

Table 1. Crystal data, structure solution and refinement for 2

Identification code	ki33
Chemical formula	$C_{25}H_{42}KN_2PSi_2$
Formula weight	496.86
Temperature	160(2) K
Radiation and wavelength	MoK α , 0.71073 Å
Crystal system, space group	monoclinic, $P2_1/n$
Unit cell dimensions	$a = 9.9165(4)$ Å $\alpha = 90^\circ$ $b = 17.7521(8)$ Å $\beta = 92.5140(10)^\circ$ $c = 15.8600(7)$ Å $\gamma = 90^\circ$
Volume	$2789.3(2)$ Å ³
Z	4
Density (calculated)	1.183 g/cm ³
Absorption coefficient μ	0.349 mm ⁻¹
F(000)	1072
Reflections for cell refinement	8933 (θ range 2.63 to 29.14°)
Crystal colour	yellow
Crystal size	$0.54 \times 0.30 \times 0.26$ mm
Data collection method	Siemens SMART CCD diffractometer, ω rotation with narrow frames
θ range for data collection	2.29 to 29.14°
Index ranges	$-13 \leq h \leq 12$, $-24 \leq k \leq 22$, $-21 \leq l \leq 19$
Reflections collected	17747
Independent reflections	6913 ($R_{int} = 0.0219$)
Reflections with $I > 2\sigma(I)$	5417
Absorption correction	semi-empirical from ψ -scans
Max. and min. transmission	0.9348 and 0.8372
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0484, 0.0924
Data / restraints / parameters	6913 / 0 / 290
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0324$, $wR2 = 0.0814$
R indices (all data)	$R1 = 0.0448$, $wR2 = 0.0838$
Goodness-of-fit on F^2	1.043
Largest and mean shift/esd	0.001 and 0.000
Largest diff. peak and hole	0.351 and -0.232 eÅ ⁻³

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

	x	y	z	U(eq)
K(1)	9268.3(3)	1732.01(18)	9814.6(2)	28.54(9)
P(1)	11477.6(3)	1282.02(18)	8471.4(2)	17.48(8)
N(1)	10212.0(12)	3133.5(7)	9040.1(8)	25.5(3)
N(2)	11414.3(12)	1158.3(7)	10834.0(8)	27.1(3)
Si(1)	9543.7(4)	1170.6(2)	6932.1(3)	24.35(9)
Si(2)	12626.9(4)	1083.6(2)	6654.9(2)	22.35(9)
C(1)	11256.6(13)	1104.2(7)	7387.3(8)	20.1(3)
C(2)	9365.2(19)	1922.3(10)	6086.7(11)	40.9(4)
C(3)	8246.5(15)	1424.7(9)	7725.9(11)	32.0(3)
C(4)	8855.9(18)	286.7(10)	6414.8(11)	41.2(4)
C(5)	13151.8(18)	2053.5(9)	6286.1(11)	36.1(4)
C(6)	14263.4(16)	621.4(10)	7025.9(10)	34.1(4)
C(7)	12128.1(17)	564.4(8)	5651.4(9)	30.8(3)
C(8)	12358.8(13)	457.4(7)	8982.5(8)	19.5(3)
C(9)	12429.3(14)	-203.5(8)	8503.4(9)	23.3(3)
C(10)	12980.0(15)	-867.7(8)	8832.8(10)	27.5(3)
C(11)	13481.0(15)	-887.7(8)	9660.6(10)	28.7(3)
C(12)	13386.2(14)	-245.0(8)	10156.7(9)	26.3(3)
C(13)	12812.8(13)	423.4(8)	9838.7(9)	21.3(3)
C(14)	12726.4(14)	1084.5(8)	10438.4(9)	24.0(3)
C(15)	11115.2(19)	487.9(11)	11328.8(13)	45.5(5)
C(16)	11467.7(19)	1812.2(10)	11400.0(11)	40.5(4)
C(17)	12810.5(13)	2021.4(7)	8578.6(8)	19.3(3)
C(18)	14182.1(14)	1853.3(8)	8732.1(9)	23.2(3)
C(19)	15177.2(15)	2404.6(8)	8734.6(10)	28.0(3)
C(20)	14823.9(16)	3150.5(9)	8590.7(10)	30.2(3)
C(21)	13474.1(16)	3332.7(8)	8449.7(9)	27.5(3)
C(22)	12454.6(14)	2788.1(7)	8450.7(8)	21.6(3)
C(23)	11013.1(14)	3042.7(8)	8277.6(9)	24.3(3)
C(24)	10866.7(17)	3667.8(9)	9630.8(10)	34.3(4)
C(25)	8878.8(16)	3435.4(9)	8773.4(12)	36.6(4)

Table 3. Bond lengths (Å) and angles (°) for 2.

