

# ORGANOMETALLICS

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Table 1. Atomic coordinates [ $x 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 5.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Si	9908(2)	2108(2)	9885(1)	25(1)
O(1)	9810(4)	1873(4)	9085(2)	28(1)
O(2)	11398(4)	3204(4)	9884(2)	28(1)
O(3)	9941(4)	2082(4)	10679(2)	26(1)
O(4)	8349(4)	3109(4)	9841(2)	29(1)
O(5)	9780(4)	2683(5)	8144(2)	42(1)
O(6)	9934(5)	3125(4)	11588(2)	42(1)
O(7)	12622(4)	-2785(4)	11039(2)	39(1)
N	10620(5)	-738(5)	10465(2)	27(1)
C(1)	10064(6)	1(6)	9889(3)	28(1)
C(2)	10388(6)	-2391(6)	10441(2)	33(2)
C(3)	11077(7)	-3111(7)	10998(3)	44(2)
C(4)	12213(6)	-404(6)	10556(3)	33(2)
C(5)	12838(7)	-1238(6)	11099(3)	36(2)
C(16)	11881(6)	4079(6)	9420(2)	23(1)
C(15)	12927(6)	5143(6)	9564(3)	31(2)
C(14)	13455(7)	6096(7)	9114(3)	42(2)
C(13)	12942(7)	5939(7)	8529(3)	40(2)
C(12)	11918(7)	4900(7)	8394(3)	37(2)
C(11)	11354(6)	3949(6)	8827(2)	23(1)
C(10)	10250(7)	2811(6)	8665(2)	27(2)
C(26)	7857(6)	4138(6)	10249(2)	26(1)
C(25)	6841(6)	5163(6)	10048(3)	30(2)
C(24)	6303(6)	6239(6)	10432(3)	37(2)
C(23)	6774(6)	6288(7)	11027(3)	33(2)
C(22)	7772(6)	5240(6)	11230(2)	32(2)
C(21)	8356(6)	4164(6)	10837(2)	25(1)
C(20)	9480(6)	3097(6)	11072(3)	31(2)

Table 2. Bond lengths [Å] and angles [°] for 5.

Si-O(2)	1.666(4)	Si-O(4)	1.671(4)
Si-O(3)	1.762(4)	Si-O(1)	1.791(4)
Si-C(1)	1.903(5)	O(1)-C(10)	1.320(7)
O(2)-C(16)	1.368(6)	O(3)-C(20)	1.330(6)
O(4)-C(26)	1.369(6)	O(5)-C(10)	1.237(6)
O(6)-C(20)	1.216(6)	O(7)-C(5)	1.414(7)
O(7)-C(3)	1.426(7)	N-H	1.16(4)
N-C(4)	1.480(7)	N-C(2)	1.504(6)
N-C(1)	1.525(7)	C(2)-C(3)	1.529(7)
C(4)-C(5)	1.528(7)	C(16)-C(15)	1.381(7)
C(16)-C(11)	1.405(7)	C(15)-C(14)	1.399(8)
C(14)-C(13)	1.386(8)	C(13)-C(12)	1.348(8)
C(12)-C(11)	1.384(8)	C(11)-C(10)	1.473(8)
C(26)-C(25)	1.374(7)	C(26)-C(21)	1.382(7)
C(25)-C(24)	1.379(8)	C(24)-C(23)	1.387(8)
C(23)-C(22)	1.379(7)	C(22)-C(21)	1.406(7)
C(21)-C(20)	1.490(8)		
O(2)-Si-O(4)	110.9(2)	O(2)-Si-O(3)	89.8(2)
O(4)-Si-O(3)	94.6(2)	O(2)-Si-O(1)	96.2(2)
O(4)-Si-O(1)	87.9(2)	O(3)-Si-O(1)	172.2(2)
O(2)-Si-C(1)	122.1(2)	O(4)-Si-C(1)	126.9(2)
O(3)-Si-C(1)	88.9(2)	O(1)-Si-C(1)	83.7(2)
C(10)-O(1)-Si	127.6(4)	C(16)-O(2)-Si	126.9(3)
C(20)-O(3)-Si	129.8(4)	C(26)-O(4)-Si	126.8(3)
C(5)-O(7)-C(3)	110.1(5)	H-N-C(4)	107(2)
H-N-C(2)	115(2)	C(4)-N-C(2)	109.9(4)
H-N-C(1)	104(2)	C(4)-N-C(1)	110.1(4)
C(2)-N-C(1)	110.9(4)	N-C(1)-Si	117.6(4)
N-C(2)-C(3)	109.6(4)	O(7)-C(3)-C(2)	111.2(5)
N-C(4)-C(5)	111.4(4)	O(7)-C(5)-C(4)	111.1(5)
O(2)-C(16)-C(15)	116.3(5)	O(2)-C(16)-C(11)	123.3(5)
C(15)-C(16)-C(11)	120.3(5)	C(16)-C(15)-C(14)	119.5(6)
C(13)-C(14)-C(15)	119.5(6)	C(12)-C(13)-C(14)	120.6(6)
C(13)-C(12)-C(11)	121.7(6)	C(12)-C(11)-C(16)	118.4(5)
C(12)-C(11)-C(10)	120.6(5)	C(16)-C(11)-C(10)	121.0(5)
O(5)-C(10)-O(1)	119.9(5)	O(5)-C(10)-C(11)	121.6(5)
O(1)-C(10)-C(11)	118.4(5)	O(4)-C(26)-C(25)	117.2(5)
O(4)-C(26)-C(21)	122.1(5)	C(25)-C(26)-C(21)	120.7(5)
C(26)-C(25)-C(24)	120.5(5)	C(25)-C(24)-C(23)	120.2(6)
C(22)-C(23)-C(24)	119.3(6)	C(23)-C(22)-C(21)	120.9(6)
C(26)-C(21)-C(22)	118.5(5)	C(26)-C(21)-C(20)	122.7(5)
C(22)-C(21)-C(20)	118.8(5)	O(6)-C(20)-O(3)	121.8(5)
O(6)-C(20)-C(21)	123.0(5)	O(3)-C(20)-C(21)	115.3(5)

