Pressure-induced structural changes in wet vitamin B12

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Electronic Supplementary Information

Contents:

Crystal data

Crystal data for "wet B12" at ambient pressure: $C_{63}H_{88}CoN_{14}O_{14}P$, 23.5($H_2O$), M = 1778.75 , red block, orthorhombic, $P2_12_12_1$, a = 15.8260(9), b = 22.4438(13), c = 25.4429(16), V = 9037.2(9), Z = 4, μ = 0.298 mm^2, ρ_{calc} = 1.307 g cm^{-3}, T = 293(2) K, 101570 reflections measured, of which 26484 were independent (R_{int} = 0.0436), 917 parameters, 168 restraints, R_1 = 0.0731[based on F and 19937 data with $I > 2\sigma(I)$], wR_2 = 0.2254 [based on F^2 and all 26484 reflections], Flack = 0.014(11), the final difference map extremes were +0.82 and –0.18 e Å^3.

Crystal data for "wet B12" at 1.0 GPa: $C_{63}H_{88}CoN_{14}O_{14}P$, 22($H_2O$), M = 1751.73, red block, orthorhombic, $P2_12_12_1$, a = 15.9455(4), b = 21.0511(5), c = 23.8739(8), V = 8013.8(4), Z = 4, μ = 0.333 mm^2, ρ_{calc} = 1.452 g cm^{-3}, T = 293(2) K, 53048 reflections measured, of which 10032 were independent (R_{int} = 0.052), 936 parameters, 168 restraints, R_1 = 0.0665 [based on F and 7534 data with $I > 2\sigma(I)$], wR_2 = 0.2165 [based on F^2 and all 10032 reflections], Flack = 0.02(2), the final difference map extremes were +0.58 and –0.52 e Å^3.

Structure refinement

Restraints:

For ADPs the same similarity and rigid-bond restraints were applied in the refinement of the two structures, namely:

Rigid-bond (DELU command in SHELXL)	**Similarity (SIMU command in SHELXL)**
C1 > C19 (corrin ring C-atoms)	C27 O28 N29 (amide side chain a)
C1R > O8R (ribose atoms)	C32 O33 N34 (amide side chain b)
N1B > C10B (benzimidazole atoms)	C38 O39 N40 (amide side chain c)
C12 C47 C46 (terminal methyl groups)	C43 O44 N45 (amide side chain d)
C1 C20 (termianl methyl group)	C50 O51 N52 (amide side chain e)
C1C N2C (cyano group)	C61 O62 N63 (amide side chain g)
C3 C30 (amide side chain b)	
C7 C37 (amide side chain c)	
C60 C61 (amide side chain g)	

Bond distances restraints were also applied, values in bracket refer to the unstrained values:

