid is attacked to 90% from the β-side and to 10% from the α-face[11]). Cobyrinic acid yields in 78% the β-methylated isomer, and the α-methylcobyrinic acid is detected in 22% yield[11]). Evidence for the predominating formation of heptamethyl β-methylcobyrinate by methylation of the corresponding Co(I)-corrinoid can be found in [10]. It is therefore reasonable to assume that cob(I)alamin (**4**(**I**)) and heptamethyl cob(I)yrinate (**5**(**I**)) are both predominantly attacked on the β-face by electrophilic substrates distinctly larger than methyl iodide.

Accordingly an analysis of the significance of a H-bond, as shown in *Figure 2*, is possible using as catalysts cob(I)alamin (**4**(**I**)) and heptamethyl cob(I)yrinate (**5**(**I**)) and as substrates an α,β-unsaturated ester and a corresponding primary amide. The enantioselective reductions of ethyl (*Z*)- and (*E*)-3-methyl-5-phenyl-2-pentenoate (**1** and **6**, respectively) are shown in *Scheme 3*. *Table 1* summarizes the results of the corresponding experiments. The reduction of the (*Z*)-isomer **1** with **4**(**I**) produced the saturated derivative **3** in 80% yield displaying the (*S*)-configuration and an enantiomeric excess of 26.7% (experiment a). In this reduction the formation of a H-bond, as discussed above, is formally possible. The C_2-side chain in ring B is present as amide and has therefore the possibility to establish a H-bond to the carbonyl oxygen of the substrate. In the analogous reduction of **1** using **5**(**I**) as catalyst such a H-bond is not feasible (experiment b). The saturated ester **3** was isolated in 43% yield showing the (*S*)-configuration and an enantiomeric excess of 15.4%, the reaction was slower, starting material was obtained in

[11]) Results from the research group of *W. Friedrich*, Hamburg, GFR, presented at The Third European Symposium on Vitamin B_{12} and Intrinsic Factor, March 1979.

31% and the isomerized ester **6** was isolated in 8% yield. The reduction of the (*E*)-isomer **6** with **4(I)** produced *rac*-**3** in 78% yield (experiment c). Using **5(I)** a distinctly slower reaction produced 52% of *rac*-**3**; the starting material was recovered in 36% yield. No isomerization occurred during the reductions of **6**.

An identical set of experiments was performed with the corresponding amides **7** and **9**, which always have the possibility to function as a H-bond donor. The (*Z*)-isomer **7** was saturated in the presence of **4(I)** in 78% yield leading to **8** showing (*S*)-configuration (enantiomeric excess: 20%). Using **5(I)** the saturation of **7** was distinctly slower, and **8** with (*S*)-configuration (enantiomeric excess: 14%) was isolated in 55% yield, in addition to 16% of isomerized starting material **9** and 14% of starting material **7**. The reduction of the (*E*)-isomer **9** with **4(I)** as catalyst led to *rac*-**8** in 95% yield. Using **5(I)** as catalyst **9** produced **8** in 56% yield showing the (*S*)-configuration with a very weak enantiomeric excess (3.7%); the starting material **9** was isolated in 21% and the isomerized starting material **7** in 6% yield.

4. Discussion. – The results of these experiments can be summarized in the following way (compare *Table 1*). The saturation of a given substrate shows to be distinctly slower if **5(I)** is used as a catalyst in place of **4(I)**. In the majority of the experiments **5(I)** produces an isomerization of the starting material. The α,β-unsaturated ester is less susceptible to isomerization than the corresponding amide. Using **5(I)** as a catalyst the excess of zinc (20 mol-equiv.) is consumed faster than in the experiments with **4(I)**. In all reductions (catalyzed with **4(I)** or **5(I)**) starting from the (*Z*)-isomer the product has (*S*)-configuration with variing enantiomeric excesses (14–26.7%), the lower ones having been obtained with **5(I)**. The isomerization of the starting material in the presence of **5(I)** can account for these lower values. A racemic product is usually obtained from the *E*-isomer; the small enantiomeric excess (*S*, 3.7%) observed in experiment h) is probably due to a reduction of the (*Z*)-isomer **7** of the starting material obtained after isomerization of **9**[12]).

To find an answer to the question concerning the significance of H-bonds as presented in *Figure 2* the experiments b) and f) have to be compared. During the reduction b) of **1** with **5(I)** as catalyst H-bonds as presented in *Figure 2* are impossible. In experiment f) the postulated H-bonds are formally possible and might have some significance. As both experiments led to a similar enantiomeric excess in the product **3** and **8**, respectively, a participation of H-bonds as shown in *Figure 2* can be ruled out.