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 5.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
Si	26(1)	26(1)	24(1)	1(1)	-3(1)	0(1)
O(1)	34(2)	28(2)	23(2)	-1(2)	-4(2)	-2(2)
O(2)	31(2)	26(2)	26(2)	7(2)	-4(2)	-8(2)
O(3)	30(2)	24(2)	22(2)	2(2)	-3(2)	-2(2)
O(4)	33(2)	28(2)	25(2)	-3(2)	-5(2)	6(2)
O(5)	46(3)	55(3)	24(2)	-5(2)	-5(2)	6(2)
O(6)	69(3)	40(3)	18(2)	5(2)	-10(2)	-1(2)
O(7)	31(3)	25(2)	60(3)	10(2)	-8(2)	0(2)
N	32(3)	17(3)	31(3)	3(2)	-1(2)	7(2)
C(1)	27(3)	30(3)	25(3)	-1(3)	1(3)	-2(3)
C(2)	34(4)	23(3)	41(4)	3(3)	-3(3)	-2(3)
C(3)	41(4)	30(4)	60(5)	24(3)	-6(4)	-3(3)
C(4)	20(3)	28(3)	51(4)	5(3)	-5(3)	-4(3)
C(5)	34(4)	31(4)	43(4)	4(3)	-8(3)	-4(3)
C(16)	22(3)	17(3)	30(3)	0(3)	4(3)	5(3)
C(15)	26(4)	33(4)	35(4)	13(3)	-1(3)	-6(3)
C(14)	28(4)	39(4)	57(4)	13(3)	4(3)	-3(3)
C(13)	49(4)	37(4)	33(4)	21(3)	16(3)	6(4)
C(12)	36(4)	40(4)	35(4)	6(3)	4(3)	14(4)
C(11)	27(3)	22(3)	20(3)	4(3)	-2(3)	13(3)
C(10)	34(4)	25(3)	23(4)	-8(3)	-3(3)	13(3)
C(26)	22(3)	32(3)	24(3)	-4(3)	-1(3)	-8(3)
C(25)	26(4)	36(4)	28(4)	-6(3)	-4(3)	-1(3)
C(24)	31(4)	35(4)	44(4)	-6(3)	-5(3)	-2(3)
C(23)	29(3)	29(4)	41(4)	-2(3)	14(3)	2(3)
C(22)	42(4)	24(3)	29(3)	-5(3)	12(3)	-16(3)
C(21)	30(3)	20(3)	26(3)	8(3)	8(3)	-11(3)
C(20)	34(4)	28(4)	30(4)	3(3)	2(3)	-13(3)

