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COMMISSION ON BIOCHEMICAL NOMENCLATURE

# NOMENCLATURE OF CORRINOIDS

(RULES APPROVED 1975)

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## NOMENCLATURE OF CORRINOIDS‡

(RULES APPROVED 1975)

1. The corrinoids are a group of compounds containing four reduced pyrrole rings joined into a macrocyclic ring by links between their  $\alpha$ -positions; three of these links are formed by one-carbon units (methylidyne radicals) and the other by a direct C $\alpha$ -C $\alpha$  bond. They include various B-12 vitamins, factors, and derivatives based upon the skeleton of **corrin**, C<sub>19</sub>H<sub>22</sub>N<sub>4</sub> (structure I). The atoms are numbered and the rings are lettered as shown in structure I. The numbering is thus the same as that of the porphyrin nucleus, number 20 being omitted to preserve the identity.

*Note.* The name "corrin" was proposed by those who established its structure because it is the *core* of the vitamin B-12 molecule; the letters "co" of corrin are *not* derived from the fact that vitamin B-12 contains cobalt. However, this does not apply to the "cob" terms below, all of which do contain "co" for cobalt.

2. Some important corrinoids that are more unsaturated than corrin itself are derivatives of octadecahydrocorrin. This has sometimes been called tetradecahydrocorrin§ because it has four additional double bonds. Although this could be indicated by the prefix "tetrakis(didehydro)", "octadecahydro" is preferred.

The octadecahydrocorrin system IA has the trivial name **corrole**.

3. Many important corrinoids have a regular pattern of substituents on the methylene carbon atoms of the reduced pyrrole rings and a cobalt atom in the center of the macrocyclic ring. The heptacarboxylic acid II is named **cobyric acid**. The carboxyl groups are designated by the locants *a-g*, as shown in II.¶ Cobyric *a,b,c,d,e,g*-hexamide, formerly sometimes referred to as *Factor V<sub>1a</sub>*, is named **cobyric acid**.¶ Substituents on the side chains may be designated by appropriate locants, e.g.  $7\beta^1$ -methylcobyric acid, if  $-\text{CH}(\text{CH}_3)\text{CO}_2\text{H}$  replaces  $-\text{CH}_2\text{CO}_2\text{H}$  at C- $7\beta$  ofobyric acid.

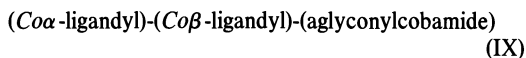
4. The compound III (R=OH, R'=H), which is the amide formed by combination ofobyric acid with D-1-amino-2-propanol at position *f*, is named **cobinic acid**;¶ its hexamide (III; R=H<sub>2</sub>N, R'=H) is named **cobinamide**.¶

5. The compound III (R=OH, R'=structure V) in which cobinic acid is further substituted at the 2 position of the aminopropanol by an  $\alpha$ -D-ribofuranose 3-phosphate residue (V) is named **cobamic acid**;¶ its hexamide (III; R=NH<sub>2</sub>, R'=V) is named **cobamide**.¶

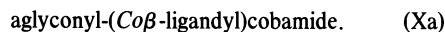
6. Glycosyls and nucleotides (which are N-glycosyl derivatives at C-1 of the ribofuranose unit) of cobamides are named by adding the name of the appropriate aglycon radical (ending in "yl") as a prefix to the name of the corrinoid allotted according to 1-5, e.g. aglyconylcobamide (VI).

7. Most of the important natural products in this series have aglycon radicals containing an imidazole nucleus, one N of the latter being covalently bonded to the ribose while the other is coordinately bonded to what is, by this attachment, defined as the cobalt- $\alpha$  position. *The latter situation (VII) is assumed to exist unless otherwise indicated.* When another ligand occupies the cobalt- $\alpha$  position, it and its locant may be indicated by, e.g. (Co $\alpha$  ligand)-aglyconylcobamide (VIII). The absence of a "Co $\alpha$ -ligand" term, as in the cobalamins (Sec. 9), indicates that the aglycon radical attached to the ribose occupies the cobalt- $\alpha$  position as well.