K(1)-N(2)	2.8067(13)	K(1)-N(1)	2.9454(12)
K(1)-P(1)	3.2227(5)	K(1)-C(11#1)	3.2513(15)
K(1)-C(16)	3.2585(19)	K(1)-C(5#2)	3.3981(16)
K(1)-C(25)	3.4589(18)	K(1)-C(3)	3.4646(17)
K(1)-C(10#1)	3.5137(14)	P(1)-C(1)	1.7524(14)
P(1)-C(17)	1.8652(14)	P(1)-C(8)	1.8712(13)
N(1)-C(24)	1.465(2)	N(1)-C(25)	1.471(2)
N(1)-C(23)	1.4845(18)	N(2)-C(15)	1.463(2)
N(2)-C(16)	1.467(2)	N(2)-C(14)	1.4750(18)
Si(1)-C(1)	1.8202(14)	Si(1)-C(4)	1.8846(17)
Si(1)-C(3)	1.8935(16)	Si(1)-C(2)	1.8944(17)
Si(2)-C(1)	1.8264(13)	Si(2)-C(7)	1.8863(15)
Si(2)-C(6)	1.8893(17)	Si(2)-C(5)	1.8984(15)
C(8)-C(9)	1.4013(19)	C(8)-C(13)	1.4130(19)
C(9)-C(10)	1.392(2)	C(10)-C(11)	1.384(2)
C(10)-K(1#1)	3.5137(14)	C(11)-C(12)	1.391(2)
C(11)-K(1#1)	3.2513(15)	C(12)-C(13)	1.4002(19)
C(13)-C(14)	1.5154(19)	C(17)-C(18)	1.4033(19)
C(17)-C(22)	1.4184(19)	C(18)-C(19)	1.3897(19)
C(19)-C(20)	1.386(2)	C(20)-C(21)	1.386(2)
C(21)-C(22)	1.3989(19)	C(22)-C(23)	1.513(2)
N(2)-K(1)-N(1)	107.46(4)	N(2)-K(1)-P(1)	76.74(3)
N(1)-K(1)-P(1)	72.30(2)	N(2)-K(1)-C(11#1)	107.96(4)
N(1)-K(1)-C(11#1)	141.40(4)	P(1)-K(1)-C(11#1)	131.07(3)
N(2)-K(1)-C(16)	26.68(4)	N(1)-K(1)-C(16)	94.06(4)
P(1)-K(1)-C(16)	93.98(3)	C(11#1)-K(1)-C(16)	111.28(4)
N(2)-K(1)-C(5#2)	95.52(4)	N(1)-K(1)-C(5#2)	82.51(4)
P(1)-K(1)-C(5#2)	149.62(3)	C(11#1)-K(1)-C(5#2)	79.31(4)
C(16)-K(1)-C(5#2)	70.70(4)	N(2)-K(1)-C(25)	131.16(4)
N(1)-K(1)-C(25)	24.95(4)	P(1)-K(1)-C(25)	88.05(3)
C(11#1)-K(1)-C(25)	116.61(4)	C(16)-K(1)-C(25)	112.78(5)
C(5#2)-K(1)-C(25)	74.95(4)	N(2)-K(1)-C(3)	132.54(4)
N(1)-K(1)-C(3)	79.58(4)	P(1)-K(1)-C(3)	60.51(3)
C(11#1)-K(1)-C(3)	87.64(4)	C(16)-K(1)-C(3)	154.48(4)
C(5#2)-K(1)-C(3)	131.77(4)	C(25)-K(1)-C(3)	70.08(4)
N(2)-K(1)-C(10#1)	88.58(4)	N(1)-K(1)-C(10#1)	147.69(3)
P(1)-K(1)-C(10#1)	139.75(3)	C(11#1)-K(1)-C(10#1)	23.19(4)
C(16)-K(1)-C(10#1)	88.23(4)	C(5#2)-K(1)-C(10#1)	67.86(4)
C(25)-K(1)-C(10#1)	127.78(4)	C(3)-K(1)-C(10#1)	110.38(4)
C(1)-P(1)-C(17)	105.89(6)	C(1)-P(1)-C(8)	108.66(6)
C(17)-P(1)-C(8)	101.27(6)	C(1)-P(1)-K(1)	129.34(5)
C(17)-P(1)-K(1)	105.36(4)	C(8)-P(1)-K(1)	103.04(4)
C(24)-N(1)-C(25)	108.39(12)	C(24)-N(1)-C(23)	110.69(12)
C(25)-N(1)-C(23)	108.15(12)	C(24)-N(1)-K(1)	114.85(9)
C(25)-N(1)-K(1)	97.45(9)	C(23)-N(1)-K(1)	116.05(8)
C(15)-N(2)-C(16)	108.56(14)	C(15)-N(2)-C(14)	111.05(12)
C(16)-N(2)-C(14)	108.76(12)	C(15)-N(2)-K(1)	115.96(10)
C(16)-N(2)-K(1)	94.10(10)	C(14)-N(2)-K(1)	116.61(8)
C(1)-Si(1)-C(4)	115.62(7)	C(1)-Si(1)-C(3)	113.65(7)
C(4)-Si(1)-C(3)	104.15(8)	C(1)-Si(1)-C(2)	112.52(7)
C(4)-Si(1)-C(2)	104.92(9)	C(3)-Si(1)-C(2)	104.93(8)
C(1)-Si(2)-C(7)	111.81(7)	C(1)-Si(2)-C(6)	117.61(7)
C(7)-Si(2)-C(6)	103.91(7)	C(1)-Si(2)-C(5)	113.55(7)
C(7)-Si(2)-C(5)	104.40(7)	C(6)-Si(2)-C(5)	104.27(8)
P(1)-C(1)-Si(1)	116.86(7)	P(1)-C(1)-Si(2)	124.28(8)
Si(1)-C(1)-Si(2)	117.16(7)	C(9)-C(8)-C(13)	117.64(12)
C(9)-C(8)-P(1)	116.98(10)	C(13)-C(8)-P(1)	124.95(10)