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

	x	y	z	U(eq)
H	9980(6)	-140(5)	10847(18)	32
H(1A)	9072	-412	9796	33
H(1B)	10736	-292	9557	33
H(2A)	10854	-2799	10073	39
H(2B)	9312	-2614	10426	39
H(3A)	10566	-2743	11364	52
H(3B)	10936	-4200	10978	52
H(4A)	12340	677	10617	40
H(4B)	12775	-688	10190	40
H(5A)	13913	-1026	11136	43
H(5B)	12342	-885	11470	43
H(15)	13286	5228	9965	37
H(14)	14159	6846	9210	50
H(13)	13316	6568	8221	48
H(12)	11574	4819	7990	44
H(25)	6508	5131	9642	36
H(24)	5607	6950	10289	44
H(23)	6413	7034	11291	39
H(22)	8069	5246	11640	38

Table 1. Atomic coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 5 x CH<sub>3</sub>CN. U(eq) is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Si	2338(1)	6648(1)	6363(1)	20(1)
O(1)	3175(1)	4894(1)	6568(1)	24(1)
O(2)	650(1)	6461(1)	7083(1)	24(1)
O(3)	1578(1)	8444(1)	6010(1)	22(1)
O(4)	3643(1)	6567(1)	7276(1)	27(1)
O(5)	3865(1)	2735(1)	7687(1)	38(1)
O(6)	1055(1)	10546(1)	6092(1)	26(1)
O(7)	2374(1)	10201(1)	1394(1)	38(1)
N	2098(1)	8163(1)	3713(1)	21(1)
C(1)	2663(2)	6818(1)	4661(1)	24(1)
C(2)	3111(2)	9103(1)	3484(1)	26(1)
C(3)	2444(2)	10424(2)	2526(2)	35(1)
C(4)	1965(2)	7959(2)	2511(1)	29(1)
C(5)	1418(2)	9319(2)	1545(1)	37(1)
C(16)	361(2)	5313(1)	7920(1)	23(1)
C(15)	-1069(2)	5454(1)	8560(1)	29(1)
C(14)	-1418(2)	4345(2)	9462(1)	33(1)
C(13)	-356(2)	3079(1)	9742(1)	32(1)
C(12)	1052(2)	2934(1)	9100(1)	28(1)
C(11)	1427(2)	4041(1)	8176(1)	23(1)
C(10)	2928(2)	3839(1)	7473(1)	23(1)
C(26)	3698(1)	7494(1)	7815(1)	23(1)
C(25)	4671(2)	7041(2)	8776(1)	30(1)
C(24)	4798(2)	7937(2)	9355(1)	35(1)
C(23)	3983(2)	9300(2)	8972(2)	35(1)
C(22)	3020(2)	9747(2)	8023(1)	29(1)
C(21)	2841(1)	8847(1)	7450(1)	22(1)
C(20)	1763(1)	9343(1)	6466(1)	20(1)
N(2)	5442(3)	9228(3)	5239(3)	43(1)
C(31)	6279(4)	8201(4)	5318(3)	36(1)
C(32)	7331(12)	6886(10)	5414(10)	67(3)
N(2')	439(4)	14228(4)	5288(4)	59(1)
C(31')	1548(4)	13571(4)	4984(3)	39(1)
C(32')	2940(10)	12765(9)	4607(9)	57(2)

Table 2. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 5 x  $\text{CH}_3\text{CN}$ .