Scheme 4 summarizes the reduction of the amides **7** and **9** using **4(I)** and **5(I)** as catalysts. It is reasonable to assume that the $3d_{z^2}$ orbitals in **4(I)** and **5(I)** show similar nucleophilicity[13]) and attack therefore the electrophiles present in the system with comparable speed. The nucleophilic alkylation[14]) of **5(I)** produces the

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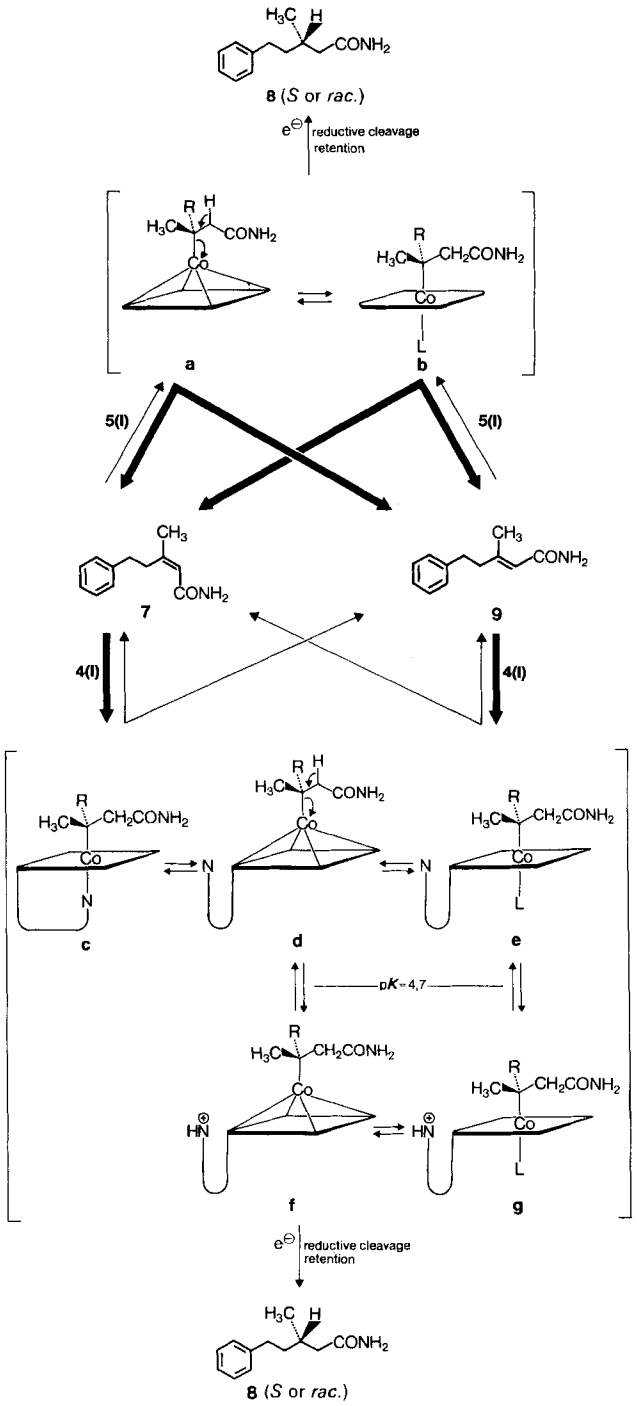
[12]) Due to the catalyst **5(I)**.

[13]) Compare [20–22].

[14]) For the terms nucleophilic alkylation, reductive fragmentation, reductive cleavage and the observation of the corresponding phenomena compare [6].

Scheme 4


8 (S or rac.)
e⊖ reductive cleavage retention
a
b
5(l)
5(l)
7
9
4(l)
4(l)
c
d
e
pK=4,7
f
g
e⊖ reductive cleavage retention
8 (S or rac.)

corresponding alkylcobalamins **a** and **b**[15]). In a second step a reductive cleavage[14]) known to proceed with retention at the C-atom involved[16]) produces the final product **8**. From the intermediate alkylcobalamins **a** and **b** a reductive fragmentation[14]) leads back to the starting material with or without isomerization. The nucleophilic alkylation of the catalyst **4(I)** results in the formation of the alkylcobalamins **c**–**g**[15]). A subsequent reductive cleavage with retention produces the saturated amide **8**. The extensive isomerization revealed by the catalyst **5(I)**, and not by **4(I)**, can be ascribed to different factors. The catalyst **5(I)** exists *a priori* in a 'base off' form and might therefore produce alkylcobalamins prone to suffer a reductive fragmentation induced by the decreased electron density on the central Co-atom. The octahedral Co-atom displays a definitely higher electron density in the 'base on' form **c**, an intermediate only formed from **4(I)**. A second explanation for the enhanced reductive fragmentation in the case of **5(I)** might be the distinctly slower reductive cleavage in the reductions catalyzed by **5(I)**. Finally a combination of the two factors cited above might also be possible.

Experimental Part

(With the assistance of *K. Bichsel, D. Süss* and *R. Unger*)

General remarks. S. [23] [24]. The procedure followed during a 'usual' or 'normal' extraction is described in [23].

The authors would like to express their gratitude to our colleagues from the Central Research Units, in particular to Dr. *A. Dirscherl* (microanalysis), *G. Oesterheld* (GC./MS.), Dr. *L. Chopard* (IR.), Dr. *G. Englert* (NMR.), Dr. *W. Arnold* (NMR.) and *W. Meister* (MS.) for the analytical and spectroscopical data.

A) Reductions using catalytic amounts of cob(I)alamin (4(I)). – *Reduction of* **1** *to ethyl (S)-3-methyl-5-phenylvalerate ((S)-3).* Following the procedure described earlier [2] 311 mg (0.1 mol-equiv.) of cyanocob(III)alamin (**4**) were transformed to the catalyst. The catalyst residue was dissolved in 10.5 ml of CH_3COOH/H_2O 6:1. To the suspension of the homogeneous catalyst and an excess of metallic zinc (20 mol-equiv.) 500 mg of ethyl (*Z*)-3-methyl-5-phenyl-2-pentenoate[17]) (**1**) in 3.5 ml of CH_3COOH/H_2O 6:1 was added. The mixture was stirred in the dark at +10° for 70 h under Ar. Following the usual extraction the crude product was purified by chromatography (SiO_2, ether/hexane 1:10): 405 mg (80%) of pure **3**[18]), (*S*)-configuration, enantiomeric excess of 26.7% ($[\alpha]^{RT.}$: −4.3 (589), −16.0 (365) (*c* = 1, ethanol)). No other products were isolated after chromatography.