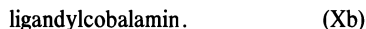
8. Cobamides bearing a ligand in the cobalt- $\beta$  position [which implies Co(III)] may be named as follows:



or, if the aglycon is attached to the cobalt- $\alpha$  position, as indicated in Section 7,

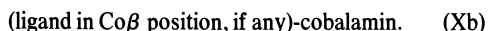


In a cobalamin (see 9 below), the latter becomes simply



See also Section 15.

9. **Cobalamins**.¶ A cobalamin is a cobamide in which 5,6-dimethylbenzimidazole is the aglycon attached by a glycosyl link from its N-1 to the C-1 of the ribose and additionally linked, as stated in 7 above, by a bond between the N-3 and the cobalt (in position  $\alpha$ ).¶ They may be named as cobamides, as above, or according to the pattern:



Examples:

Co $\alpha$  - [ $\alpha$  - (5,6-dimethylbenzimidazolyl)] - Co $\beta$  - cyanocobamide, also known as vitamin B-12, is termed **cyanocobalamin**.

Co $\alpha$  - [ $\alpha$  - (5,6-dimethylbenzimidazolyl)] - Co $\beta$  - aquacobamide, also known as vitamin B-12a, is termed **aquacobalamin**.

† *Chairman*: O. Hoffmann-Ostenhof (Austria); *Secretary*: W. E. Cohn (USA); *Members*: A. E. Braunstein (USSR), B. L. Horecker (USA), P. Karlson (FRG), B. Kiel (France), W. Klyne (UK), C. Liébecq (Belgium), E. C. Webb (Australia), W. J. Whelan (USA).

‡ Revision of the 1965 document.¶ Significant changes from the 1965 version are indicated by  $\Delta$  in the margin. An appendix on abbreviations has been added.

§ "Pentadecahydrocorrin" in the previous document<sup>1</sup> was an error.

¶ The namesobyric acid, cobinic acid, cobamic acid, and cobalamin, and names derived from them, imply the relative and absolute configurations shown in the structural formulas.  $\alpha$  and  $\beta$  are used as in Steroid Nomenclature<sup>2</sup> and the IUPAC Rules on Stereochemistry: (E-Rules<sup>3</sup>) to indicate stereochemical configuration. Epimers at C-3, C-8, and C-13 may be designated as, e.g. 13-epicobalamin.

*Coα*-[ $\alpha$ -(5,6-dimethylbenzimidazolyl)]-*Coβ*-hydroxocobamide, also known as vitamin B-12b, is termed *hydroxocobalamin*.

Note: aquacobalamin is the conjugate acid of hydroxocobalamin.

*Coα*-[ $\alpha$ -(5,6-dimethylbenzimidazolyl)]-*Coβ*-nitritocobamide, also known as vitamin B-12c, is termed *nitritocobalamin*.

10. Anion(s) associated with the corrinoids is(are) stated in the usual way after the name of the (cationic) corrinoid, e.g. cobamic dichloride (not dichlorocobamic acid).

11. The state of oxidation of the cobalt may be specified, when necessary, as follows:

vitamin B-12      cyanocob(III)alamin  
 vitamin B-12r    cob(II)alamin†  
 vitamin B-12s    cob(I)alamin†

12. Displacement of the ribosyl-bound aglycon base from its normal coordinate bonding to position  $\alpha$  of the cobalt by another ligand (or by water) may be indicated by name (see Section 6) in parentheses. (See also Section 7.) placing the name and locant of the replacing ligand before the corrinoid name and enclosing the modified corrinoid

Example:

*Coα*-aqua-*Coβ*-methyl(2-methyladenylcobamide), in which the 2-methyladenyl residue is attached to the ribose residue but is not coordinately bound to the cobalt atom, having been displaced by water. Methyl occupies the *Coβ* position.

13. Modified, derived or related compounds are named systematically from the largest of the compounds I, II, or III that is contained in them.

Examples:

cobyrinic acid *a,b,c,d,e,g*-hexaamide *f*-2-hydroxyethylamide;

3,8,13,17-tetraethyl-1,2,2,5,7,7,12,12,15,17,18-undecamethylcobalticorrin dichloride (for the dichloride of fully decarboxylated cobyrinic acid);

12 $\alpha$ <sup>1</sup>-carboxycobyrinic acid (for cobyrinic acid in which the 12 $\alpha$ -methyl group has been replaced by -CH<sub>2</sub>CO<sub>2</sub>H).