Si-O(2)	1.6700(10)	Si-O(4)	1.6732(10)
Si-O(1)	1.7709(9)	Si-O(3)	1.7830(9)
Si-C(1)	1.9058(14)	O(1)-C(10)	1.315(2)
O(2)-C(16)	1.362(2)	O(3)-C(20)	1.309(2)
O(4)-C(26)	1.360(2)	O(5)-C(10)	1.220(2)
O(6)-C(20)	1.229(2)	O(7)-C(5)	1.421(2)
O(7)-C(3)	1.424(2)	N-H	0.91(2)
N-C(2)	1.497(2)	N-C(1)	1.500(2)
N-C(4)	1.510(2)	C(1)-H(1B)	0.96(2)
C(1)-H(1A)	0.97(2)	C(2)-H(2A)	0.94(2)
C(2)-H(2B)	0.98(2)	C(2)-C(3)	1.509(2)
C(3)-H(3A)	0.95(2)	C(3)-H(3B)	1.03(2)
C(4)-H(4B)	0.98(2)	C(4)-H(4A)	0.99(2)
C(4)-C(5)	1.516(2)	C(5)-H(5A)	1.00(2)
C(5)-H(5B)	1.02(2)	C(16)-C(15)	1.395(2)
C(16)-C(11)	1.400(2)	C(15)-H(15)	0.98(2)
C(15)-C(14)	1.382(2)	C(14)-H(14)	0.99(2)
C(14)-C(13)	1.393(2)	C(13)-H(13)	0.96(2)
C(13)-C(12)	1.380(2)	C(12)-H(12)	0.97(2)
C(12)-C(11)	1.401(2)	C(11)-C(10)	1.482(2)
C(26)-C(21)	1.395(2)	C(26)-C(25)	1.396(2)
C(25)-H(25)	0.96(2)	C(25)-C(24)	1.385(2)
C(24)-H(24)	0.96(2)	C(24)-C(23)	1.393(2)
C(23)-H(23)	0.98(2)	C(23)-C(22)	1.380(2)
C(22)-H(22)	1.02(2)	C(22)-C(21)	1.402(2)
C(21)-C(20)	1.475(2)	N(2)-C(31)	1.133(4)
C(31)-C(32)	1.443(8)	N(2')-C(31')	1.138(5)
C(31')-C(32')	1.417(8)		
O(2)-Si-O(4)	114.36(5)	O(2)-Si-O(1)	95.83(5)
O(4)-Si-O(1)	87.29(5)	O(2)-Si-O(3)	88.31(5)
O(4)-Si-O(3)	94.36(5)	O(1)-Si-O(3)	174.46(5)
O(2)-Si-C(1)	119.47(6)	O(4)-Si-C(1)	126.05(6)
O(1)-Si-C(1)	84.28(5)	O(3)-Si-C(1)	90.49(5)
C(10)-O(1)-Si	128.86(8)	C(16)-O(2)-Si	126.92(8)
C(20)-O(3)-Si	132.98(8)	C(26)-O(4)-Si	129.00(8)
C(5)-O(7)-C(3)	110.40(12)	H-N-C(2)	106.9(11)
H-N-C(1)	109.7(11)	C(2)-N-C(1)	113.36(10)
H-N-C(4)	108.3(11)	C(2)-N-C(4)	108.05(11)
C(1)-N-C(4)	110.39(10)	H(1B)-C(1)-H(1A)	108(2)
H(1B)-C(1)-N	104.2(11)	H(1A)-C(1)-N	105.7(11)
H(1B)-C(1)-Si	105.0(11)	H(1A)-C(1)-Si	112.6(11)
N-C(1)-Si	120.69(8)	H(2A)-C(2)-H(2B)	109.5(14)
H(2A)-C(2)-N	106.8(11)	H(2B)-C(2)-N	107.5(10)
H(2A)-C(2)-C(3)	111.6(11)	H(2B)-C(2)-C(3)	111.9(10)
N-C(2)-C(3)	109.35(12)	H(3A)-C(3)-H(3B)	109(2)
H(3A)-C(3)-O(7)	107.7(13)	H(3B)-C(3)-O(7)	111.0(10)
H(3A)-C(3)-C(2)	108.8(13)	H(3B)-C(3)-C(2)	110.0(10)
O(7)-C(3)-C(2)	110.83(11)	H(4B)-C(4)-H(4A)	111(2)
H(4B)-C(4)-N	105.6(11)	H(4A)-C(4)-N	107.1(11)
H(4B)-C(4)-C(5)	110.5(11)	H(4A)-C(4)-C(5)	111.8(11)
N-C(4)-C(5)	110.47(12)	H(5A)-C(5)-H(5B)	106(2)
H(5A)-C(5)-O(7)	109.2(12)	H(5B)-C(5)-O(7)	111.2(11)
H(5A)-C(5)-C(4)	107.0(11)	H(5B)-C(5)-C(4)	110.7(11)
O(7)-C(5)-C(4)	112.25(12)	O(2)-C(16)-C(15)	116.79(11)
O(2)-C(16)-C(11)	123.37(12)	C(15)-C(16)-C(11)	119.82(12)
H(15)-C(15)-C(14)	120.9(11)	H(15)-C(15)-C(16)	119.1(11)
C(14)-C(15)-C(16)	120.00(12)	H(14)-C(14)-C(15)	118.9(11)
H(14)-C(14)-C(13)	120.3(11)	C(15)-C(14)-C(13)	120.77(14)