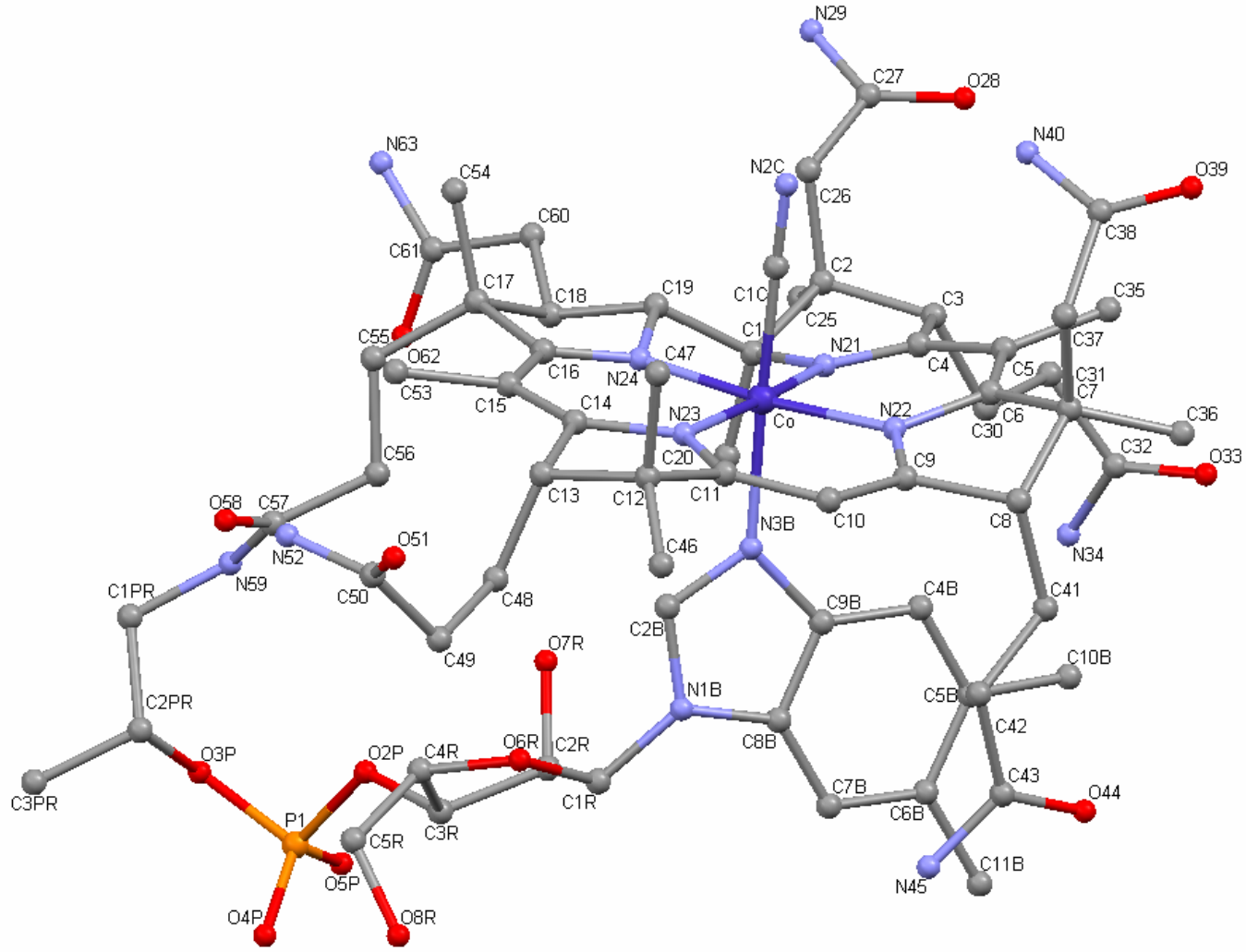
Ambient pressure

DFIX C27 N29 1.34 0.005 [1.266(7)]
DFIX C32 N34 1.34 0.005 [1.235(8)]
DFIX C43 N45 1.34 0.005 [1.287(8)]
DFIX C27 O28 1.24 0.01 [1.152(7)]
DFIX C32 O33 1.24 0.01 [1.198(7)]
DFIX C43 O44 1.24 0.01 [1.215(7)]

High pressure

DFIX C32 N34 1.34 0.01 [1.297(14)]
DFIX C38 N40 1.34 0.01 [1.302(10)]
DFIX C57 N59 1.34 0.01 [1.280(12)]
DFIX C61 O62 1.24 0.01 [1.208(11)]
DFIX C32 O33 1.24 0.01 [1.270(11)]
DFIX C1C N2C 1.16 0.01 [1.138(12)]

Structure numbering scheme



Structure comparison with the 1964 "wet B12" structure by C. Brink-Shoemaker *et al.*[1]

Water site assignment	Ambient pressure	1.0 GPa
Pocket region	OW1-OW11 + OW13	OW1-OW8 + OW10-OW11 + OW14-15 + OW22-OW23
Channel region	OW12	OW9 + OW12-OW13 + OW16-OW21 + OW24

Note: between the pocket and channel regions there is a less well-defined interface region. For example, at 1.0 GPa, atoms OW22 and OW23 belong to this region.

Water O-atom site correspondence.

Ambient pressure	Ambient pressure (1964 structure)	High pressure
1	**4**	1
2	**10**	2
3	**3**	3
4	**5**	4
5	**2**	5
6	**1**	6
7	**13**	7
8	**12**	-
9		-
10	6b	10
11	7a+7b	(12)
12	9a	17
13	6c	8

Note: In 1964, on the basis of experimental density measurements, the structure of wet B12 was assigned 22 water molecules per formula unit; using the diffraction data, 21-23 sites were then assigned, of which 8-9 (above in bold face) were assigned full and 28 half occupancy. Sites 1-5 (1964) are common to many B12 structures.

Comment on displacement parameters and site occupancy:
"Unusual high temperature factors are a sign for partially occupied solvent molecules. However, one should take into account that, due to their mobility, non-coordinating solvent molecules tend to show relatively large temperature factors. Therefore the ADPs should be significantly larger to justify a reduction of the occupation factors. A better criterion is the residual electron density map, which shows negative electron density at the nuclear positions if the occupancy is lower than one".

Extract from: http://shelx.uni-ac.gwdg.de/~peterm/tutorial/do-type.htm

[1] C. Brink-Shoemaker, D. W. J. Cruickshank, D. C. Hodgkin and M. J. Kamper, *Proc. R. Soc. London, Ser. A*, 1964, **278**, 1-26.