14. Replacement of the cobalt atom in compounds II or III by another metal or by hydrogen is indicated by replacing "co" in the "cob" part of the name with the name or the root of the name of the replacing metal followed by "o" or "i" according to its valence (e.g. cupri, cupro, zinco). When cobalt is replaced by hydrogen, "hydrogeno" replaces "co".

Examples:

ferrobamic acid  
 hydrogenobamic acid.

See Note to Section 1 concerning corrin. This replacement nomenclature does not apply to corrole (Section 2).

15. **Cofactor forms.** The coenzymatically active forms of the B-12 vitamins (Section 12) and their analogs possess an organic ligand, either methyl or 5'-deoxy-5'-adenosyl,‡ attached to the  $\beta$  position of the cobalt by a carbon-to-cobalt bond, i.e. in the position of the CN in formula IV. These adducts<sup>4</sup> should be named according to the pattern:

*Coα*-(radical in  $\alpha$  position)-*Coβ*-(ligand in  $\beta$  position) (corrinoid name) or (ligand in  $\beta$  position) cobalamin, if the radical in the  $\alpha$  position is dimethylbenzimidazole.

Examples:

*Coα*-[ $\alpha$ -(5,6-dimethylbenzimidazolyl)]-*Coβ*-adenosylcobamide,‡ or adenosylcobalamin,‡ for the compound formerly known as "coenzyme B-12".

*Coα*-[ $\alpha$ -(5,6-dimethylbenzimidazolyl)]-*Coβ*-methylcobamide or methylcobalamin, for the compound involved in several reactions, including methionine biosynthesis, where a methyl group is ligated to the cobalt in the  $\beta$  position.

*Coα*-[ $\alpha$ -(7-adenyl)]-*Coβ*-adenosylcobamide,‡ the coenzymatically active form of "pseudovitamin B-12" capable of replacing adenosylcobalamin in many systems.

16. Summary. The trivial names applied to corrinoids of varying complexity are perhaps confusing to the nonspecialist, and it seems desirable to tabulate (in outline) how they are interrelated (Table 1).

Table 1

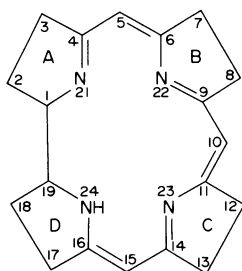
Section	Description	Specific names, in increasing order of complexity
1	Skeleton (porphyrin nucleus minus C-20)	Corrin (I)
		<i>Heptaacid</i> <i>Heptaacid, hexaamide</i>
3	1, with standard side chains and with cobalt	Cobyrinic acid (II)
4	3, with D-1-amino-2-propanol at position <i>f</i>	Cobinic acid (III)
5	4, with D-ribofuranose 3-phosphate at position 2 of the aminopropanol	Cobamic acid (III-V)
7	5, with heterocyclic base attached by N-glycosyl link at position 1 of ribose and attached as an $\alpha$ -ligand to cobalt (Sections 6, 7)	Aglyconylcobamide (VI)
9	Many "B <sub>12</sub> " vitamins and derivatives, in which the heterocyclic base is 5,6-dimethylbenzimidazole, are given the trivial name "cobalamin" (Section 9)	Cobalamin
15	"B <sub>12</sub> coenzymes", compounds in which a further organic group (X-yl) is $\beta$ -ligated to cobalt (Sections 9, 15)	X-ylcobalamin; ( <i>Coα</i> -ligandyl)- ( <i>Coβ</i> -X-yl)cobamide (X)

†The previous document<sup>1</sup> erred in prefixing "cyano" to these names.

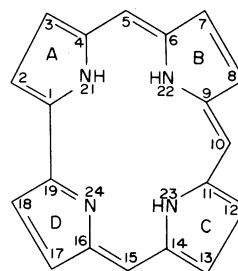
‡For brevity, 5'-deoxy-5'-adenosyl may be replaced by adenosyl, with definition, as is commonly seen in S-adenosylmethionine. The intermediate form, 5'-deoxyadenosyl, should not be used.

