

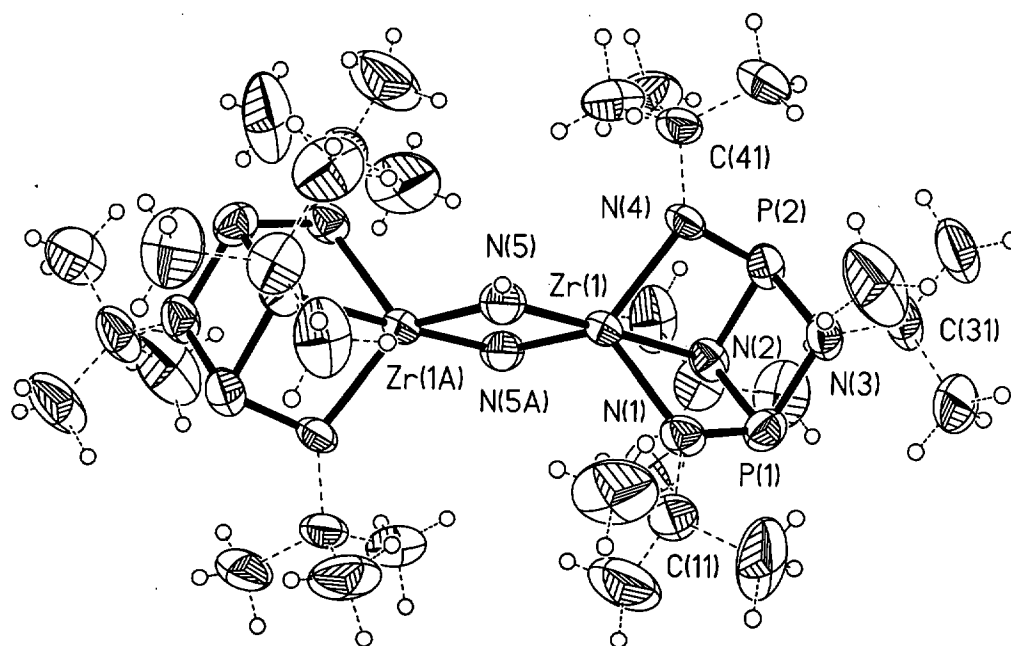


Table 1. Crystal data and structure refinement for **2**.

Identification code	2	
Empirical formula	C ₃₂ H ₇₄ N ₁₀ P ₄ Zr ₂	
Formula weight	905.33	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.618(7) Å	α = 90°.
	b = 18.426(7) Å	β = 90.25(3)°.
	c = 18.479(8) Å	γ = 90°.
Volume	4637(3) Å ³	
Z	4	
Density (calculated)	1.297 Mg/m ³	
Absorption coefficient	0.620 mm ⁻¹	
F(000)	1904	
Crystal size	0.90 x 0.90 x 0.60 mm ³	
Theta range for data collection	3.64 to 23.75°.	
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 0, -19 ≤ l ≤ 20	
Reflections collected	6971	
Independent reflections	6913 [R(int) = 0.0614]	
Completeness to theta = 23.75°	97.9 %	
Max. and min. transmission	0.7072 and 0.6052	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6913 / 0 / 457	
Goodness-of-fit on F ²	1.107	
Final R indices [I > 2σ(I)]	R ₁ = 0.0859, wR ₂ = 0.2027	
R indices (all data)	R ₁ = 0.1078, wR ₂ = 0.2203	
Largest diff. peak and hole	1.418 and -1.109 e.Å ⁻³	

