

Table 1. Crystal data and structure refinement for 1.

Identification code	EK2_250495
Empirical formula	C ₃₄ H ₂₈ Co ₁ N ₁ O ₃ P ₂
Formula weight	619.49
Temperature	253 K
Wavelength	.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 13.073(3) Å alpha = 90 deg. b = 9.705(6) Å beta = 101.20(2) deg. c = 11.637(3) Å gamma = 90 deg.
Volume	1448(1) Å ³
Z	2.00
Density (calculated)	1.42 Mg/m ³
Absorption coefficient	0.734 mm ⁻¹
F(000)	640
Crystal size	0.58 x 0.15 x 0.04 mm
Theta range for data collection	2.6 to 30.0 deg.
Index ranges	-16 ≤ h ≤ 1, 0 ≤ k ≤ 12, -16 ≤ l ≤ 18
Reflections collected	4226
Independent reflections	2039 [R(int) = 0.016]
Absorption correction	Numerical
Max. and min. transmission	0.972 and 0.901
Refinement method	Full-matrix least-squares on F
Data / restraints / parameters	1393 / 59 / 141
Final R indices [I > 1sigma(I)]	R ₁ = 0.080, wR = 0.069
Largest diff. peak	0.45 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Co	0	0	0	34(1)
P	2515(1)	-249(2)	1533(1)	40(1)
C(1)	1118(4)	-53(7)	1512(5)	37(2)
C(2)	577(5)	1237(7)	1372(5)	43(2)
C(3)	-488(5)	992(8)	1348(5)	51(2)
C(4)	-639(5)	-448(8)	1412(6)	48(2)
C(5)	343(5)	-1077(7)	1527(5)	39(2)
C(10)	3082(5)	786(7)	2819(5)	38(2)
C(11)	2556(5)	1243(7)	3658(5)	43(2)
C(12)	3073(6)	2014(7)	4601(6)	49(2)
C(13)	4115(7)	2285(8)	4719(7)	63(2)
C(14)	4639(7)	1826(9)	3898(7)	70(2)
C(15)	4132(6)	1107(8)	2922(6)	54(2)
C(20)	2728(5)	-1995(7)	2079(5)	37(2)
C(21)	3196(5)	-2377(7)	3193(5)	45(2)
C(22)	3357(6)	-3741(8)	3499(6)	55(2)
C(23)	3052(6)	-4750(8)	2692(6)	58(2)
C(24)	2529(6)	-4420(9)	1592(7)	67(2)
C(25)	2393(6)	-3049(8)	1263(7)	55(2)
N	-140(1)	130(2)	5100(1)	54(3)
O(1)	-320(1)	-1080(1)	4940(2)	157(7)
O(2)	-500(1)	740(1)	5820(1)	88(4)
O(3)	354(9)	820(1)	4505(9)	95(4)
H(2)	898	2136	1294	55
H(3)	-1036	1691	1297	66
H(4)	-1305	-919	1393	62
H(5)	462	-2073	1604	50
H(11)	1815	1023	3591	56
H(12)	2691	2352	5189	65
H(13)	4491	2811	5389	82
H(14)	5384	2027	3982	91
H(15)	4517	829	2316	70
H(21)	3405	-1649	3775	59
H(22)	3733	-3987	4285	71
H(23)	3141	-5716	2934	75
H(24)	2272	-5148	1024	87
H(25)	2093	-2785	455	72

Table 3. Bond lengths [Å] and angles [deg] for 1.

Co-C(1)	2.058(4)
Co-C(2)	2.022(6)

Co-C(3)	2.045(6)
Co-C(4)	2.029(6)
Co-C(5)	2.035(6)
P-C(1)	1.832(5)
P-C(10)	1.836(6)
P-C(20)	1.813(6)
C(1)-C(2)	1.431(8)
C(1)-C(5)	1.421(8)
C(2)-C(3)	1.408(9)
C(2)-H(2)	.9800
C(3)-C(4)	1.41(1)
C(3)-H(3)	.9800
C(4)-C(5)	1.404(9)
C(4)-H(4)	.9800
C(5)-H(5)	.9800
C(10)-C(11)	1.373(7)
C(10)-C(15)	1.389(8)
C(11)-C(12)	1.390(7)
C(11)-H(11)	.9800
C(12)-C(13)	1.367(9)
C(12)-H(12)	.9800
C(13)-C(14)	1.355(9)
C(13)-H(13)	.9800
C(14)-C(15)	1.387(9)
C(14)-H(14)	.9800
C(15)-H(15)	.9800
C(20)-C(21)	1.372(7)
C(20)-C(25)	1.407(8)
C(21)-C(22)	1.376(8)
C(21)-H(21)	.9800
C(22)-C(23)	1.362(8)
C(22)-H(22)	.9800
C(23)-C(24)	1.367(8)
C(23)-H(23)	.9800
C(24)-C(25)	1.386(9)
C(24)-H(24)	.9800
C(25)-H(25)	.9800
N-O(1)	1.20(4)
N-O(2)	1.20(2)
N-O(3)	1.23(3)