#### NOTES ON FORMULAS

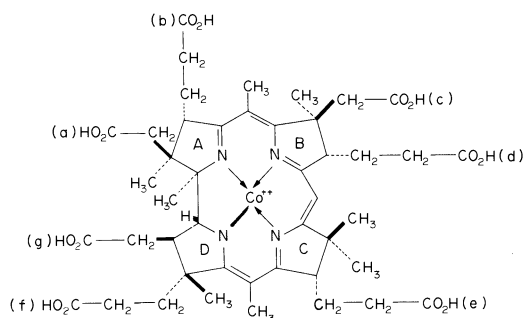
1. In formulas II and III, the corrin nucleus is represented as being roughly in the plane of the paper. Bonds joining peripheral substituents to the nucleus are shown by the same convention as in the steroid series,<sup>2</sup> i.e. full (heavy) lines are bonds lying *above* the plane of



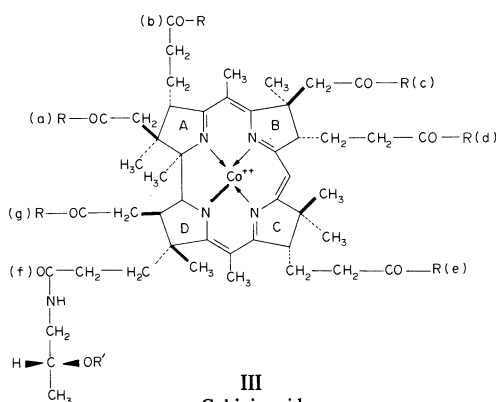
I  
Corrin



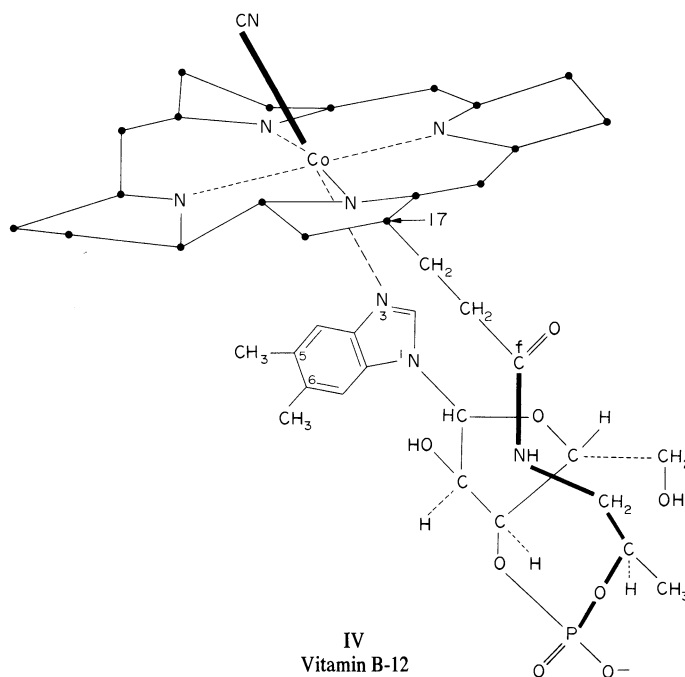
IA  
Corrole



II  
Cobyrinic acid



III  
Cobinamic acid



IV  
Vitamin B-12

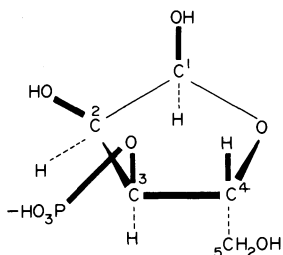
IV. Sketch based on Hodgkin *et al.*<sup>5</sup> Detail of substituents on corrin nucleus (except side chain at C-17) is omitted for the sake of clarity.

the ring system, while dashed (broken) lines are bonds lying *below* this plane.

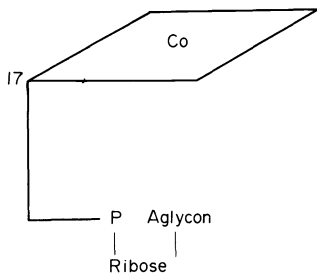
2. Formulas II, III, and IV represent the true absolute stereochemical configuration of the structures as determined by X-ray work.<sup>5,6</sup> The CN is in the  $\beta$ -position of the cobalt, the ribose-bound heterocyclic base in the  $\alpha$ -position, in formula IV. When adenine is the heterocyclic

base, it is usually bound to the ribose by its N-7, the opposite from what is seen in the nucleic acids.