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zr(1)	4389(1)	4635(1)	630(1)	41(1)
P(1)	2835(2)	4787(1)	1777(1)	49(1)
P(2)	2950(2)	3497(1)	1137(1)	46(1)
N(1)	3930(5)	5166(4)	1586(4)	46(2)
N(2)	2692(5)	4411(4)	890(4)	44(2)
N(3)	2998(6)	3878(4)	1989(4)	50(2)
N(4)	4078(5)	3510(4)	761(4)	42(2)
N(5)	5804(6)	4860(4)	353(4)	49(2)
C(11)	4274(9)	5826(6)	2008(6)	67(3)
C(12)	5390(11)	5861(9)	1946(10)	123(6)
C(13)	3872(16)	6482(8)	1661(10)	139(7)
C(14)	3920(20)	5822(11)	2762(9)	194(13)
C(21)	1781(7)	4570(7)	459(6)	65(3)
C(22)	866(9)	4315(9)	874(8)	97(5)
C(23)	1860(9)	4199(8)	-260(6)	83(4)
C(24)	1744(9)	5408(8)	368(7)	86(4)
C(31)	3156(11)	3537(6)	2682(6)	75(4)
C(32)	2781(16)	3982(8)	3294(7)	131(7)
C(33)	4280(13)	3465(9)	2793(7)	116(6)
C(34)	2770(14)	2787(7)	2701(7)	114(6)
C(41)	4512(8)	2812(5)	505(5)	54(2)
C(42)	4032(11)	2571(7)	-194(7)	94(4)
C(43)	4415(12)	2213(6)	1050(8)	94(5)

C(44)	5594(10)	2948(7)	365(8)	89(4)
Zr(2)	9389(1)	4637(1)	4370(1)	41(1)
P(3)	7954(2)	3503(1)	3863(1)	47(1)
P(4)	7834(2)	4793(1)	3225(1)	48(1)
N(6)	9082(6)	3517(4)	4247(4)	45(2)
N(7)	8004(6)	3882(4)	3005(4)	49(2)
N(8)	8913(6)	5168(4)	3413(4)	47(2)
N(9)	7693(5)	4426(4)	4102(4)	45(2)
N(10)	10801(5)	4845(4)	4640(4)	46(2)
C(61)	9530(9)	2820(5)	4497(6)	61(3)
C(62)	9445(13)	2205(6)	3936(8)	104(5)
C(63)	10607(10)	2949(7)	4650(8)	89(4)
C(64)	8998(12)	2586(7)	5186(7)	98(5)
C(71)	8168(11)	3540(6)	2328(5)	76(4)
C(72)	9317(14)	3476(9)	2217(8)	127(7)
C(73)	7796(15)	2774(8)	2305(9)	132(7)
C(74)	7772(16)	3994(8)	1722(8)	130(7)
C(81)	9266(9)	5817(5)	2996(6)	63(3)
C(82)	8909(17)	5810(10)	2227(9)	165(10)
C(83)	10351(12)	5872(10)	3057(11)	140(8)
C(84)	8857(17)	6492(8)	3325(11)	148(8)
C(91)	6773(7)	4606(7)	4544(6)	68(3)
C(92)	6852(9)	4223(7)	5259(6)	78(4)
C(93)	6747(9)	5434(7)	4628(7)	81(4)
C(94)	5864(9)	4321(12)	4115(8)	121(7)

Table 3. Bond lengths [Å] and angles [°] for 2.

Zr(1)-N(5)	2.039(8)
Zr(1)-N(5)#1	2.057(8)
Zr(1)-N(1)	2.116(7)
Zr(1)-N(4)	2.129(7)
Zr(1)-N(2)	2.399(7)
Zr(1)-P(1)	3.015(3)
Zr(1)-P(2)	3.023(3)
Zr(1)-Zr(1)#1	3.168(2)
P(1)-N(1)	1.686(8)
P(1)-N(3)	1.733(8)
P(1)-N(2)	1.789(8)
P(1)-P(2)	2.660(4)
P(2)-N(4)	1.689(8)
P(2)-N(3)	1.726(8)
P(2)-N(2)	1.781(8)
N(1)-C(11)	1.516(12)
N(2)-C(21)	1.500(12)
N(3)-C(31)	1.441(13)
N(4)-C(41)	1.493(11)
N(5)-Zr(1)#1	2.057(8)
C(11)-C(14)	1.479(16)
C(11)-C(13)	1.47(2)
C(11)-C(12)	1.527(18)
C(21)-C(23)	1.499(16)
C(21)-C(22)	1.539(16)
C(21)-C(24)	1.554(17)
C(31)-C(34)	1.480(16)
C(31)-C(32)	1.488(17)
C(31)-C(33)	1.55(2)
C(41)-C(42)	1.512(15)
C(41)-C(43)	1.501(15)