PLATON[2] "SQUEEZE" and "CALC SOLV" calculations:

From the PLATON manual:
"The number of recovered electrons in the solvent area is strongly dependent on the quality of the low-angle reflections. Supply COMPLETE data sets!"
"As far as the refinement goes, the method tolerates in general the absence of a limited number of reflections."

If strong/low-angle reflections are missing, the squeeze procedure tends to underestimate the electron count. The electron count in from the squeeze calculation also strongly depends on the quality of the difference map.

Ambient pressure calculation, PLATON(V-210110):
1) All O-water atoms deleted from the input file:

N: Number of moved primary input atoms: 181
W: Low density (check!) of 0.996 gcm-3
N: Total Potential Solvent Accessible Void Vol ..... 2978.6 Ang^3
N: Electron Count / Cell = 973 - To be included in D(calc), F000 & Mol.Wght.
(convergence reached in 24 cycles)
→ *ca.* 24 water molecules per B12 formula unit

2) All O-water atoms deleted from the input file, apart from the 5 fully occupied ones:

N: Number of moved primary input atoms: 186
N: Total Potential Solvent Accessible Void Vol ..... 2531.6 Ang^3
N: Electron Count / Cell = 856 - To be included in D(calc), F000 & Mol.Wght.
Missing Reflections below sin(theta)/lambda=0.3 *(partially obscured by the beamstop)*
→ *ca.* 21.5 + 5 = 26.5 water molecules per B12 formula unit

3) All O-water atoms kept in the input file:

N: Number of moved primary input atoms: 194
N: Total Potential Solvent Accessible Void Vol ..... 1678.3 Ang^3
N: Electron Count / Cell = 581 - To be included in D(calc), F000 & Mol.Wght.
(convergence reached in 11 cycles)
→ *ca.* 14.5 + 9 = 23.5 water molecules per B12 formula unit

1.0 GPa calculation, PLATON(V-210110):
1) All O-water atoms deleted from the input file:

N: Number of moved primary input atoms: 181
N: Total Potential Solvent Accessible Void Vol ..... 2149.9 Ang^3
N: Electron Count / Cell = 681 - To be included in D(calc), F000 & Mol.Wght.
(convergence reached in 8 cycles)
:: Number of Missing Low Order Reflections = 116
→ *ca.* 17 water molecules per B12 formula unit

[2] P. v. d. Sluis and A. L. Spek, *Acta Crystallogr., Sect. A: Found. Crystallogr.*, 1990, **46**, 194-201. A. L. Spek, *J. Appl. Cryst.*, 2003, **36**, 7-13; A. L. Spek, *Acta Crystallogr., Sect. D: Biol. Crystallogr.*, 2009, **65**, 148-155.

2) All O-water atoms deleted from the input file apart from the ones with the 12 lowest U_{iso}:

N: Number of moved primary input atoms: 193
N: Total Potential Solvent Accessible Void Vol ..... 1038.3 Ang^3
N: Electron Count / Cell = 304 - To be included in D(calc), F000 & Mol.Wght.
(convergence reached in 6 cycles)
→ *ca.* 7.5 + 12 = 19.5 water molecules per B12 formula unit

The same calculations using a previous version of the PLATON executable give different results
PLATON(V-180105)

Ambient pressure calculation, PLATON(V-180105):
1) All O-water atoms deleted from the input file:

N: Number of moved primary input atoms: 181
N: Total Potential Solvent Accessible Void Vol ..... 2978.6 Ang^3
N: Electron Count / Cell = 927 - To be included in D(calc), F000 & Mol.Wght.
→ *ca.* 23 water molecules per B12 formula unit

2) All O-water atoms kept the input file:

N: Number of moved primary input atoms: 194
N: Total Potential Solvent Accessible Void Vol ..... 1678.3 Ang^3
N: Electron Count / Cell = 575 - To be included in D(calc), F000 & Mol.Wght.
→ *ca.* 14.5 + 9 = 23.5 water molecules per B12 formula unit