H(13)-C(13)-C(12)	120.2(11)	H(13)-C(13)-C(14)	120.5(11)
C(12)-C(13)-C(14)	119.31(13)	H(12)-C(12)-C(13)	120.4(12)
H(12)-C(12)-C(11)	118.6(12)	C(13)-C(12)-C(11)	120.96(12)
C(16)-C(11)-C(12)	119.12(12)	C(16)-C(11)-C(10)	121.29(12)
C(12)-C(11)-C(10)	119.58(11)	O(5)-C(10)-O(1)	121.31(12)
O(5)-C(10)-C(11)	121.88(12)	O(1)-C(10)-C(11)	116.75(10)
O(4)-C(26)-C(21)	123.20(11)	O(4)-C(26)-C(25)	117.07(12)
C(21)-C(26)-C(25)	119.73(13)	H(25)-C(25)-C(24)	123.7(13)
H(25)-C(25)-C(26)	116.3(13)	C(24)-C(25)-C(26)	120.06(14)
H(24)-C(24)-C(25)	120.1(12)	H(24)-C(24)-C(23)	119.3(12)
C(25)-C(24)-C(23)	120.62(13)	H(23)-C(23)-C(22)	118.9(11)
H(23)-C(23)-C(24)	121.7(11)	C(22)-C(23)-C(24)	119.33(14)
H(22)-C(22)-C(23)	121.4(12)	H(22)-C(22)-C(21)	117.6(12)
C(23)-C(22)-C(21)	120.90(13)	C(26)-C(21)-C(22)	119.29(12)
C(26)-C(21)-C(20)	120.95(11)	C(22)-C(21)-C(20)	119.76(12)
O(6)-C(20)-O(3)	121.04(11)	O(6)-C(20)-C(21)	121.79(11)
O(3)-C(20)-C(21)	117.16(10)	N(2)-C(31)-C(32)	179.3(5)
N(2')-C(31')-C(32')	179.2(5)		

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Table 3. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for  $5 \times \text{CH}_3\text{CN}$ .  
 The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
Si	19(1)	16(1)	21(1)	-3(1)	-1(1)	-3(1)
O(1)	25(1)	18(1)	25(1)	-4(1)	3(1)	-3(1)
O(2)	22(1)	17(1)	27(1)	-1(1)	1(1)	-3(1)
O(3)	25(1)	18(1)	22(1)	-5(1)	-4(1)	-4(1)
O(4)	25(1)	21(1)	31(1)	-6(1)	-7(1)	-2(1)
O(5)	37(1)	20(1)	38(1)	-2(1)	7(1)	5(1)
O(6)	25(1)	19(1)	33(1)	-8(1)	-2(1)	-2(1)
O(7)	42(1)	34(1)	25(1)	2(1)	7(1)	-7(1)
N	21(1)	20(1)	19(1)	-4(1)	1(1)	-4(1)
C(1)	28(1)	17(1)	24(1)	-4(1)	-1(1)	-4(1)
C(2)	28(1)	26(1)	27(1)	-8(1)	5(1)	-11(1)
C(3)	42(1)	23(1)	33(1)	-5(1)	12(1)	-9(1)
C(4)	32(1)	34(1)	22(1)	-10(1)	-1(1)	-9(1)
C(5)	32(1)	46(1)	22(1)	-2(1)	-2(1)	-6(1)
C(16)	24(1)	20(1)	22(1)	-3(1)	-2(1)	-6(1)
C(15)	23(1)	25(1)	33(1)	-4(1)	1(1)	-4(1)
C(14)	28(1)	33(1)	33(1)	-3(1)	5(1)	-11(1)
C(13)	39(1)	26(1)	28(1)	-2(1)	3(1)	-12(1)
C(12)	35(1)	20(1)	25(1)	-3(1)	-2(1)	-6(1)
C(11)	26(1)	19(1)	21(1)	-5(1)	-2(1)	-4(1)
C(10)	27(1)	18(1)	22(1)	-5(1)	-2(1)	-3(1)
C(26)	19(1)	26(1)	22(1)	-5(1)	1(1)	-9(1)
C(25)	25(1)	36(1)	26(1)	-1(1)	-5(1)	-10(1)
C(24)	27(1)	55(1)	26(1)	-10(1)	-4(1)	-16(1)
C(23)	29(1)	51(1)	34(1)	-23(1)	1(1)	-13(1)
C(22)	25(1)	36(1)	32(1)	-18(1)	1(1)	-8(1)
C(21)	18(1)	26(1)	22(1)	-7(1)	2(1)	-7(1)
C(20)	18(1)	20(1)	21(1)	-7(1)	4(1)	-6(1)
N(2)	36(1)	51(2)	47(2)	-20(1)	6(1)	-17(1)
C(31)	36(2)	43(2)	35(2)	-13(1)	0(1)	-18(2)
C(32)	95(6)	46(4)	64(4)	-20(3)	-32(4)	-5(3)
N(2')	45(2)	62(2)	85(3)	-41(2)	-6(2)	-13(2)
C(31')	39(2)	40(2)	44(2)	-15(2)	-4(1)	-16(1)
C(32')	49(3)	59(5)	60(4)	-13(3)	19(3)	-25(4)