C(10)-C(9)-C(8)	122.27(14)	C(11)-C(10)-C(9)	119.78(14)
C(11)-C(10)-K(1#1)	67.70(8)	C(9)-C(10)-K(1#1)	110.50(9)
C(10)-C(11)-C(12)	119.03(13)	C(10)-C(11)-K(1#1)	89.11(9)
C(12)-C(11)-K(1#1)	98.92(9)	C(11)-C(12)-C(13)	121.84(14)
C(12)-C(13)-C(8)	119.32(13)	C(12)-C(13)-C(14)	117.61(12)
C(8)-C(13)-C(14)	123.07(12)	N(2)-C(14)-C(13)	114.26(11)
C(18)-C(17)-C(22)	117.51(12)	C(18)-C(17)-P(1)	122.94(10)
C(22)-C(17)-P(1)	119.43(10)	C(19)-C(18)-C(17)	122.24(13)
C(20)-C(19)-C(18)	119.86(14)	C(21)-C(20)-C(19)	119.01(13)
C(20)-C(21)-C(22)	122.11(13)	C(21)-C(22)-C(17)	119.21(13)
C(21)-C(22)-C(23)	118.06(12)	C(17)-C(22)-C(23)	122.67(12)
N(1)-C(23)-C(22)	114.82(12)		

Symmetry transformations used to generate equivalent atoms:

#1: $-x+2, -y, -z+2$ #2: $x-1/2, -y+1/2, z+1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 2.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2(h^2 a^{*2} U_{11} + \dots + 2hka^*b^* U_{12}).$$