C(41)-C(44)	1.518(16)
Zr(2)-N(10)	2.020(7)
Zr(2)-N(10)#2	2.080(7)
Zr(2)-N(6)	2.119(7)
Zr(2)-N(8)	2.121(7)
Zr(2)-N(9)	2.393(7)
Zr(2)-P(4)	3.002(3)
Zr(2)-P(3)	3.008(3)
Zr(2)-Zr(2)#2	3.152(2)
P(3)-N(6)	1.689(8)
P(3)-N(7)	1.734(7)
P(3)-N(9)	1.793(8)
P(3)-P(4)	2.658(4)
P(4)-N(8)	1.659(8)
P(4)-N(7)	1.742(8)
P(4)-N(9)	1.768(7)
N(6)-C(61)	1.493(12)
N(7)-C(71)	1.420(13)
N(8)-C(81)	1.503(12)
N(9)-C(91)	1.534(12)
N(10)-Zr(2)#2	2.080(7)
C(61)-C(63)	1.511(17)
C(61)-C(62)	1.539(15)
C(61)-C(64)	1.531(16)
C(71)-C(74)	1.497(17)
C(71)-C(73)	1.501(16)
C(71)-C(72)	1.58(2)
C(81)-C(84)	1.493(19)
C(81)-C(83)	1.486(19)
C(81)-C(82)	1.499(18)
C(91)-C(92)	1.501(16)
C(91)-C(93)	1.534(17)
C(91)-C(94)	1.558(17)

N(5)-Zr(1)-N(5)#1	78.7(3)
N(5)-Zr(1)-N(1)	113.5(3)
N(5)#1-Zr(1)-N(1)	119.4(3)
N(5)-Zr(1)-N(4)	114.5(3)
N(5)#1-Zr(1)-N(4)	121.1(3)
N(1)-Zr(1)-N(4)	107.2(3)
N(5)-Zr(1)-N(2)	176.4(3)
N(5)#1-Zr(1)-N(2)	97.8(3)
N(1)-Zr(1)-N(2)	67.9(3)
N(4)-Zr(1)-N(2)	67.5(3)
N(5)-Zr(1)-P(1)	145.6(2)
N(5)#1-Zr(1)-P(1)	119.4(2)
N(1)-Zr(1)-P(1)	32.8(2)
N(4)-Zr(1)-P(1)	82.5(2)
N(2)-Zr(1)-P(1)	36.39(18)
N(5)-Zr(1)-P(2)	146.5(2)
N(5)#1-Zr(1)-P(2)	120.5(2)
N(1)-Zr(1)-P(2)	82.4(2)
N(4)-Zr(1)-P(2)	32.8(2)
N(2)-Zr(1)-P(2)	36.08(18)
P(1)-Zr(1)-P(2)	52.28(7)
N(5)-Zr(1)-Zr(1)#1	39.5(2)
N(5)#1-Zr(1)-Zr(1)#1	39.1(2)
N(1)-Zr(1)-Zr(1)#1	125.1(2)
N(4)-Zr(1)-Zr(1)#1	127.0(2)
N(2)-Zr(1)-Zr(1)#1	136.86(18)
P(1)-Zr(1)-Zr(1)#1	148.21(7)