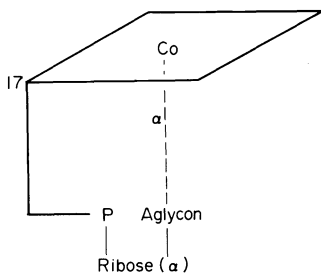
3. Formula V represents the absolute stereochemical configuration of the ribofuranose residue. For convenience in comparing it with formula IV, it is written with the  $\alpha$ -substituent at C-1 *above* the plane of the ring (i.e. the reverse of the usual carbohydrate method).<sup>7</sup>



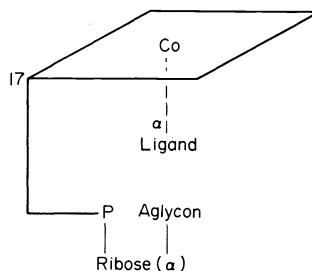
V  
 $\alpha$ -D-Ribofuranose  
 3-phosphate residue



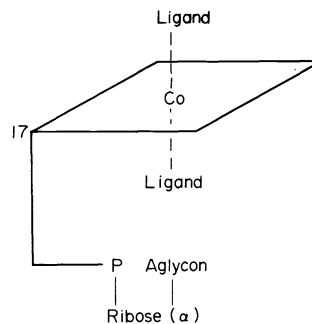
VI  
 Aglyconylcobamide  
 (III: R'=P-Rib-aglycon).



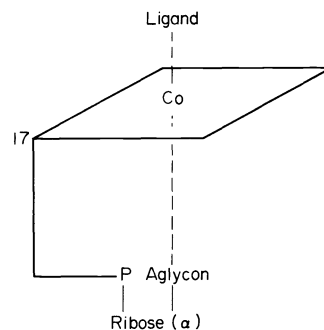
VII. Aglyconylcobamide, with aglyconyl ligated to cobalt (IV without CN and with dimethylbenzimidazole as aglycon).



VIII. ( $Co\alpha$ -Ligandyl)-aglyconylcobamide (ligand has "displaced" aglycon of VII).



IX. ( $Co\alpha$ -Ligandyl)-( $Co\beta$ -ligandyl)aglyconylcobamide (VIII with additional ligand in  $Co\beta$  position).



X. (a) Aglyconyl-( $Co\beta$ -ligandyl)cobamide (VII with additional ligand in  $Co\beta$  position; IV with dimethylbenzimidazole as aglycon, CN as  $Co\beta$  ligand). (b) Ligandylcobalamin (if aglycon is dimethylbenzimidazole as in IV).

#### REFERENCES

- <sup>1</sup>IUPAC *Information Bull.* **26**, 19 (1966); *Biochem. J.* **102**, 19 (1966).  
<sup>2</sup>*Pure Appl. Chem.* **31**, 283 (1972).  
<sup>3</sup>*Pure Appl. Chem.* **45**, 11 (1976).  
<sup>4</sup>L. Ljungdahl *et al.*, *Fed. Proc., Fed. Amer. Soc. Exp. Biol.* **25**, 1642 (1966).

<sup>5</sup>D. C. Hodgkin *et al.*, *Proc. Roy. Soc. (Lond.)* **A242**, 228 (1957).

<sup>6</sup>D. C. Hodgkin, *Science* **150**, 979 (1965).

<sup>7</sup>Tentative Nomenclature Appendix No. 7 (Sept. 1970) to IUPAC *Information Bull.*; *Europ. J. Biochem.* **21**, 455 (1971).

#### APPENDIX: ABBREVIATIONS FOR CORRINOIDS

This appendix was inspired by the burgeoning literature concerning corrinoid compounds, many of which have long and unwieldy names—a fact that has led to a variety of *ad hoc* abbreviations that in turn has led to difficulties for the reader.