Table 4. Hydrogen coordinates (  $\times 10^4$  ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5 x CH<sub>3</sub>CN.

	x	y	z	U(eq)
H	1160(2)	8595(17)	3963(16)	27(4)
H(1B)	2110(2)	6239(18)	4540(17)	34(4)
H(1A)	3730(2)	6490(18)	4422(17)	34(4)
H(2B)	3178(19)	9239(17)	4264(16)	27(4)
H(2A)	4090(2)	8655(18)	3220(17)	32(4)
H(3B)	1370(2)	10886(18)	2834(17)	34(4)
H(3A)	3100(2)	11010(2)	2390(2)	52(6)
H(4B)	3000(2)	7485(18)	2277(17)	32(4)
H(4A)	1240(2)	7383(18)	2667(17)	35(5)
H(5B)	300(2)	9769(18)	1741(17)	37(5)
H(5A)	1440(2)	9127(19)	758(19)	41(5)
H(15)	-1820(2)	6345(18)	8357(17)	35(5)
H(14)	-2420(2)	4469(19)	9918(18)	38(5)
H(13)	-600(2)	2312(19)	10366(18)	36(5)
H(12)	1820(2)	2072(19)	9307(18)	39(5)
H(25)	5210(2)	6100(2)	9000(2)	48(5)
H(24)	5480(2)	7630(2)	10005(19)	43(5)
H(23)	4100(2)	9958(19)	9344(18)	40(5)
H(22)	2450(2)	10740(2)	7690(2)	48(5)
H(32A)	6869	6172	5968	101
H(32B)	8287	6835	5738	101
H(32C)	7551	6759	4602	101
H(32D)	3804	12881	4937	86
H(32E)	3059	13052	3710	86
H(32F)	2921	11806	4913	86

Table 1. Atomic coordinates [ $x \cdot 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \cdot 10^3$ ] for 6.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
Si	1605(1)	2106(1)	1021(1)	26(1)
O(1)	11(2)	1512(2)	620(1)	31(1)
O(2)	2254(2)	3513(2)	732(1)	31(1)
O(3)	3195(2)	2538(2)	1457(1)	31(1)
O(4)	122(2)	2462(2)	1338(1)	32(1)
O(5)	-1497(2)	1239(2)	-24(1)	45(1)
O(6)	4534(2)	3795(2)	2012(1)	48(1)
N	4179(2)	-182(2)	1225(1)	26(1)
C(1)	2551(3)	200(3)	961(1)	32(1)
C(10)	-334(3)	1820(3)	199(1)	33(1)
C(11)	755(3)	2930(3)	17(1)	33(1)
C(12)	522(3)	3231(3)	-434(1)	47(1)
C(13)	1435(4)	4299(4)	-616(1)	56(1)
C(14)	2605(4)	5083(3)	-344(1)	54(1)
C(15)	2878(3)	4806(3)	103(1)	42(1)
C(16)	1945(3)	3721(2)	287(1)	32(1)
C(20)	3247(3)	3453(2)	1798(1)	29(1)
C(21)	1617(3)	3981(2)	1907(1)	28(1)
C(22)	1536(3)	5011(3)	2246(1)	39(1)
C(23)	35(4)	5467(3)	2364(1)	46(1)
C(24)	-1398(3)	4879(3)	2145(1)	39(1)
C(25)	-1354(3)	3868(3)	1807(1)	31(1)
C(26)	168(3)	3428(2)	1682(1)	26(1)
C(31)	4076(3)	-1507(3)	1541(1)	44(1)
C(32)	5740(4)	-1653(4)	1822(1)	57(1)
C(33)	7200(4)	-1744(3)	1556(1)	50(1)
C(34)	7214(3)	-380(3)	1267(1)	43(1)
C(35)	5649(3)	-163(2)	947(1)	30(1)
C(36)	2796(5)	-1071(4)	1848(1)	77(1)
C(37)	3570(4)	-2948(3)	1292(1)	63(1)
C(38)	5481(3)	-1329(3)	583(1)	44(1)
C(39)	5678(3)	1392(3)	745(1)	48(1)

Table 2. Bond lengths [ $\text{\AA}$ ] and angles [ $^{\circ}$ ] for 6.