Reduction of **6**[18]) *to* rac-**3**. Following the same procedure as for **1**→**3** with **4**, 394 mg (78%) of pure racemic **3**[18]) were obtained. No other products were isolated after chromatography.

Reduction of **7** *to (S)-3-methyl-5-phenylvaleramide ((S)-8).* Following the procedure described earlier [2] 358 mg (0.1 mol-equiv.) of **4** were transformed to the catalyst. The catalyst residue was dissolved in 10.5 ml of CH_3COOH/H_2O 6:1. To the suspension of the homogeneous catalyst and an excess of metallic zinc (20 mol-equiv.) 500 mg of (*Z*)-3-methyl-5-phenyl-2-pentenamide (**7**)[19]) in 3.5 ml of CH_3COOH/H_2O 6:1 were added. The mixture was stirred in the dark at +10° for 24 h under Ar. Following the usual extraction the crude product was purified by chromatography

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15) Only the diastereomer after *re* attack is shown.

16) See [1].

17) For the preparation and the data of **1** compare [2].

18) For the analytical, chiroptical and spectroscopical data, and the proof of the absolute configuration see [2].

19) See [3].

(SiO_2, ethyl acetate/hexane 20:1): 295 mg (78%) of pure **8**[19]), (*S*)-configuration, enantiomeric excess of 20% ($[\alpha]^{RT}$·: −2.9 (589), −3.9 (365) ($c = 1$, ethanol)). No additional products could be isolated after chromatography.

Reduction of **9**[19]) *to* rac-**8**. Following the same procedure as for **7**→**8** using **4**, with the exception of a prolonged reaction time of 90 h, 480 mg (95%) of pure racemic **8**[19]) were obtained. No other products could be isolated after chromatography.

B) Reductions using catalytic amounts of heptamethyl cob(I)yrinate (5(I)). – *Reduction of* **1** *to (*S*)-***3***.* Analogously to the procedure described earlier [2] 249.5 mg (0.1 mol-equiv.) of heptamethyl dicyano-cob(III)yrinate (**5**)[20]) were transformed to the catalyst. The catalyst residue was dissolved in 10.5 ml of CH_3COOH/H_2O 6:1. To the suspension of the homogenous catalyst and an excess of metallic zinc (20 mol-equiv.) 500 mg of **1**[17]) in 3.5 ml of CH_3COOH/H_2O 6:1 were added. The mixture was stirred in the dark at +10° for 90 h under Ar. Following the usual extraction the crude product was purified by chromatography (SiO_2, ether/hexane 1:10) giving 151 mg (31%) of **1**[18]), 40 mg (8%) of **6** (*E*)-configuration and 215 mg (43%) of **3** of (*S*)-configuration and an enantiomeric excess of 15.4% ($[\alpha]^{RT}$·: −2.5 (589), −9.5 (365) ($c = 1$, ethanol)). No additional products were isolated after chromatography.

Reduction of **6**[18]) *to* rac-**3**. Following an identical procedure to the one for **1**→**3** with **5**, 260 mg (52%) of racemic **3** and 180 mg (36%) of **6**[18]) were obtained. Neither the (*Z*)-configurated isomer of **6** nor other products have been isolated after chromatography.

Reduction of **7** *to (*S*)-***8***.* Analogously to the procedure described earlier [2] 287.5 mg (0.1 mol-equiv.) of **5** were transformed to the catalyst. The catalyst residue was dissolved in 10.5 ml of CH_3COOH/H_2O 6:1. To the suspension of the homogeneous catalyst and an excess of metallic zinc (20 mol-equiv.) 500 mg of **7**[19]) in 3.5 ml of CH_3COOH/H_2O 6:1 were added. The mixture was stirred in the dark at +10° for 46 h under Ar. Following the usual extraction the crude product was purified by chromatography (SiO_2, ethyl acetate/hexane 20:1) giving 70 mg (14%) of **7**[19]), 80 mg (16%) of **9** ((*E*)-configuration) and 278 mg (55%) of **8**[19]) showing (*S*)-configuration and an enantiomeric excess of 14% ($[\alpha]^{RT}$·: −2.0 (589), −2.7 (365) ($c = 1$, ethanol)). Additional products could not be detected.

Reduction of **9**[19]) *to (*S*)-***8***.* Following an identical procedure to the one for **7**→**8** with **5**, 105 mg (21%) of **9**[19]), 30 mg (6%) of **7**[19]) ((*Z*)-configuration) and 285 mg (56%) of **8** with (*S*)-configuration and a rather weak enantiomeric excess of 3.7% ($[\alpha]^{RT}$·: −0.5 (589), −0.8 (365) ($c = 1$, ethanol)) were obtained. No additional products could be detected.

C) Results of X-ray analysis.