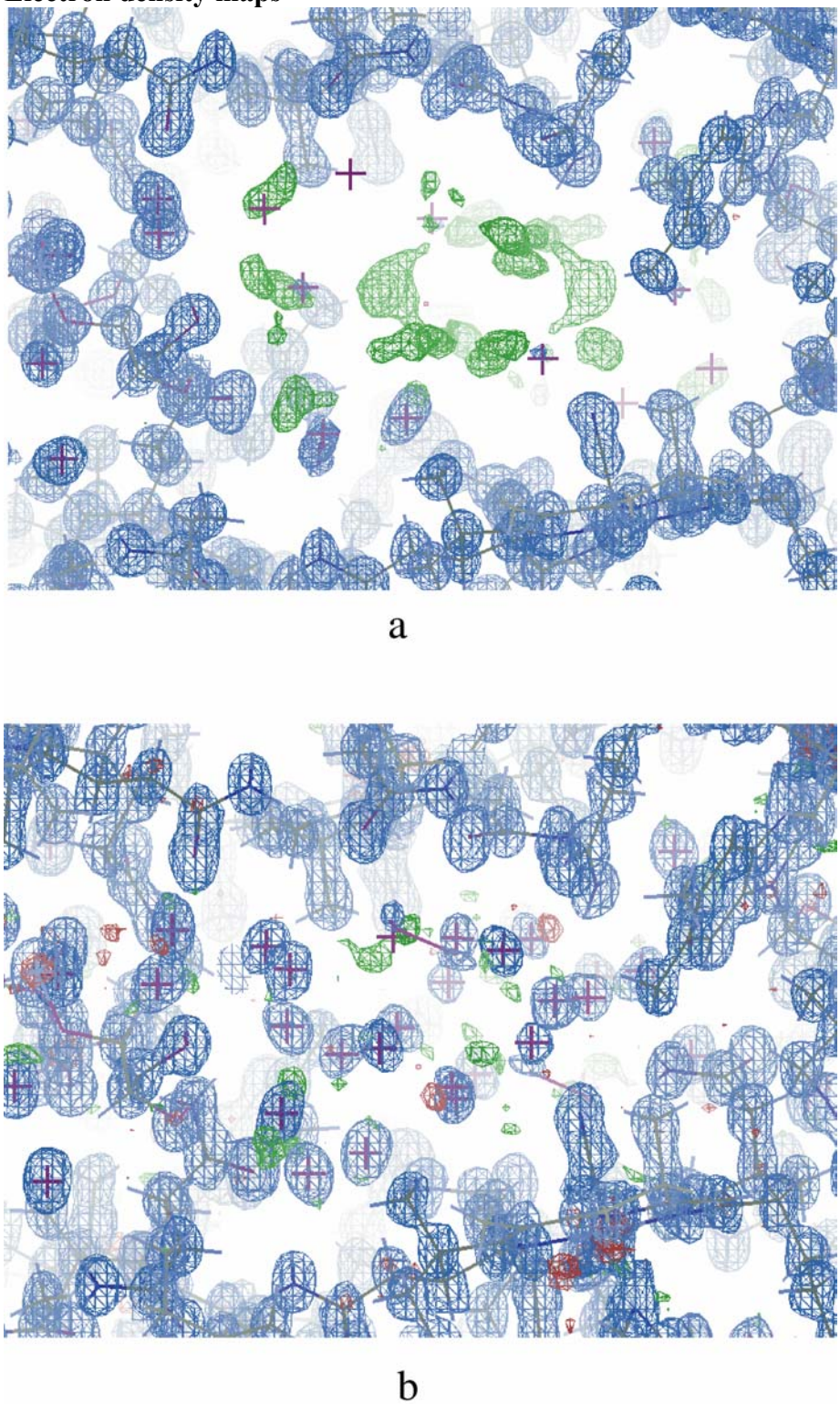
1.0 GPa calculation, PLATON(V-180105):
1) All O-water atoms deleted from the input file:

N: Number of moved primary input atoms: 181
N: Total Potential Solvent Accessible Void Vol ..... 2149.9 Ang^3
N: Electron Count / Cell = 599 - To be included in D(calc), F000 & Mol.Wght.
→ *ca.* 15 water molecules per B12 formula unit

2) All O-water atoms deleted from the input file apart from the ones with the 11 lowest U_{iso}:

N: Number of moved primary input atoms: 192
N: Total Potential Solvent Accessible Void Vol ..... 1176.7 Ang^3
N: Electron Count / Cell = 316 - To be included in D(calc), F000 & Mol.Wght.
→ *ca.* 8 + 11 = 19 water molecules per B12 formula unit

Electron density maps



Electron density maps generated with COOT[3] for wet B12 at a) ambient pressure and b) at 1.0 GPa viewed along the solvent channel. 2Fo-Fc (also called sigma A) map in blue; Fo-Fc maps in red (-ve, indicating density is misplaced in the model) and green (+ve, indicating density is missing in the model). Contour levels: Fo-Fc maps at 3σ [a) 0.55 $e^-/Å^3$, b) 0.38 $e^-/Å^3$]; 2Fo-Fc maps at 1.5 σ [a) 1.37 $e^-/Å^3$, b) 1.46 $e^-/Å^3$]. Note that at high pressure there is considerably less positive density in the channel.