Many individuals, including, but not limited to those whose names appear in the references, have assisted in the development of the system and symbols here proposed. They are not here named, but a special acknowledgment is made of the assistance of B.M. Babior to CBN in the construction of this appendix.

In accordance with several preceding CBN documents,<sup>1-3</sup> as well as with standard chemical practice, the abbreviations are constructed by assembling symbols representing the various radicals involved, rather than from combinations of letters drawn haphazardly from the complete names of the compounds. The use of symbols reflects the actual structure of a compound and facilitates the writing of equations for its chemical transformations. In particular, the use of DBC, DMBC, etc., is discouraged, as is the use of B-12 (except as vitamin B-12), coenzyme B-12, and "factor" terms.

## I. NAMES AND SYMBOLS

Names		Symbols
of free acid	Corrin of hexaamide	Crn (for the hexaamide)
cobyrinic acid	cobyric acid	Cby
cobinic acid	cobinamide	Cbi
cobamic acid	cobamide	Cba
	cobalamin	Cbl†

## II. DESIGNATION OF SUBSTITUENTS ATTACHED TO COBALT

Ligands coordinated to the  $\alpha$  and  $\beta$  position of the cobalt (below and above the plane of the corrin residue, respectively, as shown in structure IV) are represented by terms that precede the symbol for the corrinoid residue. If the positions of the ligands are *unknown or not specified*, the two terms representing the ligands in the  $\alpha$  and  $\beta$  position are enclosed in one set of parentheses and are separated by a *comma*. If the positions are *known and specified*, the  $\alpha$  ligand precedes and is set apart by parentheses; the  $\beta$  is enclosed (separately) only if its complexity may make it ambiguous. If the ligands are identical, a single term followed by the subscript 2 is used.

## A. Anion substituents

The chemical symbol for the anion is used. Aqua is abbreviated aq. *Examples*:

(Me)aqCbi (methyl)aquacobinamide (Ref. 4) (methyl in  $\alpha$  position)  
 (CN)MeCbi (cyano)methylcobinamide (methyl in  $\beta$  position)  
 (CN,aq)Cbi or (aq,CN)Cbi cyanoaquacobinamide (ligand location unspecified)

## B. Alkyl substituents

1. Primary substituents are designated by naming the alkyl group‡ without denoting the position attached to the cobalt, as it is always 1. *Examples*:

(aq)EtCbi (aqua)ethylcobinamide  
 (CN)(2-OAcBu)Cbi (cyano)(2-acetoxybutyl)cobinamide

2. Secondary substituents are named similarly, except that the position attached to the cobalt is given by a locant suffixed to the name of the alkyl group (as in the -x-yl name). *Examples*:

(aq)(Bu-2)Cbi or (aq)Bu‡Cbi (aqua)(*sec*-butyl)cobinamide<sup>5</sup>  
 (aq)(3-OAcBu-2)Cby (aqua)(3-acetoxybut-2-yl)cobyric acid

3. Alicyclic groups are indicated by a small "c" before the symbol for the alkyl residue. In these compounds, cobalt is always assumed to be substituted in position 1 of the ring. *Examples*:

(aq)cHxCbi (aqua)cyclohexylcobinamide<sup>5</sup>  
 (CN)(2-HOcPe)Cby (cyano)(2-hydroxycyclopentyl)-cobyric acid

4. 5'-Deoxy-5'-adenosyl in the  $\beta$  coordination position, as in "coenzyme B-12", is represented by the symbol Ado for "adenosyl" (see † footnote on p. 3) a 2'-deoxyadenosine residue by dAdo (Ref. 3). Unusual deoxyadenosyl residues can be indicated by superscripts (e.g. d<sup>3</sup>Ado, d<sup>2-3</sup>Ado). See C below.

## C. Cobamides of the cobalamin† type

As the symbol Cbl designates  $\alpha$ -(5,6-dimethylbenzimidazolyl)cobamide [cob(III)alamin], only those cobamides having this base utilize Cbl. Those containing another base are named as cobamides, utilizing the symbol Cba. Hence, Cbl is preceded by only a single term, the one representing the  $\beta$ -substituent. Examples are in Table 1A.