Table 2. *Final coordinates (with standard deviations) and thermal parameters*

Atom	x	y	z	B
C(1)	0.3964 (7)	0.6154 (9)	0.6944 (7)	2.4
C(2)	0.4126 (7)	0.6599 (9)	0.6020 (8)	2.7
C(3)	0.3222 (7)	0.7068 (9)	0.5431 (8)	2.5
C(4)	0.2625 (7)	0.6445 (9)	0.5768 (8)	2.4
C(5)	0.1669 (7)	0.6381 (9)	0.5234 (8)	2.5
C(6)	0.1149 (7)	0.5855 (8)	0.5606 (7)	2.3
C(7)	0.0166 (7)	0.5695 (9)	0.5100 (8)	2.8
C(8)	−0.0116 (7)	0.5284 (9)	0.5993 (8)	3.1

Table 2 (continued).

Atom	x	y	z	B
C(15)	0.3777 (7)	0.3662 (10)	0.9231 (8)	2.9
C(16)	0.4219 (7)	0.4212 (9)	0.8671 (8)	2.7
C(17)	0.5189 (8)	0.4176 (10)	0.8825 (8)	2.9
C(18)	0.5265 (7)	0.5057 (13)	0.8122 (8)	3.4
C(19)	0.4341 (7)	0.5127 (10)	0.7352 (7)	2.9
N(20)	0.2324 (6)	0.4045 (8)	0.8128 (7)	2.6
N(21)	0.1407 (6)	0.5299 (7)	0.6483 (6)	2.5
N(22)	0.3009 (6)	0.5951 (7)	0.6566 (6)	2.3
N(23)	0.3790 (6)	0.4742 (7)	0.7920 (6)	2.8
C(24)	0.2546 (9)	0.6011 (10)	0.8220 (10)	3.2
C(25)	0.2537 (8)	0.3959 (10)	0.6335 (9)	3.2
N(26)	0.2473 (9)	0.6585 (11)	0.8789 (10)	5.1
N(27)	0.2528 (10)	0.3326 (12)	0.5793 (12)	5.7
Co(28)	0.2591 (1)	0.5000 (0)	0.7281 (1)	[a])
C(29)	0.4147 (8)	0.6942 (10)	0.7790 (9)	3.1
C(30)	0.5991 (8)	0.4935 (14)	0.7698 (9)	4.2
C(31)	0.6862 (10)	0.5315 (11)	0.8357 (11)	4.3
O(32)	0.6970 (9)	0.5907 (11)	0.8998 (10)	7.0
O(33)	0.7502 (7)	0.4903 (10)	0.8148 (8)	5.3
C(34)	0.8368 (12)	0.5239 (16)	0.8707 (14)	6.7
C(35)	0.5818 (9)	0.4375 (11)	0.9883 (10)	3.8
C(36)	0.5568 (10)	0.5332 (13)	1.0323 (12)	5.2
C(37)	0.5934 (10)	0.5318 (11)	1.1448 (11)	4.3
O(38)	0.5901 (7)	0.4618 (9)	1.1960 (8)	5.3
O(39)	0.6311 (8)	0.6200 (11)	1.1761 (9)	6.7
C(40)	0.6642 (16)	0.6348 (21)	1.2867 (18)	8.8
C(41)	0.5394 (10)	0.3116 (12)	0.8512 (11)	4.7
C(42)	0.4321 (9)	0.3118 (11)	1.0210 (10)	3.9
C(43)	0.2454 (9)	0.3862 (12)	1.0414 (10)	4.1
C(44)	0.2356 (11)	0.3324 (13)	1.1309 (12)	5.4
C(45)	0.2292 (11)	0.4046 (14)	1.2043 (12)	5.0
O(46)	0.2417 (9)	0.3625 (12)	1.2907 (10)	7.4
O(47)	0.2037 (10)	0.4895 (15)	1.1884 (11)	8.8
C(48)	0.2200 (15)	0.4295 (19)	1.3666 (17)	8.1
C(49)	0.0703 (11)	0.3117 (14)	0.9165 (12)	5.4
C(50)	0.1443 (11)	0.1924 (14)	0.8343 (13)	5.7
C(51)	−0.0480 (10)	0.6057 (12)	0.6492 (11)	4.5
C(52)	0.0190 (10)	0.6870 (12)	0.7100 (11)	4.5
C(53)	−0.0131 (10)	0.7505 (12)	0.7728 (11)	4.3
O(54)	0.0309 (9)	0.8327 (12)	0.7964 (10)	7.5
O(55)	−0.0735 (12)	0.7355 (15)	0.7967 (13)	9.6
C(56)	0.0131 (14)	0.9047 (18)	0.8588 (16)	7.4
C(57)	0.0122 (8)	0.4806 (10)	0.4359 (9)	3.6
C(58)	−0.0753 (9)	0.4346 (11)	0.3866 (10)	4.0
O(59)	−0.1173 (7)	0.4760 (8)	0.3029 (7)	5.0
O(60)	−0.1048 (8)	0.3643 (10)	0.4227 (8)	5.7
C(61)	−0.2003 (13)	0.4250 (17)	0.2466 (15)	6.5
C(62)	−0.0411 (9)	0.6593 (12)	0.4599 (10)	4.2
C(63)	0.1327 (8)	0.6917 (10)	0.4257 (9)	3.4
C(64)	0.3078 (9)	0.8225 (11)	0.5536 (10)	3.8
C(65)	0.3359 (10)	0.8832 (13)	0.4805 (11)	4.9
C(66)	0.2983 (9)	0.9895 (13)	0.4700 (10)	4.3