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
K(1)	26.60(17)	32.00(17)	27.58(17)	-0.79(13)	7.53(13)	1.76(13)
P(1)	19.06(17)	16.78(16)	16.76(16)	-0.17(12)	2.46(12)	-0.30(12)
N(1)	25.3(6)	22.9(6)	28.7(7)	-0.5(5)	4.6(5)	1.6(5)
N(2)	26.9(6)	30.8(6)	24.0(6)	-0.5(5)	4.7(5)	-2.3(5)
Si(1)	24.1(2)	26.0(2)	22.6(2)	-3.06(15)	-2.44(15)	0.79(15)
Si(2)	28.1(2)	19.78(18)	19.62(19)	-0.57(14)	6.51(15)	1.17(15)
C(1)	22.0(7)	20.9(6)	17.5(6)	-0.6(5)	1.6(5)	0.7(5)
C(2)	42.6(10)	45.5(10)	34.0(9)	7.5(8)	-6.9(7)	11.9(8)
C(3)	21.9(7)	35.9(8)	38.0(9)	-5.2(7)	1.0(6)	0.4(6)
C(4)	39.1(10)	45.9(10)	38.2(10)	-13.1(8)	-1.8(8)	-8.5(8)
C(5)	47.3(10)	25.0(8)	37.7(9)	-1.2(7)	19.9(8)	-3.9(7)
C(6)	29.5(8)	41.9(9)	31.7(8)	-3.4(7)	9.1(7)	5.9(7)
C(7)	44.2(9)	26.8(7)	21.8(7)	-2.6(6)	6.9(6)	2.9(7)
C(8)	18.3(6)	18.8(6)	21.6(7)	2.6(5)	3.4(5)	-1.6(5)
C(9)	25.7(7)	21.1(7)	23.3(7)	1.0(5)	4.0(6)	-1.5(5)
C(10)	31.7(8)	18.5(6)	33.0(8)	1.1(6)	8.2(6)	-0.5(6)
C(11)	25.0(7)	24.5(7)	36.7(8)	10.3(6)	4.2(6)	2.7(6)
C(12)	22.9(7)	30.7(7)	25.4(7)	8.1(6)	0.0(6)	-1.0(6)
C(13)	18.6(6)	23.3(7)	22.2(7)	2.7(5)	2.3(5)	-3.8(5)
C(14)	24.6(7)	28.0(7)	19.4(7)	0.1(6)	1.1(5)	-5.0(6)
C(15)	41.5(10)	48.1(11)	48.4(11)	12.1(9)	20.5(8)	-4.4(8)
C(16)	42.3(10)	47.6(10)	32.1(9)	-11.2(8)	6.8(7)	1.5(8)
C(17)	22.9(7)	20.4(6)	14.9(6)	-1.5(5)	3.3(5)	-1.7(5)
C(18)	24.1(7)	22.4(7)	23.3(7)	1.9(5)	3.6(5)	-0.6(5)
C(19)	21.7(7)	32.6(8)	29.9(8)	0.9(6)	3.8(6)	-3.6(6)
C(20)	30.8(8)	28.8(8)	31.4(8)	0.9(6)	6.1(6)	-11.7(6)
C(21)	36.4(8)	19.2(7)	27.5(8)	1.6(6)	7.9(6)	-3.9(6)
C(22)	27.4(7)	21.3(6)	16.4(6)	-0.3(5)	4.0(5)	0.2(5)
C(23)	29.0(8)	19.7(6)	24.2(7)	1.3(5)	1.7(6)	3.5(6)
C(24)	34.6(9)	39.0(9)	30.0(8)	-8.3(7)	7.5(7)	-2.5(7)
C(25)	29.8(8)	31.8(8)	48.3(10)	-5.2(7)	2.7(7)	5.8(7)

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

	x	y	z	U
H(2A)	9586	2415	6334	61
H(2B)	8435	1928	5852	61
H(2C)	9983	1813	5637	61
H(3A)	8223	1031	8159	48
H(3B)	7355	1467	7438	48
H(3C)	8489	1907	7992	48
H(4A)	9355	179	5909	62
H(4B)	7898	357	6256	62
H(4C)	8958	-136	6810	62
H(5A)	12396	2290	5968	54
H(5B)	13922	2006	5924	54
H(5C)	13408	2366	6777	54
H(6A)	14633	883	7529	51
H(6B)	14911	649	6577	51
H(6C)	14095	93	7164	51
H(7A)	11812	58	5790	46
H(7B)	12910	526	5297	46
H(7C)	11403	840	5346	46
H(9)	12089	-198	7934	28
H(10)	13012	-1306	8491	33
H(11)	13884	-1334	9887	34
H(12)	13720	-260	10727	32
H(14A)	13443	1031	10889	29
H(14B)	12906	1554	10125	29
H(15A)	10941	61	10948	68
H(15B)	10317	582	11656	68
H(15C)	11888	372	11714	68
H(16A)	10614	1853	11686	61
H(16B)	11612	2270	11071	61
H(16C)	12212	1750	11821	61
H(18)	14439	1345	8838	28
H(19)	16098	2271	8835	34
H(20)	15497	3531	8589	36
H(21)	13233	3844	8349	33
H(23A)	11025	3530	7975	29
H(23B)	10553	2672	7898	29
H(24A)	11764	3479	9808	52
H(24B)	10319	3724	10126	52
H(24C)	10956	4157	9353	52
H(25A)	8301	3451	9259	55
H(25B)	8464	3111	8335	55
H(25C)	8983	3945	8549	55