[3] P. Emsley and K. Cowtan, *Acta Crystallogr., Sect. D: Biol. Crystallogr.*, 2004, **60**, 2126–2132.

Side chains torsion angles

Table 1 Selected torsion angles (°) of amide side chains a-g.

Side chain a	C2-C26-C27-O28	C2-C26-C27-N29	C1-C2-C26-C27
0.1 MPa	-52.1(10)	130.5(5)	175.9(3)
1.0 GPa	-61.2(11)	116.6(9)	-177.1(6)
Side chain b	C30-C31-C32-O33	C30-C31-C32-N34	C3-C30-C31-C32
0.1 MPa	-89.3(8)	93.4(6)	172.9(4)
1.0 GPa	-94.8(9)	83.3(10)	166.3(7)
Side chain c	C7-C37-C38-O39	C7-C37-C38-N40	C8-C7-C37-C38
0.1 MPa	-82.5(7)	94.6(6)	67.2(4)
1.0 GPa	-85.9(11)	92.2(9)	-173.2(6)
Side chain d	C41-C42-C43-O44	C41-C42-C43-N45	C8-C41-C42-C43
0.1 MPa	30.6(9)	-156.0(6)	-178.3(4)
1.0 GPa	21.1(12)	-159.7(7)	175.5(6)
Side chain e	C48-C49-C50-O51	C48-C49-C50-N52	C13-C48-C49-C50
0.1 MPa	-114.0(7)	66.6(8)	45.5(7)
1.0 GPa	-111.7(9)	69.0(11)	42.9(10)
Side chain f	C455-C56-C57-O58	C55-C56-C57-N59	C56-C57-N59-C1PR
0.1 MPa	-59.3(5)	120.3(4)	177.1(3)
1.0 GPa	-63.3(11)	112.0(10)	178.1(7)
Side chain g	C18-C60-C61-O62	C18-C60-C61-N63	C17-C18-C60-C61
0.1 MPa	-37.2(6)	143.8(4)	-77.5(4)
1.0 GPa	-43.3(12)	140.0(8)	-69.8(11)

H-bonding parameters

Table 2 H-bonding parameters (Å, °) for wet cyanocobalamin at conditions of ambient and high pressure, where cyanocobalamin is the H-bonding donor.

	D...A D-H...A[a]	0.1 MPa	0.98 GPa
Ribose	O7R-H7R..OW1	2.779(5) 172	2.691(8) 171
	O8R-H8R..OW4	*3.332(13)*[b] *176*	2.903(13) 153
Side chain a	N29-H29A...O44	3.075(8) 172	2.937(9) 161
	N29-H29B...OW7	3.095(17) 145	3.168(10) 145
Side chain b	N34-H34A...OW2	3.142(9) 143	2.972(17) [14]a 149
Side chain c	N40-H40A...O5P	2.985(6) 167	-
	N40-H40A...OW	-	3.164(17) [10]a 150
	N40-H40A...OW	-	3.15(3) [22]a,b 126
	N40-H40B...OW4	2.890(8) 142	-
	N40-H40B...N2C (intra)	-	3.152(11) 164
Side chain d	N45-H45A OW	-	2.957(15) [9]a,b 177
	N45-H45B...OW6	3.005(19) 170	3.148(11) 168
Side chain e	N52-H52A...O28	2.886(8) 145	2.900(9) 139
	N52-H52B...OW5	2.986(10) 161	2.887(13) 160
Side chain f	N59-H59...OW2	2.922(6) 162	2.981(13) 164
Side chain g	N63-H63A...O51	2.960(6) 159	2.973(9) 168
	N63-H63B...OW8c	2.975(17) 161	-
	N63-H63B...O33	-	2.892(12) 155

cont.

Table 2 (cont.) H-bonding parameters (Å, °) for wet cyanocobalamin at conditions of ambient and high pressure, where cyanocobalamin is the H-bonding donor.