P(2)-Zr(1)-Zr(1)#1	149.98(6)
N(1)-P(1)-N(3)	109.6(4)
N(1)-P(1)-N(2)	93.5(4)
N(3)-P(1)-N(2)	81.2(4)
N(1)-P(1)-P(2)	102.9(3)
N(3)-P(1)-P(2)	39.6(3)
N(2)-P(1)-P(2)	41.7(2)
N(1)-P(1)-Zr(1)	42.8(3)
N(3)-P(1)-Zr(1)	88.8(3)
N(2)-P(1)-Zr(1)	52.7(2)
P(2)-P(1)-Zr(1)	64.00(7)
N(4)-P(2)-N(3)	109.8(4)
N(4)-P(2)-N(2)	93.4(3)
N(3)-P(2)-N(2)	81.6(4)
N(4)-P(2)-P(1)	103.0(2)
N(3)-P(2)-P(1)	39.8(3)
N(2)-P(2)-P(1)	41.9(2)
N(4)-P(2)-Zr(1)	43.1(2)
N(3)-P(2)-Zr(1)	88.7(3)
N(2)-P(2)-Zr(1)	52.5(2)
P(1)-P(2)-Zr(1)	63.71(8)
C(11)-N(1)-P(1)	119.7(7)
C(11)-N(1)-Zr(1)	135.0(6)
P(1)-N(1)-Zr(1)	104.4(3)
C(21)-N(2)-P(2)	118.9(6)
C(21)-N(2)-P(1)	119.8(7)
P(2)-N(2)-P(1)	96.4(4)
C(21)-N(2)-Zr(1)	131.0(6)
P(2)-N(2)-Zr(1)	91.4(3)
P(1)-N(2)-Zr(1)	90.9(3)
C(31)-N(3)-P(2)	129.6(7)
C(31)-N(3)-P(1)	129.8(7)
P(2)-N(3)-P(1)	100.5(4)
C(41)-N(4)-P(2)	118.6(6)
C(41)-N(4)-Zr(1)	136.3(6)
P(2)-N(4)-Zr(1)	104.1(3)
Zr(1)-N(5)-Zr(1)#1	101.3(3)
C(14)-C(11)-C(13)	106.9(15)
C(14)-C(11)-N(1)	112.3(10)
C(13)-C(11)-N(1)	108.8(10)
C(14)-C(11)-C(12)	113.8(14)
C(13)-C(11)-C(12)	107.5(13)
N(1)-C(11)-C(12)	107.5(9)
C(23)-C(21)-N(2)	108.6(9)
C(23)-C(21)-C(22)	111.3(10)
N(2)-C(21)-C(22)	110.2(10)
C(23)-C(21)-C(24)	111.1(10)
N(2)-C(21)-C(24)	106.1(8)
C(22)-C(21)-C(24)	109.4(11)
N(3)-C(31)-C(34)	112.2(10)
N(3)-C(31)-C(32)	112.6(11)
C(34)-C(31)-C(32)	111.9(11)
N(3)-C(31)-C(33)	107.4(9)
C(34)-C(31)-C(33)	105.5(13)
C(32)-C(31)-C(33)	106.8(13)
N(4)-C(41)-C(42)	110.7(9)
N(4)-C(41)-C(43)	112.7(8)
C(42)-C(41)-C(43)	108.5(10)
N(4)-C(41)-C(44)	107.3(8)
C(42)-C(41)-C(44)	108.6(10)
C(43)-C(41)-C(44)	108.9(10)