*Notes*: i. The hyphenation in the case of secondary alkyl substituents and similar situations of potential confusion may make it necessary to enclose the  $\beta$  substituent in parentheses, or set it off by a hyphen.

ii. If the replacing base (in  $\alpha$  position) is unspecified, the term (?) is used, e.g. (?)MeCba. The term (OH)/base indicates that the ribose residue is not attached to the Co $\alpha$ -linked base.

iii. If the  $\alpha$ -substituent (the "base") is displaced from the cobalt by another ligand, but remains attached to the ribosyl residue, the same system is used. *Example*:

(2-MeAde/aq)MeCba Co $\alpha$ -aqua-Co $\beta$ -methyl(2-methyladenylcobamide)  
 (Ade/CN)CN-Cba Co $\alpha$ -cyano-Co $\beta$ -cyano-(adenylcobamide) or dicyanoadenylcobamide

In abbreviating cobalamin derivatives, the base need not be specified. Replacement of the base by another Co $\alpha$  ligand is indicated by merely adding to the abbreviation a term corresponding to the replacing ligand. *Examples*:

(OH)MeCbl Co $\alpha$ -hydroxo-Co $\beta$ -methylcobalamin or Co $\alpha$ -hydroxo-Co $\beta$ -methyl(dimethylbenzimidazolylcobamide)  
 (CN)<sub>2</sub>Cbl Co $\alpha$ -cyano-Co $\beta$ -cyanocobalamin or dicyanocobalamin

iv. Cobalt valences of II or I may be indicated by superscripts (e.g. Cbl<sup>II</sup>).

## III. DESIGNATION OF ALTERATIONS AND SUBSTITUENTS ON THE CORRIN RING

Substituents on the ring itself are represented by symbols following the symbol for the corrinoid, with locants indicating the positions of the substituents. Epimerization is indicated in a similar manner. Symbols representing replacements on the carboxyl groups at the periphery of the corrin residue follow those that designate substituents directly on the ring. The location of the substituent is indicated by the letter corresponding to the

†A cobalamin is a cobamide in which 5,6-dimethylbenzimidazole is covalently bonded to the ribose in  $\alpha$ -glycosidic linkage; it is thus a dimethylbenzimidazolylcobamide and can be symbolized as such. However, it is often convenient to have a short symbol for this complex, hence Cbl. Cbl is recommended in place of the former B<sub>12</sub> or B-12 for chemical use.

‡Symbols for alkyl groups are Me, Et, Pr, Pr', Bu, Bu\*, Bu', Pe, Hx, Hp, ...

Table 1A

CN-Cbl	cyanocob(III)alamin (vitamin B-12)
AdoCbl	adenosylcob(III)alamin <sup>6,7</sup>
PrCbl	<i>n</i> -propylcob(III)alamin; methyl-, etc. similarly <sup>8,9</sup>
(Ade)(Pr-2)Cba or (Ade)Pr <sup>1</sup> -Cba†	<i>Coα</i> -[α-(aden-9-yl)]- <i>Coβ</i> -isopropylcobamide
(Bza)MeCba‡	<i>Coα</i> -(α-benzimidazolyl)- <i>Coβ</i> -methylcobamide
2-(MeOOC)EtCbl	(2-methoxycarbonylethyl)cob(III)alamin <sup>8</sup>
(Ade-7)AdoCba†	<i>Coα</i> -[α-(aden-7-yl)] <i>Coβ</i> -adenosylcobamide <sup>10</sup>
(2-SHAde-7AdoCba†	<i>Coα</i> -[α-(2-thiaaden-7-yl)]- <i>Coβ</i> -adenoxylcobamide <sup>11</sup>
(5-MeOBza)MeCba	<i>Coα</i> -(5-methoxybenzimidazolyl)- <i>Coβ</i> -methylcobamide <sup>11,13</sup>
(2-MeAde-7)CN-Cba†	<i>Coα</i> -[α-(2-methyladen-7-yl)]- <i>Coβ</i> -cyanocobamide <sup>11,14</sup>
(Ade)CN-Cba†	<i>Coα</i> -[α-(aden-9-yl)]- <i>Coβ</i> -cyanocobamide (pseudovitamin B-12)
(Ade)OH-Cba†	<i>Coα</i> -[α-(aden-9-yl)]- <i>Coβ</i> -hydroxocobamide (hydroxopseudovitamin B-12)
(Ade)MeCba†	<i>Coα</i> -[α-(aden-9-yl)]- <i>Coβ</i> -methylcobamide
[4-(Ade-9)Bu]Cbl§	[4-(aden-9-yl)butyl]cob(III)alamin <sup>6</sup>
(6MeSPur)AdoCba	<i>Coα</i> -(α-6-methylthiopurinyloxy)- <i>Coβ</i> -adenosylcobamide <sup>15</sup>