C(1)-P-C(10)	101.4(2)
C(1)-P-C(20)	100.8(3)
C(10)-P-C(20)	102.4(3)
Co-C(1)-P	123.7(3)
Co-C(1)-C(2)	68.2(3)
Co-C(1)-C(5)	68.8(3)
P-C(1)-C(2)	124.1(5)
P-C(1)-C(5)	129.6(5)
C(2)-C(1)-C(5)	106.0(5)
Co-C(2)-C(1)	70.8(3)
Co-C(2)-C(3)	70.6(4)
Co-C(2)-H(2)	123.81
C(1)-C(2)-C(3)	108.6(6)
C(1)-C(2)-H(2)	125.37

C(3)-C(2)-H(2)	126.03
Co-C(3)-C(2)	68.9(3)
Co-C(3)-C(4)	69.1(4)
Co-C(3)-H(3)	127.76
C(2)-C(3)-C(4)	108.2(6)
C(2)-C(3)-H(3)	126.36
C(4)-C(3)-H(3)	125.43
Co-C(4)-C(3)	70.3(4)
Co-C(4)-C(5)	70.0(3)
Co-C(4)-H(4)	125.82
C(3)-C(4)-C(5)	107.5(6)
C(3)-C(4)-H(4)	126.23
C(5)-C(4)-H(4)	126.26
Co-C(5)-C(1)	70.5(3)
Co-C(5)-C(4)	69.6(4)
Co-C(5)-H(5)	126.21
C(1)-C(5)-C(4)	109.5(6)
C(1)-C(5)-H(5)	126.22
C(4)-C(5)-H(5)	124.24
P-C(10)-C(11)	125.3(4)
P-C(10)-C(15)	115.4(5)
C(11)-C(10)-C(15)	119.3(5)
C(10)-C(11)-C(12)	120.0(6)
C(10)-C(11)-H(11)	119.82
C(12)-C(11)-H(11)	120.18
C(11)-C(12)-C(13)	120.4(6)
C(11)-C(12)-H(12)	119.70
C(13)-C(12)-H(12)	119.88
C(12)-C(13)-C(14)	119.7(7)
C(12)-C(13)-H(13)	121.12
C(14)-C(13)-H(13)	119.19
C(13)-C(14)-C(15)	121.1(7)
C(13)-C(14)-H(14)	119.56
C(15)-C(14)-H(14)	119.31
C(10)-C(15)-C(14)	119.3(6)
C(10)-C(15)-H(15)	120.88
C(14)-C(15)-H(15)	119.79
P-C(20)-C(21)	126.4(5)
P-C(20)-C(25)	115.9(4)
C(21)-C(20)-C(25)	117.7(6)
C(20)-C(21)-C(22)	121.5(6)
C(20)-C(21)-H(21)	118.13
C(22)-C(21)-H(21)	120.40
C(21)-C(22)-C(23)	120.2(6)
C(21)-C(22)-H(22)	119.99
C(23)-C(22)-H(22)	119.66
C(22)-C(23)-C(24)	120.3(7)
C(22)-C(23)-H(23)	119.15
C(24)-C(23)-H(23)	120.22
C(23)-C(24)-C(25)	119.8(7)
C(23)-C(24)-H(24)	120.41
C(25)-C(24)-H(24)	119.77
C(20)-C(25)-C(24)	120.3(6)
C(20)-C(25)-H(25)	118.11
C(24)-C(25)-H(25)	121.48

O(1)-N-O(2)	120(3)
O(1)-N-O(3)	123(2)
O(2)-N-O(3)	116(3)

Table 4. Hydrogen coordinates and isotropic displacement parameters ($\text{\AA}^2$) for 1.

	x	y	z	U(eq)
H2	0.0898	0.2136	0.1294	0.0551
H3	-0.1036	0.1691	0.1297	0.0658
H4		-0.1305	-0.0919	0.1393
H5		0.0462	-0.2073	0.1604
H11	0.1815	0.1023	0.3591	0.0560
H12	0.2691	0.2352	0.5189	0.0645
H13	0.4491	0.2811	0.5389	0.0819
H14	0.5384	0.2027	0.3982	0.0912
H15	0.4517	0.0829	0.2316	0.0705
H21	0.3405	-0.1649	0.3775	0.0590
H22	0.3733	-0.3987	0.4285	0.0709
H23	0.3141	-0.5716	0.2934	0.0753
H24	0.2272	-0.5148	0.1024	0.0869
H25	0.2093	-0.2785	0.0455	0.0722

Table 5. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Co	32(1)	41(1)	28(1)	-4(1)	0(1)	4(1)
P	36(1)	49(1)	32(1)	1(1)	3(1)	1(1)
C(1)	40(3)	40(3)	26(3)	0(3)	-9(2)	3(4)
C(2)	50(4)	48(4)	26(3)	-4(3)	-2(3)	6(3)
C(3)	41(4)	72(5)	37(3)	-14(4)	2(3)	15(4)
C(4)	34(3)	69(5)	38(3)	7(3)	0(3)	3(3)
C(5)	39(3)	44(4)	33(3)	11(3)	6(3)	-2(3)
O(1)	110(1)	55(7)	280(2)	-60(1)	-30(1)	-5(8)
O(2)	95(9)	104(9)	63(7)	-14(7)	11(6)	-10(8)
O(3)	91(7)	105(8)	104(7)	60(6)	59(5)	6(7)