Table 2 (continued)

Atom	x	y	z	B
O(67)	0.2314 (10)	1.0101 (14)	0.4932 (11)	8.3
O(68)	0.3403 (7)	1.0561 (9)	0,4435 (7)	5.0
C(69)	0.3006 (11)	1.1556 (14)	0.4163 (13)	5.9
C(70)	0.4883 (9)	0.7335 (12)	0.6282 (11)	4.3
C(71)	0.4277 (9)	0.5692 (11)	0.5389 (10)	3.9
C(72)	0.4341 (10)	0.5959 (13)	0.4399 (11)	4.5
O(73)	0.4337 (7)	0.5155 (11)	0.3899 (8)	6.3
O(74)	0.4352 (10)	0.6822 (12)	0.4059 (10)	7.6
C(75)	0.4383 (13)	0.5262 (17)	0.2870 (15)	7.0
O(76)	0.7893 (12)	0.2716 (15)	0.9794 (14)	4.2
O(77)	0.8072 (13)	0.1974 (16)	0.9230 (14)	4.2

[a]) Anisotropic temperature factor: $T = \exp-(B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{23}kl + B_{13}hl + B_{12}hk)$

Atom	B_{11}	B_{22}	B_{33}	B_{23}	B_{13}	B_{12}
Co(28)	0.0023	0.0040	0.0021	0.0003	0.0012	0.0001

Table 3. *Bond lengths (with standard deviations) in Å*

C(2),C(1)	1.566 (0.009)	C(14),C(13)	1.513 (0.010)	O(38),C(37)	1.200 (0.010)
C(19),C(1)	1.525 (0.010)	C(43),C(13)	1.548 (0.012)	O(39),C(37)	1.325 (0.012)
N(22),C(1)	1.496 (0.008)	C(15),C(14)	1.360 (0.010)	C(40),O(39)	1.519 (0.016)
C(29),C(1)	1.558 (0.010)	N(20),C(14)	1.357 (0.009)	C(44),C(43)	1.533 (0.013)
C(3),C(2)	1.565 (0.009)	C(16),C(15)	1.453 (0.010)	C(45),C(44)	1.458 (0.014)
C(70),C(2)	1.519 (0.012)	C(42),C(15)	1.570 (0.011)	O(46),C(45)	1.321 (0.012)
C(71),C(2)	1.577 (0.011)	C(17),C(16)	1.530 (0.010)	O(47),C(45)	1.192 (0.014)
C(4),C(3)	1.483 (0.009)	N(23),C(16)	1.284 (0.008)	C(48),O(46)	1.545 (0.016)
C(64),C(3)	1.563 (0.011)	C(18),C(17)	1.580 (0.011)	C(52),C(51)	1.576 (0.013)
C(5),C(4)	1.495 (0.009)	C(35),C(17)	1.551 (0.011)	C(53),C(52)	1.460 (0.013)
N(22),C(4)	1.290 (0.009)	C(41),C(17)	1.544 (0.012)	O(54),C(53)	1.285 (0.012)
C(6),C(5)	1.347 (0.009)	C(19),C(18)	1.548 (0.009)	O(55),C(53)	1.171 (0.013)
C(63),C(5)	1.510 (0.010)	C(30),C(18)	1.521 (0.010)	C(56),O(54)	1.410 (0.015)
C(7),C(6)	1.542 (0.009)	N(23),C(19)	1.501 (0.008)	C(58),C(57)	1.498 (0.011)
N(21),C(6)	1.402 (0.008)	Co(28),N(20)	1.911 (0.006)	O(59),C(58)	1.295 (0.010)
C(8),C(7)	1.609 (0.010)	Co(28),N(21)	1.931 (0.005)	O(60),C(58)	1.241 (0.011)
C(57),C(7)	1.577 (0.011)	Co(28),N(22)	1.898 (0.006)	C(61),O(59)	1.489 (0.014)
C(62),C(7)	1.537 (0.011)	Co(28),N(23)	1.897 (0.005)	C(65),C(64)	1.519 (0.013)
C(9),C(8)	1.483 (0.010)	N(26),C(24)	1.157 (0.011)	C(66),C(65)	1.521 (0.015)
C(51),C(8)	1.487 (0.012)	Co(28),C(24)	1.925 (0.008)	O(67),C(66)	1.281 (0.011)
C(10),C(9)	1.380 (0.010)	N(27),C(25)	1.144 (0.011)	O(68),C(66)	1.255 (0.011)
N(21),C(9)	1.349 (0.009)	Co(28),C(25)	1.923 (0.008)	C(69),O(68)	1.462 (0.013)
C(11),C(10)	1.394 (0.010)	C(31),C(30)	1.508 (0.012)	C(72),C(71)	1.514 (0.012)
C(12),C(11)	1.497 (0.011)	O(32),C(31)	1.182 (0.011)	O(73),C(72)	1.286 (0.012)
N(20),C(11)	1.367 (0.009)	O(33),C(31)	1.304 (0.011)	O(74),C(72)	1.245 (0.013)
C(13),C(12)	1.553 (0.011)	C(34),O(33)	1.444 (0.013)	C(75),O(73)	1.523 (0.014)
C(49),C(12)	1.560 (0.013)	C(36),C(35)	1.534 (0.013)	O(77),O(76)	1.370 (0.016)
C(50),C(12)	1.547 (0.014)	C(37),C(36)	1.533 (0.013)		