†Ade alone represents adenine bonded to the ribosyl moiety through its 7 position (i.e. a 7-α-D-ribofuranosyladenine). Bonding to the cobalt is thus through N-9. When these positions are reversed, Ade-7 and aden-7-yl are used (i.e. the locant specifies the N linked to cobalt).

‡Bza = benzimidazolyl.

§As this is a cobalamin, the adenine residue is not in the *Coα* position, but is attached (-9-yl) to a but-4-yl residue that is in turn linked to the β position of the cobalt. Named as a cobamide, it would be (Me<sub>2</sub>Bza)[4-(Ade-9)Bu]Cba.

¶Factor III<sub>m</sub>.<sup>12,13</sup>

carboxyl group that carries it. *Examples*:

CN-Cbl(13-epi) cyano(13-epi)cobalamin  
 CN-Cbl(13epi-*e*OH) *Coα* - (α - 5,6 - dimethyl-  
 benzimidazolyl)-*Coβ*-cyano (13-epi) cobamic  
*a,b,c,d,g*-pentaamide  
 Ado - Cbl (10 - Cl) adenosyl - 10 - chlorocobalamin  
 (aq) AdoCbi(*e* - PhNH) *Coα* - aqua - *Coβ* -  
 adenosylcobinic *a,b,c,d,g* - pentaamide - *e* - anilide  
 (CN)Cl-Cby(8-NH-*c*-lactam)  
 (CN)<sub>2</sub>Cby(OMe)<sub>7</sub> Dicyanoeoobyrinicheptamethylester<sup>16</sup>

If the location of the carboxyl substituent(s) is unknown, a term of the following structure should be used:



where *a* : *g* indicates a substitution at the periphery of the ring, X is the replacing group, and *n* refers to the number of carboxyl groups substituted. *Examples*:

(CN,aq)Cby[*a* : *g*-(NH<sub>2</sub>)<sub>5</sub>] cyanoaquacobyrinic acid  
 pentaamide<sup>17</sup>  
 (CN)<sub>2</sub>Cby[10-Cl-*a* : *g*-(NH<sub>2</sub>)<sub>5</sub>] 10-chloro derivative of  
 the above.

#### IV. REPLACEMENT OF COBALT BY OTHER METALS<sup>18,19</sup>

Corrinoids containing metals other than cobalt are symbolized by placing the symbol of the replacing metal in square brackets preceding and attached to the symbol of the corrinoid. Thus, a hydrogenocobamide utilizes [H]Cba, a nickelocobalamin [Ni]Cbl<sup>II</sup>, a zincocobinamide [Zn]Cbi<sup>II</sup>, etc. Phenylcupribamide<sup>19,20</sup> could be indicated as (Ph)[Cu]Cba<sup>II</sup>. I, II, and III may be added as superscripts when needed.

#### V. ISOTOPIC LABELING

A labeled position is indicated in the usual fashion,<sup>21</sup> e.g.

(Bza)Me[<sup>57</sup>Co]Cba *Coα*-(α-benzimidazolyl)-*Coβ*-  
 methyl[<sup>57</sup>Co]cobamide  
 (Bza)[<sup>14</sup>C]MeCba *Coα*-(α-benzimidazolyl)-*Coβ*-  
 [<sup>14</sup>C]methylcobamide

([4-<sup>3</sup>H]Bza)MeCba *Coα*-(α-[4-<sup>3</sup>H]benzimidazolyl)-  
*Coβ*-methylcobamide.

#### VI. METALLOCORRINS

As corrin contains no metal (the name "corrin" being derived from "core", not "cobalt"), complexes of metals with corrin require specification of both terms. Example: Cu<sup>II</sup>Crn for copper(II) corrin.

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