Si-O(2)	1.664(2)	Si-O(4)	1.6741(14)
Si-O(1)	1.758(2)	Si-O(3)	1.786(2)
Si-C(1)	1.893(2)	O(1)-C(10)	1.312(3)
O(2)-C(16)	1.363(3)	O(3)-C(20)	1.323(3)
O(4)-C(26)	1.358(2)	O(5)-C(10)	1.217(3)
O(6)-C(20)	1.209(3)	N-H	0.94(3)
N-C(1)	1.510(3)	N-C(31)	1.539(3)
N-C(35)	1.556(2)	C(10)-C(11)	1.488(3)
C(11)-C(16)	1.390(3)	C(11)-C(12)	1.392(3)
C(12)-C(13)	1.372(4)	C(13)-C(14)	1.380(5)
C(14)-C(15)	1.378(4)	C(15)-C(16)	1.396(3)
C(20)-C(21)	1.492(3)	C(21)-C(26)	1.388(3)
C(21)-C(22)	1.393(3)	C(22)-C(23)	1.385(4)
C(23)-C(24)	1.382(4)	C(24)-C(25)	1.377(3)
C(25)-C(26)	1.403(3)	C(31)-C(32)	1.523(4)
C(31)-C(37)	1.530(4)	C(31)-C(36)	1.539(3)
C(32)-C(33)	1.527(4)	C(33)-C(34)	1.509(4)
C(34)-C(35)	1.525(3)	C(35)-C(38)	1.519(3)
C(35)-C(39)	1.526(3)		
O(2)-Si-O(4)	117.66(8)	O(2)-Si-O(1)	96.78(8)
O(4)-Si-O(1)	86.04(7)	O(2)-Si-O(3)	88.84(8)
O(4)-Si-O(3)	92.41(7)	O(1)-Si-O(3)	174.25(8)
O(2)-Si-C(1)	118.09(9)	O(4)-Si-C(1)	124.23(9)
O(1)-Si-C(1)	86.40(9)	O(3)-Si-C(1)	89.91(9)
C(10)-O(1)-Si	132.1(2)	C(16)-O(2)-Si	126.8(2)
C(20)-O(3)-Si	132.17(14)	C(26)-O(4)-Si	127.99(14)
H-N-C(1)	101(2)	H-N-C(31)	103.2(14)
C(1)-N-C(31)	113.4(2)	H-N-C(35)	106.0(14)
C(1)-N-C(35)	113.4(2)	C(31)-N-C(35)	117.2(2)
N-C(1)-Si	119.8(2)	O(5)-C(10)-O(1)	121.0(2)
O(5)-C(10)-C(11)	122.8(2)	O(1)-C(10)-C(11)	116.1(2)
C(16)-C(11)-C(12)	119.2(2)	C(16)-C(11)-C(10)	121.8(2)
C(12)-C(11)-C(10)	118.9(2)	C(13)-C(12)-C(11)	121.3(3)
C(12)-C(13)-C(14)	119.0(2)	C(15)-C(14)-C(13)	121.3(3)
C(14)-C(15)-C(16)	119.5(3)	O(2)-C(16)-C(11)	123.5(2)
O(2)-C(16)-C(15)	116.8(2)	C(11)-C(16)-C(15)	119.7(2)
O(6)-C(20)-O(3)	121.6(2)	O(6)-C(20)-C(21)	122.9(2)
O(3)-C(20)-C(21)	115.4(2)	C(26)-C(21)-C(22)	119.2(2)
C(26)-C(21)-C(20)	120.7(2)	C(22)-C(21)-C(20)	120.1(2)
C(23)-C(22)-C(21)	120.9(2)	C(24)-C(23)-C(22)	119.2(2)
C(25)-C(24)-C(23)	121.0(2)	C(24)-C(25)-C(26)	119.6(2)
O(4)-C(26)-C(21)	123.4(2)	O(4)-C(26)-C(25)	116.6(2)
C(21)-C(26)-C(25)	119.9(2)	C(32)-C(31)-C(37)	112.1(2)
C(32)-C(31)-N	107.7(2)	C(37)-C(31)-N	111.8(2)
C(32)-C(31)-C(36)	108.0(2)	C(37)-C(31)-C(36)	110.8(3)
N-C(31)-C(36)	106.3(2)	C(31)-C(32)-C(33)	114.3(2)
C(34)-C(33)-C(32)	109.3(2)	C(33)-C(34)-C(35)	114.3(2)
C(38)-C(35)-C(34)	111.9(2)	C(38)-C(35)-C(39)	109.7(2)
C(34)-C(35)-C(39)	108.8(2)	C(38)-C(35)-N	112.6(2)
C(34)-C(35)-N	107.2(2)	C(39)-C(35)-N	106.4(2)