	D...A D-H...A[a]	0.1 MPa	1.0 GPa
C-H...A H-bonds[d]	C1R-H1R...O39	-	3.203(12) 132
	C1R-H1R...OW10	*3.465(18)* *168*	-
	C3-H3...O28 (intra)	2.962(9) 135	3.023(10) 133
	C3R-H3R...O4P (intra)	-	2.949(10) 104
	C3PR-H3PR...O39	*3.357(7)* *139*	-
	C8-H8...O39 (intra)	3.094(6) 133	-
	C10-H10...O58	-	*3.434(9)* *156*
	C18-H18...O62 (intra)	2.917(5) 101	-
	C20-H20C...N3B (intra)	3.200(4) 137	3.174(8) 137

[a] Water O-atoms (OW) numbering scheme in this column given according to OW sites found in the ambient-pressure structure. Where no correspondence between atomic sites is observed at high-pressure, the high-pressure site number is given in square brackets in the last column. [b] Values in italics indicate long contacts. [c] Site disordered over two positions. [d] Further C-H(methyl)...O H-bonds are observed in the high-pressure structures. All standard uncertainties calculated with PLATON.[2]

Table 3 H-bonding distances (Å) for wet cyanocobalamin at conditions of ambient and high pressure, where cyanocobalamin is the H-bonding acceptor.

	A...D[a]	0.1 MPa	1.0 GPa
Side chain a	O28...N52^{R}	2.886(8)	2.897(9)
	O28...OW	-	3.189(15) [19][a]
	O28...OW	-	2.99(3) [22][a,b] 2.74(2) [23][a,b]
Side chain b	O33...OW8[b]	2.574(15) 2.81(2) [9][b]	2.905(7) [3][a]
	O33...OW	-	2.893(11) [9][a]
	O33...N63^{R}	-	2.886(12)
	O39...OW3	2.634(8)	3.090(10) [4][a]

cont.

Table 3 (cont.) H-bonding distances (Å) for wet cyanocobalamin at conditions of ambient and high pressure, where cyanocobalamin is the H-bonding acceptor.

	A...D[a]	0.1 MPa	1.0 GPa
Side chain c	O39...OW		2.931(10) [8][a]
Side chain d	O44...N29[R]	3.075(8)	2.938(9)
	O44...OW	-	2.689(15) [19][a]
Side chain e	O51...N63[R]	2.960(6)	2.974(9)
	O51...OW11	2.45(3)	2.69(4) [21][a]
		-	3.08(3) [23][a,b]
Side chain f	O58...OW5	2.759(8)	2.733(8)
	O62...OW2	2.943(9)	2.753(17) [15][a]
Side chain g	O62...OW4	2.772(8)	2.788(12)
Phosphate	O4P...OW1	2.712(6)	2.774(8)
	O4P...OW4	2.740(8)	2.682(10)
	O5P...OW3	2.676(8)	2.674(8)
	O5P...N34[R]	2.984(8)	3.016(12)
	O5P...N40[R]	2.985(6)	-
Ribose	O8R...OW	-	3.124(12) [2][a]
	O8R...OW		2.832(13) [11][a]
Cyanide	N2C...OW12	3.10(2)	3.063(16) [9][a]
	N2C...OW	-	3.150(15) [16][a]
	N2C...OW	-	3.065(19) [17][a]
	N2C...N40[R]	-	3.160(11)

[a] Water O-atoms (OW) numbering scheme in this column given according to OW sites found in the ambient-pressure structure. Where no correspondence between atomic sites is observed at high-pressure, the high-pressure site number is given in square brackets in the last column. [b] Site disordered over two positions. [R] Contact also present in Table 2. All standard uncertainties calculated with PLATON.[2]

Table 4a H-bonding distances (Å) for wet cyanocobalamin at conditions of ambient pressure: OW…OW and OW…Y contacts as calculated by PLATON.[2] Only unique contacts have been considered for creating Fig. 7 in the manuscript.

At(I)[1555.03]	At(J)	[ARU(J)]	D(I-J)
OW1	.... OW2	[ ]	2.790(10)
OW1	.... O7R	[ ]	2.779(5)
OW1	.... OW3	[3566]	2.779(9)
OW1	.... O4P	[3566]	2.712(6)
OW2	.... OW1	[ ]	2.790(10)
OW2	.... O62	[ ]	2.943(9)
OW2	.... N59	[ ]	2.922(6)
OW2	.... N34	[3466]	3.142(9)
OW3	.... OW5	[ ]	2.884(11)
OW3	.... OW1	[3466]	2.779(9)
OW3	.... O5P	[3466]	2.676(8)
OW3	.... O39	[4545]	2.634(8
OW4	.... N40	[ ]	2.890(8)
OW4	.... O4P	[2574]	2.740(8)
OW4	.... *OW13	[2574]	2.78(2)
OW4	.... O62	[4655]	2.772(8)
OW5	.... OW3	[ ]	2.884(11)
OW5	.... O58	[ ]	2.759(8)
OW5	.... N52	[ ]	2.986(10)
*OW6	.... N45	[ ]	3.005(19)
*OW7	.... *OW8	[ ]	2.78(2)
*OW7	.... *OW9	[ ]	2.56(3)
*OW7	.... N29	[ ]	3.095(17)
*OW8	.... *OW7	[ ]	2.78(2)
*OW8	.... N63	[ ]	2.975(17)
*OW8	.... O33	[4645]	2.574(15)
*OW9	.... *OW7	[ ]	2.56(3)
*OW9	.... N63	[ ]	2.78(2)
*OW9	.... O33	[4645]	2.81(2)
*OW10	.... *OW13	[ ]	2.66(3)
*OW11	.... O51	[ ]	2.45(3)
*OW11	.... *OW13	[2475]	2.96(3)
*OW12	.... N2C	[ ]	3.10(2)
*OW13	.... *OW10	[ ]	2.66(3)
*OW13	.... *OW11	[2475]	2.96(3)

