S3a: Fractional atomic coordinates and mean−square atomic displacement parameters for the non−hydrogen atoms.

	Fractional atomic coordinates			Mean−square atomic displacement parameters [Å]					
Atom	x/*a*	*y*/*b*	*z*/*c*	*U*11	*U*22	*U*33	*U*12	*U*13	*U*23
Si(2)	0.302283(9)	0.263099(13)	−0.086250(9)	0.01521(4)	0.01959(5)	0.02321(5)	−0.00064(3)	−0.00003(3)	−0.00526(4)
Si(1)	0.360087(10)	0.364467(12)	0.142651(9)	0.01713(4)	0.02092(5)	0.01712(4)	0.00037(4)	−0.00047(3)	0.00369(4)
N	0.32170(4)	0.65175(5)	0.01422(4)	0.01575(14)	0.01575(16)	0.02033(15)	0.00046(12)	−0.00024(12)	−0.00178(13)
C(1)	0.34445(3)	0.40747(4)	0.00109(3)	0.01391(12)	0.01611(14)	0.01614(13)	0.00126(11)	0.00004(10)	−0.00010(11)
C(2)	0.21836(5)	0.35769(7)	0.20396(4)	0.0262(2)	0.0590(4)	0.02440(18)	0.0003(2)	0.00801(16)	0.0090(2)
C(3)	0.44800(8)	0.49177(8)	0.22359(5)	0.0428(3)	0.0346(3)	0.01996(19)	−0.0082(3)	−0.0073(2)	−0.0005(2)
C(4)	0.43410(5)	0.19839(7)	0.16947(5)	0.0370(3)	0.0277(2)	0.0389(3)	0.0071(2)	−0.0079(2)	0.01062(19)
C(5)	0.25199(5)	0.31911(7)	−0.22208(4)	0.0315(2)	0.0485(3)	0.02199(18)	−0.0046(2)	−0.00559(16)	−0.00591(19)
C(6)	0.18768(5)	0.14550(5)	−0.04195(5)	0.02615(19)	0.02222(18)	0.0453(3)	−0.00720(16)	0.00334(18)	−0.00462(17)
C(7)	0.43079(6)	0.15207(8)	−0.10675(7)	0.0243(2)	0.0278(3)	0.0458(3)	0.0046(2)	0.0023(2)	−0.0152(3)
C(11)	0.27294(3)	0.53035(4)	−0.01261(3)	0.01226(12)	0.01619(14)	0.01658(13)	0.00037(11)	0.00075(10)	0.00121(11)
C(12)	0.15600(4)	0.52954(5)	−0.04788(4)	0.01265(12)	0.01972(16)	0.0349(2)	0.00008(11)	−0.00214(12)	0.00216(13)
C(13)	0.09272(4)	0.64778(5)	−0.05310(4)	0.01447(13)	0.02391(19)	0.0407(2)	0.00346(13)	−0.00146(14)	0.00497(16)
C(14)	0.14460(4)	0.77001(5)	−0.02328(4)	0.01988(16)	0.01992(17)	0.03251(19)	0.00554(13)	0.00302(13)	0.00352(14)
C(15)	0.25923(4)	0.76603(5)	0.00900(3)	0.02103(16)	0.01679(16)	0.02521(17)	0.00222(14)	0.00148(12)	−0.00099(12)
Li	0.519190	0.392970	−0.052800	0.015314	0.040846	0.029042	0.002015	0.001001	−0.001989