N(10)-Zr(2)-N(10)#2	79.6(3)
N(10)-Zr(2)-N(6)	113.5(3)
N(10)#2-Zr(2)-N(6)	121.1(3)
N(10)-Zr(2)-N(8)	113.9(3)
N(10)#2-Zr(2)-N(8)	118.9(3)
N(6)-Zr(2)-N(8)	107.4(3)
N(10)-Zr(2)-N(9)	177.2(3)
N(10)#2-Zr(2)-N(9)	97.6(3)
N(6)-Zr(2)-N(9)	68.2(3)
N(8)-Zr(2)-N(9)	67.1(3)
N(10)-Zr(2)-P(4)	145.4(2)
N(10)#2-Zr(2)-P(4)	119.1(2)
N(6)-Zr(2)-P(4)	83.0(2)
N(8)-Zr(2)-P(4)	32.3(2)
N(9)-Zr(2)-P(4)	36.07(18)
N(10)-Zr(2)-P(3)	145.5(2)
N(10)#2-Zr(2)-P(3)	120.6(2)
N(6)-Zr(2)-P(3)	33.1(2)
N(8)-Zr(2)-P(3)	82.2(2)
N(9)-Zr(2)-P(3)	36.59(19)
P(4)-Zr(2)-P(3)	52.50(7)
N(10)-Zr(2)-Zr(2)#2	40.5(2)
N(10)#2-Zr(2)-Zr(2)#2	39.1(2)
N(6)-Zr(2)-Zr(2)#2	126.6(2)
N(8)-Zr(2)-Zr(2)#2	125.4(2)
N(9)-Zr(2)-Zr(2)#2	136.71(18)
P(4)-Zr(2)-Zr(2)#2	148.07(7)
P(3)-Zr(2)-Zr(2)#2	149.83(6)
N(6)-P(3)-N(7)	109.8(4)
N(6)-P(3)-N(9)	93.7(3)
N(7)-P(3)-N(9)	81.5(4)
N(6)-P(3)-P(4)	103.2(3)
N(7)-P(3)-P(4)	40.2(3)
N(9)-P(3)-P(4)	41.4(2)
N(6)-P(3)-Zr(2)	43.2(2)
N(7)-P(3)-Zr(2)	88.7(3)
N(9)-P(3)-Zr(2)	52.7(2)
P(4)-P(3)-Zr(2)	63.64(8)
N(8)-P(4)-N(7)	109.3(4)
N(8)-P(4)-N(9)	93.8(4)
N(7)-P(4)-N(9)	82.0(4)
N(8)-P(4)-P(3)	103.1(3)
N(7)-P(4)-P(3)	40.0(2)
N(9)-P(4)-P(3)	42.1(3)
N(8)-P(4)-Zr(2)	43.1(3)
N(7)-P(4)-Zr(2)	88.7(3)
N(9)-P(4)-Zr(2)	52.8(2)
P(3)-P(4)-Zr(2)	63.86(8)
C(61)-N(6)-P(3)	119.2(6)
C(61)-N(6)-Zr(2)	136.4(6)
P(3)-N(6)-Zr(2)	103.8(4)
C(71)-N(7)-P(3)	129.3(7)
C(71)-N(7)-P(4)	130.9(7)
P(3)-N(7)-P(4)	99.8(4)
C(81)-N(8)-P(4)	120.6(7)
C(81)-N(8)-Zr(2)	134.2(6)
P(4)-N(8)-Zr(2)	104.5(4)
C(91)-N(9)-P(4)	119.9(7)
C(91)-N(9)-P(3)	119.9(7)
P(4)-N(9)-P(3)	96.6(4)
C(91)-N(9)-Zr(2)	130.1(6)