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code
[2575]	= 1/2-x,2-y,1/2+z
[2475]	= -1/2-x,2-y,1/2+z
[3466]	= -1/2+x,3/2-y,1-z
[3566]	= 1/2+x,3/2-y,1-z
[1655]	= 1+x,y,z
[4655]	= 1-x,1/2+y,1/2-z
[4555]	= -x,1/2+y,1/2-z
[4545]	= -x,-1/2+y,1/2-z
[4645]	= 1-x,-1/2+y,1/2-z
[2574]	= 1/2-x,2-y,-1/2+z
[1455]	= -1+x,y,z
[1655]	= 1+x,y,z

Table 4b H-bonding distances (Å) for wet cyanocobalamin at conditions at 1.0 GPa: OW…OW and OW…Y contacts as calculated by PLATON.[2] Only unique contacts have been considered for creating Fig. 7 in the manuscript.

At(I)[1555.03]	At(J)	[ARU(J)]	D(I-J)
OW1	.... OW2	[ ]	2.685(11)
OW1	.... O7R	[ ]	2.691(8)
OW1	.... OW3	[2575]	2.944(10)
OW1	.... O4P	[3566]	2.776(8)
OW2	.... OW1	[ ]	2.685(11)
OW2	.... OW15	[ ]	2.856(16)
OW2	.... N59	[ ]	2.981(13)
OW2	.... O8R	[3566]	3.124(12)
OW3	.... OW1	[2574]	2.944(10)
OW3	.... O5P	[2574]	2.673(8)
OW3	.... OW5	[4555]	2.804(11)
OW4	.... O4P	[ ]	2.681(10)
OW4	.... OW8	[ ]	2.960(12)
OW4	.... O8R	[ ]	2.903(13)
OW4	.... O39	[2575]	3.091(10)
OW4	.... O62	[3466]	2.787(12)
OW5	.... O58	[ ]	2.735(8)
OW5	.... N52	[ ]	2.888(13)
OW5	.... OW3	[4545]	2.804(11)
OW6	.... OW11	[ ]	3.041(14)
OW6	.... N1B	[ ]	3.220(11)
OW6	.... N45	[ ]	3.148(11)
OW6	.... OW10	[2575]	2.98(2)
OW7	.... OW16	[ ]	2.721(16)
OW7	.... N29	[ ]	3.168(10)
OW7	.... O33	[4645]	2.908(10)
OW8	.... OW4	[ ]	2.960(12)
OW8	.... *OW22	[ ]	2.94(3)
OW8	.... *OW23	[ ]	2.67(2
OW8	.... OW10	[2575]	2.810(18)
OW8	.... O39	[2575]	2.930(10)
OW8	.... OW15	[3466]	2.680(15)
OW9	.... OW19	[ ]	3.027(17)
OW9	.... *OW24	[ ]	2.75(2)
OW9	.... N45	[ ]	2.957(15)
OW9	.... N2C	[2575]	3.058(16)
OW9	.... OW13	[4555]	2.876(19)
OW10	.... N40	[ ]	3.164(17)
OW10	.... OW6	[2574]	2.98(2)
OW10	.... OW8	[2574]	2.810(18)
OW10	.... OW20	[4645]	2.76(2)
OW11	.... OW6	[ ]	3.041(14)
OW11	.... O8R	[ ]	2.831(13)
OW11	.... O33	[1455]	2.890(12)
OW11	.... OW12	[4555]	2.88(2)

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code
[3466]	= -1/2+x,3/2-y,1-z
[2575]	= 1/2-x,2-y,1/2+z
[1655]	= 1+x,y,z
[2574]	= 1/2-x,2-y,-1/2+z
[4645]	= 1-x,-1/2+y,1/2-z
[4655]	= 1-x,1/2+y,1/2-z
[2574]	= 1/2-x,2-y,-1/2+z
[4555]	= -x,1/2+y,1/2-z
[1455]	= -1+x,y,z
[2474]	= -1/2-x,2-y,-1/2+z
[4545]	= -x,-1/2+y,1/2-z
[3566]	= 1/2+x,3/2-y,1-z
[3476]	= -1/2+x,5/2-y,1-z
[3565]	= 1/2+x,3/2-y,-z
[3576]	= 1/2+x,5/2-y,1-z
[3465]	= -1/2+x,3/2-y,-z

cont.