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 6.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^* b^* U_{12} ]$$

	U11	U22	U33	U23	U13	U12
Si	19(1)	28(1)	31(1)	-4(1)	6(1)	0(1)
O(1)	22(1)	38(1)	34(1)	-6(1)	4(1)	-1(1)
O(2)	25(1)	29(1)	39(1)	0(1)	5(1)	-1(1)
O(3)	24(1)	32(1)	37(1)	-9(1)	6(1)	3(1)
O(4)	23(1)	37(1)	36(1)	-9(1)	8(1)	-1(1)
O(5)	26(1)	63(1)	45(1)	-20(1)	-3(1)	4(1)
O(6)	28(1)	65(1)	48(1)	-21(1)	-4(1)	0(1)
N	21(1)	28(1)	30(1)	-3(1)	6(1)	2(1)
C(1)	20(1)	35(1)	40(1)	-7(1)	3(1)	2(1)
C(10)	22(1)	42(1)	36(1)	-11(1)	4(1)	10(1)
C(11)	24(1)	39(1)	37(1)	-1(1)	9(1)	13(1)
C(12)	41(2)	62(2)	39(1)	-1(1)	6(1)	28(1)
C(13)	65(2)	61(2)	47(2)	18(1)	26(2)	38(2)
C(14)	64(2)	39(2)	68(2)	23(1)	39(2)	26(1)
C(15)	36(2)	32(1)	61(2)	11(1)	20(1)	10(1)
C(16)	27(1)	30(1)	41(1)	5(1)	14(1)	12(1)
C(20)	29(1)	28(1)	31(1)	-2(1)	1(1)	1(1)
C(21)	31(1)	28(1)	26(1)	2(1)	7(1)	3(1)
C(22)	42(2)	37(1)	36(1)	-5(1)	3(1)	1(1)
C(23)	54(2)	47(2)	38(1)	-11(1)	12(1)	10(1)
C(24)	40(2)	43(1)	37(1)	-3(1)	16(1)	13(1)
C(25)	26(1)	34(1)	33(1)	4(1)	9(1)	7(1)
C(26)	28(1)	25(1)	27(1)	3(1)	7(1)	3(1)
C(31)	49(2)	39(1)	48(1)	15(1)	22(1)	10(1)
C(32)	70(2)	59(2)	41(1)	11(1)	5(1)	19(2)
C(33)	44(2)	52(2)	51(1)	1(1)	-11(1)	17(1)
C(34)	26(1)	40(1)	62(2)	-3(1)	1(1)	4(1)
C(35)	20(1)	32(1)	41(1)	2(1)	11(1)	4(1)
C(36)	90(3)	70(2)	83(2)	35(2)	59(2)	25(2)
C(37)	51(2)	34(2)	108(2)	11(2)	20(2)	-4(1)
C(38)	42(2)	54(2)	37(1)	-6(1)	9(1)	20(1)
C(39)	37(2)	46(2)	65(2)	20(1)	26(1)	10(1)

Table 4. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 6.

	x	y	z	U(eq)
H	4330(3)	640(3)	1416(7)	32(6)
H(1A)	1740	-552	1033	38
H(1B)	2682	66	645	38
H(12)	-285	2688	-620	57
H(13)	1265	4495	-924	68
H(14)	3235	5829	-467	65
H(15)	3695	5349	285	50
H(22)	2524	5406	2397	46
H(23)	-9	6176	2594	55
H(24)	-2429	5178	2228	47
H(25)	-2347	3471	1659	37
H(32A)	5729	-2561	2006	68
H(32B)	5897	-785	2023	68
H(33A)	8239	-1799	1759	60
H(33B)	7111	-2655	1371	60
H(34A)	8160	-453	1094	52
H(34B)	7385	513	1458	52
H(36A)	2871	-1762	2099	115
H(36B)	1691	-1123	1685	115
H(36C)	3013	-52	1957	115
H(37A)	4549	-3435	1203	95
H(37B)	2802	-2713	1029	95
H(37C)	3037	-3620	1484	95
H(38A)	6317	-1154	385	66
H(38B)	4383	-1260	416	66
H(38C)	5634	-2326	714	66
H(39A)	5595	2145	974	71
H(39B)	4747	1500	512	71
H(39C)	6710	1532	618	71