Table 4. *Bond angles (with standard deviations) in degrees*

C(19)–C(1)–C(2)	120.1 (0.6)	C(42)–C(15)–C(16)	119.7 (0.6)
N(22)–C(1)–C(2)	102.4 (0.5)	C(17)–C(16)–C(15)	126.4 (0.6)
N(22)–C(1)–C(19)	102.6 (0.5)	N(23)–C(16)–C(15)	120.8 (0.6)
C(29)–C(1)–C(2)	112.1 (0.6)	N(23)–C(16)–C(17)	112.6 (0.6)
C(29)–C(1)–C(19)	110.3 (0.5)	C(18)–C(17)–C(16)	100.8 (0.6)
C(29)–C(1)–N(22)	107.9 (0.5)	C(35)–C(17)–C(16)	116.6 (0.6)
C(3)–C(2)–C(1)	102.1 (0.5)	C(35)–C(17)–C(18)	109.9 (0.6)
C(70)–C(2)–C(1)	112.9 (0.6)	C(41)–C(17)–C(16)	107.7 (0.6)
C(70)–C(2)–C(3)	115.0 (0.6)	C(41)–C(17)–C(18)	114.1 (0.6)
C(71)–C(2)–C(1)	108.4 (0.6)	C(41)–C(17)–C(35)	107.9 (0.7)
C(71)–C(2)–C(3)	106.9 (0.6)	C(19)–C(18)–C(17)	103.6 (0.6)
C(71)–C(2)–C(70)	110.9 (0.6)	C(30)–C(18)–C(17)	115.1 (0.7)
C(4)–C(3)–C(2)	102.1 (0.5)	C(30)–C(18)–C(19)	115.1 (0.6)
C(64)–C(3)–C(2)	118.8 (0.6)	C(18)–C(19)–C(1)	120.0 (0.7)
C(64)–C(3)–C(4)	111.9 (0.6)	N(23)–C(19)–C(1)	105.9 (0.5)
C(5)–C(4)–C(3)	123.6 (0.6)	N(23)–C(19)–C(18)	102.1 (0.5)
N(22)–C(4)–C(3)	113.6 (0.6)	C(14)–N(20)–C(11)	109.3 (0.6)
N(22)–C(4)–C(5)	122.8 (0.6)	Co(28)–N(20)–C(11)	124.0 (0.5)
C(6)–C(5)–C(4)	121.0 (0.6)	Co(28)–N(20)–C(14)	126.3 (0.5)
C(63)–C(5)–C(4)	116.7 (0.6)	C(9)–N(21)–C(6)	111.3 (0.5)
C(63)–C(5)–C(6)	122.3 (0.6)	Co(28)–N(21)–C(6)	125.6 (0.4)
C(7)–C(6)–C(5)	125.5 (0.6)	Co(28)–N(21)–C(9)	122.5 (0.5)
N(21)–C(6)–C(5)	126.6 (0.6)	C(4)–N(22)–C(1)	111.6 (0.6)
N(21)–C(6)–C(7)	107.8 (0.5)	Co(28)–N(22)–C(1)	116.4 (0.4)
C(8)–C(7)–C(6)	101.7 (0.5)	Co(28)–N(22)–C(4)	131.9 (0.5)
C(57)–C(7)–C(6)	102.9 (0.5)	C(19)–N(23)–C(16)	113.0 (0.5)
C(57)–C(7)–C(8)	109.6 (0.6)	Co(28)–N(23)–C(16)	133.6 (0.5)
C(62)–C(7)–C(6)	119.7 (0.6)	Co(28)–N(23)–C(19)	112.8 (0.4)
C(62)–C(7)–C(8)	110.0 (0.6)	Co(28)–C(24)–N(26)	175.6 (0.8)
C(62)–C(7)–C(57)	112.1 (0.6)	Co(28)–C(25)–N(27)	177.8 (0.8)
C(9)–C(8)–C(7)	100.2 (0.5)	N(21)–Co(28)–N(20)	96.7 (0.2)
C(51)–C(8)–C(7)	115.4 (0.6)	N(22)–Co(28)–N(20)	172.3 (0.2)
C(51)–C(8)–C(9)	113.1 (0.6)	N(22)–Co(28)–N(21)	90.8 (0.2)
C(10)–C(9)–C(8)	121.2 (0.7)	N(23)–Co(28)–N(20)	89.6 (0.2)
N(21)–C(9)–C(8)	112.2 (0.6)	N(23)–Co(28)–N(21)	172.7 (0.2)
N(21)–C(9)–C(10)	126.4 (0.7)	N(23)–Co(28)–N(22)	83.1 (0.2)
C(11)–C(10)–C(9)	126.3 (0.7)	C(24)–Co(28)–N(20)	86.2 (0.3)
C(12)–C(11)–C(10)	123.7 (0.7)	C(24)–Co(28)–N(21)	90.5 (0.3)
N(20)–C(11)–C(10)	124.0 (0.7)	C(24)–Co(28)–N(22)	91.9 (0.3)
N(20)–C(11)–C(12)	112.3 (0.6)	C(24)–Co(28)–N(23)	93.5 (0.3)
C(13)–C(12)–C(11)	100.1 (0.6)	C(25)–Co(28)–N(20)	91.1 (0.3)
C(49)–C(12)–C(11)	112.6 (0.7)	C(25)–Co(28)–N(21)	85.8 (0.3)
C(49)–C(12)–C(13)	117.7 (0.7)	C(25)–Co(28)–N(22)	91.3 (0.3)
C(50)–C(12)–C(11)	109.3 (0.7)	C(25)–Co(28)–N(23)	90.5 (0.3)
C(50)–C(12)–C(13)	108.3 (0.7)	C(25)–Co(28)–C(24)	175.1 (0.4)
C(50)–C(12)–C(49)	108.4 (0.8)	C(31)–C(30)–C(18)	114.3 (0.7)
C(14)–C(13)–C(12)	102.6 (0.6)	O(32)–C(31)–C(30)	125.0 (0.9)
C(43)–C(13)–C(12)	114.4 (0.7)	O(33)–C(31)–C(30)	112.1 (0.8)
C(43)–C(13)–C(14)	108.8 (0.6)	O(33)–C(31)–O(32)	122.8 (0.9)
C(15)–C(14)–C(13)	123.4 (0.6)	C(34)–O(33)–C(31)	117.1 (0.8)
N(20)–C(14)–C(13)	109.9 (0.6)	C(36)–C(35)–C(17)	111.7 (0.7)
N(20)–C(14)–C(15)	126.6 (0.7)	C(37)–C(36)–C(35)	111.6 (0.8)
C(16)–C(15)–C(14)	121.9 (0.7)	O(38)–C(37)–C(36)	125.7 (0.8)
C(42)–C(15)–C(14)	118.4 (0.7)	O(39)–C(37)–C(36)	108.8 (0.8)