Table 4b (cont.)

At(I)[1555.03]	At(J)	[ARU(J)]	D(I-J)
OW12	.... OW16	[ ]	2.87(2)
OW12	.... *OW21	[3565]	2.88(4)
OW12	.... OW11	[4545]	2.879(19)
OW13	.... *OW21	[ ]	2.45(3)
OW13	.... OW18	[2574]	2.82(2)
OW13	.... OW20	[2574]	2.848(19)
OW13	.... OW9	[4545]	2.876(19)
OW14	.... OW18	[ ]	2.902(18)
OW14	.... N34	[ ]	2.972(17)
OW14	.... OW15	[3566]	2.862(19)
OW15	.... OW2	[ ]	2.856(16)
OW15	.... O62	[ ]	2.751(17)
OW15	.... OW8	[3566]	2.680(15)
OW15	.... OW14	[3466]	2.862(19)
OW15	.... *OW21	[4545]	3.06(3)
OW16	.... OW7	[ ]	2.721(16)
OW16	.... OW12	[ ]	2.87(2)
OW16	.... N2C	[ ]	3.150(15)
OW16	.... *OW24	[2574]	3.07(2)
OW16	.... OW18	[4645]	3.12(2)
OW17	.... OW18	[ ]	2.92(2)
OW17	.... OW19	[ ]	2.60(2)
OW17	.... OW20	[ ]	2.62(2)
OW17	.... N2C	[2575]	3.065(19)
OW18	.... OW14	[ ]	2.902(18)
OW18	.... OW17	[ ]	2.92(2)
OW18	.... OW13	[2575]	2.82(2)
OW18	.... OW16	[4655]	3.12(2)
OW19	.... OW9	[ ]	3.027(17)
OW19	.... OW17	[ ]	2.60(2)
OW19	.... O44	[ ]	2.690(15)
OW19	.... *OW23	[3576]	3.14(3)
OW19	.... *OW21	[4555]	2.96(3)
OW19	.... O28	[4655]	3.189(15)
OW20	.... OW17	[ ]	2.62(2)
OW20	.... OW13	[2575]	2.848(19)
OW20	.... OW10	[4655]	2.76(2)

At(I)[1555.03]	At(J)	[ARU(J)]	D(I-J)
*OW21	.... OW13	[ ]	2.45(3)
*OW21	.... O51	[ ]	2.70(4)
*OW21	.... OW12	[3465]	2.88(4)
*OW21	.... OW15	[4555]	3.06(3)
*OW21	.... OW19	[4545]	2.96(3)
*OW21	.... OW23*	[ ]	2.63(4)
*OW22	.... OW8	[ ]	2.94(3)
*OW22	.... O28	[2575]	2.99(4)
*OW22	.... N40	[2575]	3.15(3)
*OW23	.... OW8	[ ]	2.67(2)
*OW23	.... O28	[2575]	2.74(2)
*OW23	.... O51	[2475]	3.08(3)
*OW23	.... OW19	[3476]	3.14(3)
*OW23	.... OW24*	[ ]	2.76(3)
*OW24	.... OW9	[ ]	2.75(2)
*OW24	.... OW16	[2575]	3.07(2)
*OW24	.... OW23*	[ ]	2.76(3)

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[2574]	= 1/2-x,2-y,-1/2+z
[4645]	= 1-x,-1/2+y,1/2-z
[4655]	= 1-x,1/2+y,1/2-z
[2574]	= 1/2-x,2-y,-1/2+z
[4555]	= -x,1/2+y,1/2-z
[1455]	= -1+x,y,z
[2474]	= -1/2-x,2-y,-1/2+z
[4545]	= -x,-1/2+y,1/2-z
[3566]	= 1/2+x,3/2-y,1-z
[3476]	= -1/2+x,5/2-y,1-z
[3565]	= 1/2+x,3/2-y,-z
[3576]	= 1/2+x,5/2-y,1-z
[3465]	= -1/2+x,3/2-y,-z