P(4)-N(9)-Zr(2)	91.1(3)
P(3)-N(9)-Zr(2)	90.7(3)
Zr(2)-N(10)-Zr(2)#2	100.4(3)
N(6)-C(61)-C(63)	108.6(8)
N(6)-C(61)-C(62)	113.3(9)
C(63)-C(61)-C(62)	108.2(11)
N(6)-C(61)-C(64)	107.8(9)
C(63)-C(61)-C(64)	110.5(11)
C(62)-C(61)-C(64)	108.5(10)
N(7)-C(71)-C(74)	110.7(11)
N(7)-C(71)-C(73)	112.8(10)
C(74)-C(71)-C(73)	112.6(12)
N(7)-C(71)-C(72)	107.8(10)
C(74)-C(71)-C(72)	107.3(12)
C(73)-C(71)-C(72)	105.1(13)
C(84)-C(81)-C(83)	106.5(13)
C(84)-C(81)-N(8)	109.5(10)
C(83)-C(81)-N(8)	109.6(9)
C(84)-C(81)-C(82)	105.8(14)
C(83)-C(81)-C(82)	113.0(14)
N(8)-C(81)-C(82)	112.1(9)
C(92)-C(91)-C(93)	112.2(10)
C(92)-C(91)-N(9)	108.2(9)
C(93)-C(91)-N(9)	106.7(9)
C(92)-C(91)-C(94)	110.0(11)
C(93)-C(91)-C(94)	111.7(12)
N(9)-C(91)-C(94)	107.8(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z #2 -x+2,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Zr(1)	53(1)	27(1)	44(1)	-2(1)	7(1)	-3(1)
P(1)	55(1)	52(2)	39(1)	-4(1)	3(1)	5(1)
P(2)	61(2)	45(1)	33(1)	-1(1)	-3(1)	-17(1)
N(1)	57(5)	35(4)	45(4)	-7(3)	-5(3)	-9(3)
N(2)	49(4)	43(4)	41(4)	4(3)	-8(3)	-4(3)
N(3)	69(5)	48(5)	34(4)	7(4)	3(3)	-11(4)
N(4)	60(4)	23(3)	44(4)	1(3)	1(3)	-3(3)
N(5)	54(5)	44(4)	49(5)	-2(4)	1(3)	4(3)
C(11)	106(9)	50(6)	45(6)	-15(5)	6(5)	-16(6)
C(12)	106(12)	105(12)	156(16)	-61(12)	-14(10)	-37(9)
C(13)	250(20)	50(8)	111(14)	-16(9)	8(14)	-24(11)
C(14)	370(30)	145(17)	71(11)	-67(11)	99(15)	-160(20)
C(21)	50(6)	84(8)	61(7)	-1(6)	-14(5)	-1(5)
C(22)	57(7)	135(13)	98(11)	6(9)	-10(6)	-13(8)
C(23)	89(8)	116(11)	44(7)	9(7)	-24(6)	-31(8)
C(24)	76(8)	111(11)	71(8)	2(8)	-23(6)	29(7)
C(31)	134(11)	54(7)	36(6)	8(5)	4(6)	-32(7)
C(32)	270(20)	76(10)	45(8)	0(7)	56(10)	-5(12)
C(33)	184(17)	104(12)	60(9)	31(8)	-58(9)	-35(11)
C(34)	240(19)	56(8)	47(8)	8(6)	19(9)	-41(10)
C(41)	88(7)	31(5)	45(6)	-6(4)	4(5)	5(5)