Table 4 (continued).

O(39)–C(37)–O(38)	125.5 (0.8)	O(59)–C(58)–C(57)	113.1 (0.7)
C(40)–O(39)–C(37)	115.6 (1.0)	O(60)–C(58)–C(57)	123.4 (0.8)
C(44)–C(43)–C(13)	113.9 (0.8)	O(60)–C(58)–O(59)	123.5 (0.8)
C(45)–C(44)–C(43)	111.5 (0.9)	C(61)–O(59)–C(58)	114.6 (0.8)
O(46)–C(45)–C(44)	112.8 (1.0)	C(65)–C(64)–C(3)	111.0 (0.7)
C(47)–C(45)–C(44)	125.6 (1.0)	C(66)–C(65)–C(64)	110.5 (0.8)
O(47)–C(45)–O(46)	120.7 (1.0)	O(67)–C(66)–C(65)	121.6 (1.0)
C(48)–O(46)–C(45)	115.7 (1.0)	O(68)–C(66)–C(65)	115.7 (0.8)
C(52)–C(51)–C(8)	115.0 (0.7)	O(68)–C(66)–O(67)	122.6 (1.0)
C(53)–C(52)–C(51)	114.2 (0.8)	C(69)–C(68)–C(66)	118.3 (0.8)
O(54)–C(53)–C(52)	111.3 (0.9)	C(72)–C(71)–C(2)	116.5 (0.7)
O(55)–C(53)–C(52)	127.4 (1.1)	O(73)–C(72)–C(71)	110.6 (0.8)
O(55)–C(53)–O(54)	121.3 (1.1)	O(74)–C(72)–C(71)	127.1 (0.9)
C(56)–O(54)–C(53)	121.6 (0.9)	O(74)–C(72)–O(73)	122.2 (0.9)
C(58)–C(57)–C(7)	116.2 (0.6)	C(75)–O(73)–C(72)	118.8 (0.9)