C(42)	144(13)	71(9)	66(9)	-35(7)	-9(8)	14(8)
C(43)	158(13)	36(6)	88(10)	10(6)	29(9)	16(7)
C(44)	102(10)	56(7)	110(11)	-18(7)	26(8)	18(7)
Zr(2)	53(1)	27(1)	44(1)	1(1)	-7(1)	-3(1)
P(3)	61(2)	45(1)	35(1)	1(1)	3(1)	-17(1)
P(4)	54(1)	49(1)	40(1)	6(1)	-3(1)	4(1)
N(6)	70(5)	26(4)	37(4)	1(3)	-4(3)	-5(3)
N(7)	72(5)	45(4)	29(4)	2(3)	-6(3)	-9(4)
N(8)	63(5)	40(4)	37(4)	5(3)	6(3)	-1(3)
N(9)	47(4)	52(5)	36(4)	1(3)	7(3)	3(3)
N(10)	45(4)	45(4)	47(5)	-5(4)	-1(3)	4(3)
C(61)	99(8)	24(5)	60(7)	1(4)	4(6)	8(5)
C(62)	192(16)	39(7)	80(10)	-13(6)	-28(9)	19(8)
C(63)	104(10)	57(7)	105(11)	14(7)	-16(8)	23(7)
C(64)	166(15)	59(8)	70(9)	30(7)	18(8)	5(8)
C(71)	146(12)	60(7)	23(5)	-3(5)	4(6)	-31(7)
C(72)	191(18)	122(14)	67(10)	-31(9)	69(11)	-37(12)
C(73)	250(20)	63(9)	82(11)	-3(8)	-22(12)	-65(11)
C(74)	260(20)	72(9)	55(9)	-11(7)	-60(11)	-2(11)
C(81)	101(8)	40(6)	46(6)	8(5)	-4(5)	-16(5)
C(82)	290(30)	131(15)	72(11)	40(10)	-44(13)	-127(17)
C(83)	120(13)	116(14)	184(19)	81(13)	18(12)	-44(11)
C(84)	260(20)	52(9)	131(16)	21(9)	23(15)	8(12)
C(91)	48(6)	98(9)	57(7)	-12(6)	13(5)	-4(6)
C(92)	84(8)	96(10)	55(7)	-9(7)	24(6)	-26(7)
C(93)	71(7)	86(9)	85(9)	-12(7)	17(6)	24(6)
C(94)	47(7)	240(20)	80(10)	-23(12)	11(6)	-12(9)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H(5A)	6345	4767	587	59
H(12A)	5677	5427	2156	184
H(12B)	5632	6285	2201	184
H(12C)	5572	5893	1440	184
H(13A)	3161	6453	1650	208
H(13B)	4118	6518	1171	208
H(13C)	4071	6907	1934	208
H(14A)	4222	5426	3025	291
H(14B)	3209	5760	2763	291
H(14C)	4085	6279	2993	291
H(22A)	897	3793	942	145
H(22B)	281	4437	599	145
H(22C)	845	4552	1342	145
H(23A)	2419	4392	-521	125
H(23B)	1265	4283	-538	125
H(23C)	1948	3682	-186	125
H(24A)	2355	5576	158	129
H(24B)	1653	5634	837	129
H(24C)	1201	5537	52	129
H(32A)	2070	3954	3305	196
H(32B)	2982	4483	3230	196
H(32C)	3047	3798	3746	196
H(33A)	4597	3916	2660	174
H(33B)	4527	3075	2492	174

H(33C)	4419	3358	3297	174
H(34A)	2066	2794	2618	171
H(34B)	2908	2573	3170	171
H(34C)	3083	2501	2326	171
H(42A)	3382	2382	-93	141
H(42B)	4427	2195	-416	141
H(42C)	3978	2981	-520	141
H(43A)	3752	2021	1035	141
H(43B)	4553	2401	1530	141
H(43C)	4877	1829	938	141
H(44A)	5923	3061	818	134
H(44B)	5664	3353	33	134
H(44C)	5886	2518	154	134
H(10A)	11338	4746	4407	55
H(62A)	9821	2331	3509	155
H(62B)	8761	2139	3803	155
H(62C)	9699	1759	4143	155
H(63A)	10939	3075	4204	133
H(63B)	10896	2511	4850	133
H(63C)	10677	3343	4995	133
H(64A)	9035	2972	5542	147
H(64B)	9306	2152	5379	147
H(64C)	8315	2484	5074	147
H(72A)	9599	3958	2178	190
H(72B)	9449	3206	1778	190
H(72C)	9607	3226	2628	190
H(73A)	7087	2774	2357	198
H(73B)	8089	2498	2698	198
H(73C)	7970	2554	1846	198
H(74A)	8123	4452	1705	195
H(74B)	7079	4086	1800	195
H(74C)	7857	3739	1267	195
H(82A)	8992	6289	2018	248
H(82B)	8219	5678	2215	248
H(82C)	9284	5459	1952	248
H(83A)	10571	6318	2829	210
H(83B)	10652	5460	2819	210
H(83C)	10540	5876	3564	210
H(84A)	9088	6911	3058	221
H(84B)	9072	6528	3825	221
H(84C)	8145	6475	3306	221
H(92A)	6840	3703	5181	117
H(92B)	6304	4362	5562	117
H(92C)	7463	4358	5495	117
H(93A)	7340	5595	4873	121
H(93B)	6178	5572	4911	121
H(93C)	6708	5659	4154	121
H(94A)	5982	3824	3964	182
H(94B)	5757	4622	3692	182
H(94C)	5289	4338	4422	182

Table 6. Torsion angles [°] for **2**.