Table 5. *Some torsion angles*

C(1)–C(2)–C(3)–C(4)	– 26.28	C(19)–N(23)–C(16)–C(17)	3.99
C(2)–C(3)–C(4)–N(22)	17.17	N(23)–C(16)–C(17)–C(18)	13.85
C(3)–C(4)–N(22)–C(1)	0.66	N(22)–Co(28)–N(23)–C(18)	– 0.74
C(4)–N(22)–C(1)–C(2)	– 18.19	N(22)–Co(28)–N(23)–C(19)	– 17.69
N(22)–C(1)–C(2)–C(3)	26.73	Co(28)–N(23)–C(19)–C(1)	40.75
C(4)–C(5)–C(6)–N(21)	– 1.66	N(23)–C(19)–C(1)–N(22)	– 44.57
C(5)–C(6)–N(21)–Co(28)	– 9.05	C(19)–C(1)–N(22)–Co(28)	34.03
C(6)–N(21)–Co(28)–N(22)	12.20	C(1)–C(2)–C(3)–C(4)	– 26.28
N(21)–Co(28)–N(22)–C(4)	– 9.90	C(2)–C(3)–C(4)–C(5)	–162.18
Co(28)–N(22)–C(4)–C(5)	3.18	C(3)–C(4)–C(5)–C(6)	–175.70
N(22)–C(4)–C(5)–C(6)	5.01	C(4)–C(5)–C(6)–C(7)	–176.94
C(6)–C(7)–C(8)–C(9)	– 24.33	C(5)–C(6)–C(7)–C(8)	–165.81
C(7)–C(8)–C(9)–N(21)	24.65	C(6)–C(7)–C(8)–C(9)	– 24.33
C(8)–C(9)–N(21)–C(6)	– 14.38	C(7)–C(8)–C(9)–C(10	–159.56
C(9)–N(21)–C(6)–C(7)	– 3.84	C(8)–C(9)–C(10)–C(11)	–173.52
N(21)–C(6)–C(7)–C(8)	18.18	C(9)–C(10)–C(11)–C(12)	–179.46
C(9)–C(10)–C(11)–N(20)	– 1.14	C(10)–C(11)–C(12)–C(13)	–161.63
C(10)–C(11)–N(20)–Co(28)	0.14	C(11)–C(12)–C(13)–C(14)	– 22.85
C(11)–N(20)–Co(28)–N(21)	0.29	C(12)–C(13)–C(14)–C(15)	–162.98
N(20)–Co(28)–N(21)–C(9)	0.10	C(13)–C(14)–C(15)–C(16)	–174.05
Co(28)–N(21)–C(9)–C(10)	– 0.99	C(14)–C(15)–C(16)–C(17)	–169.73
N(21)–C(9)–C(10)–C(11)	1.63	C(15)–C(16)–C(17)–C(18)	–170.94
C(11)–C(12)–C(13)–C(14)	– 22.85	C(16)–C(17)–C(18)–C(19)	– 24.90
C(12)–C(13)–C(14)–N(20)	20.88	C(17)–C(18)–C(19)–C(1)	143.69
C(13)–C(14)–N(20)–C(11)	– 9.00	C(18)–C(19)–C(1)–C(2)	88.28
C(14)–N(20)–C(11)–C(12)	– 7.71	C(19)–C(1)–C(2)–C(3)	139.45
N(20)–C(11)–C(12)–C(13)	19.88	C(19)–C(1)–C(2)–C(71)	26.84
C(14)–C(15)–C(16)–N(23)	5.12	C(1)–C(2)–C(71)–C(72)	173.04
C(15)–C(16)–N(23)–Co(28)	– 1.11	C(2)–C(71)–C(72)–O(73)	–170.76
C(16)–N(23)–Co(28)–N(20)	– 5.73	C(71)–C(72)–O(73)–C(75)	179.02
N(23)–Co(28)–N(20)–C(14)	11.38	C(1)–C(2)–C(3)–C(64)	97.29
Co(28)–N(20)–C(14)–C(15)	– 11.50	C(2)–C(3)–C(64)–C(65)	87.30
N(20)–C(14)–C(15)–C(16)	1.42	C(3)–C(64)–C(65)–C(66)	163.47
C(16)–C(17)–C(18)–C(19)	– 24.90	C(64)–C(65)–C(66)–O(68)	154.06
C(17)–C(18)–C(19)–N(23)	27.16	C(65)–C(66)–O(68)–C(69)	169.99
C(18)–C(19)–N(23)–C(16)	– 20.42	C(3)–C(4)–C(5)–C(63)	5.42

Table 5 (continued).

C(5)–C(6)–C(7)–C(57)	80.65	C(44)–C(45)–O(46)–C(48)	–169.52
C(6)–C(7)–C(57)–C(58)	169.90	C(13)–C(14)–C(15)–C(42)	4.38
C(7)–C(57)–C(58)–O(59)	92.47	C(15)–C(16)–C(17)–C(35)	– 52.01
C(57)–C(58)–O(59)–C(61)	173.54	C(16)–C(17)–C(35)–C(36)	– 49.42
C(6)–C(7)–C(8)–C(51)	97.46	C(17)–C(35)–C(36)–C(37)	157.89
C(7)–C(8)–C(51)–C(52)	– 68.65	C(35)–C(36)–C(37)–O(39)	132.14
C(8)–C(51)–C(52)–C(53)	–169.22	C(36)–C(37)–O(39)–C(40)	174.98
C(51)–C(52)–C(53)–O(54)	–160.10	C(16)–C(17)–C(18)–C(30)	–151.48
C(52)–C(53)–O(54)–C(56)	–178.34	C(17)–C(18)–C(30)–C(31)	– 84.96
C(10)–C(11)–C(12)–C(50)	84.79	C(18)–C(30)–C(31)–O(33)	158.03
C(10)–C(11)–C(12)–C(49)	– 35.84	C(30)–C(31)–O(33)–C(34)	177.68
C(11)–C(12)–C(13)–C(43)	94.80	C(19)–C(1)–C(2)–C(70)	– 96.45
C(12)–C(13)–C(43)–C(44)	91.01	C(5)–C(6)–C(7)–C(62)	– 44.48
C(13)–C(43)–C(44)–C(45)	–173.00	C(15)–C(16)–C(17)–C(41)	69.29
C(43)–C(44)–C(45)–O(46)	–164.65		

Table 6. *Least squares plane of the corrin system*

Plane calculated using atoms C(1) through C(19), N(20) through N(23) and Co(28)
Equation of this plane: $0.2246x - 0.7664y - 0.6019z = -10.8220$
Deviations from this plane: C(1) –0.414, C(2) 0.055, C(3) –0.206, C(4) –0.108, C(5) 0.102, C(6) 0.098, C(7) 0.369, C(8) –0.149, C(9) –0.011, C(10) 0.061, C(11) 0.065, C(12) 0.156, C(3) –0.363, C(14) –0.102, C(15) –0.085, C(16) 0.042, C(17) 0.292, C(18) 0.081, C(19) 0.386, N(20) 0.018, N(21) –0.060, N(22) –0.208, N(23) 0.045, Co(28) –0.064, C(24) –1.977, and C(25) 1.852 Å

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