S4: Kappa and multipole parameters for [{2−(Me$_3$Si)$_2$C(Li)C$_5$H$_4$N}$_2$]

Symmetry forbidden multipoles are denoted by an asterisk (*)

Atom	κ’	κ’’	P_v	P_{11+}	P_{11-}	P_{10}
Si(2)	1.051(7)	1.00[b]	3.26(10)	−0.05(2)	0.13(2)	0.06(2)
Si(1)	1.031(7)	1.00[b]	3.23(11)	0.07(2)	−0.01(2)	0.02(2)
N	0.983(2)	1.00[b]	5.33(5)	−0.009(13)	−0.064(12)	0.004(11)
C(1)	0.966[b]	1.00[b]	4.52(4)	0.024(13)	−0.024(13)	−0.019(13)
C(2)[a]	0.986(3)	1.00[b]	4.44(6)	*	*	0.018(12)
C(3)	0.984[b]	1.00[b]	4.46(4)	0.06(2)	0.025(16)	0.029(17)
C(5)[a]	0.984(3)	1.00[b]	4.59(7)	*	*	0.014(12)
C(7)	0.985(5)	1.00[b]	4.54(10)	0.10(2)	0.006(17)	0.024(17)
C(11)	1.030(4)	1.00[b]	3.79(5)	0.000(11)	0.028(13)	−0.040(14)
C(12)[a]	1.009(2)	1.00[b]	4.13(3)	0.005(11)	−0.019(10)	*
C(15)	1.009(2)	1.00[b]	4.02(4)	0.036(15)	0.040(15)	*

[a] the multipole population coefficients of C(2), C(5) and C(12) were set equal to the corresponding coefficients of C(4), C(6) and C(13) / C(14), respectively (chemically constrained model).

[b] fixed values.

Atom	P_{20}	P_{21+}	P_{21-}	P_{22+}	P_{22-}
Si(2)	−0.02(2)	0.00(2)	−0.01(2)	−0.03(2)	−0.11(2)
Si(1)	−0.07(2)	0.17(2)	−0.03(2)	0.05(2)	0.02(2)
N	−0.119(13)	0.018(11)	0.006(11)	0.022(12)	0.019(12)
C(1)	−0.029(13)	−0.014(12)	−0.021(12)	−0.002(13)	−0.045(12)
C(2)[a]	0.043(12)	*	*	*	*
C(3)	0.052(16)	−0.042(19)	0.005(14)	0.012(16)	0.077(19)
C(5)[a]	0.049(11)	*	*	*	*
C(7)	0.019(16)	−0.007(19)	0.049(15)	0.014(18)	0.053(19)
C(11)	0.044(15)	−0.006(12)	0.016(13)	−0.143(12)	0.011(11)
C(12)[a]	−0.193(9)	*	*	0.007(10)	0.002(8)
C(15)	−0.182(15)	*	*	−0.021(14)	0.021(15)

[a] the multipole population coefficients of C(2), C(5) and C(12) were set equal to the corresponding coefficients of C(4), C(6) and C(13) / C(14), respectively (chemically constrained model).

Atom	P_{30}	P_{31+}	P_{31-}	P_{32+}	P_{32-}	P_{33+}	P_{33-}
Si(2)	−0.01(3)	−0.22(3)	−0.30(3)	0.06(3)	0.01(2)	0.36(3)	−0.01(2)
Si(1)	−0.09(3)	−0.21(3)	−0.43(3)	0.13(2)	−0.09(3)	0.28(3)	0.04(3)
N	0.002(11)	−0.013(11)	−0.018(11)	−0.004(10)	0.015(10)	0.137(11)	0.014(11)
C(1)	−0.035(14)	−0.054(13)	−0.097(13)	−0.015(13)	0.091(13)	0.107(13)	0.000(13)
C(2)[a]	0.175(13)	*	*	*	*	0.004(11)	0.127(12)
C(3)	0.176(16)	−0.039(17)	0.003(14)	−0.007(15)	0.006(17)	−0.017(16)	0.225(16)
C(5)[a]	0.236(12)	*	*	*	*	0.020(11)	0.144(11)
C(7)	0.179(19)	−0.065(16)	0.007(15)	0.005(17)	−0.033(17)	−0.047(16)	0.163(17)
C(11)	0.184(16)	0.013(14)	−0.004(15)	0.180(14)	−0.022(13)	0.032(12)	−0.013(12)
C(12)[a]	*	0.032(10)	0.029(9)	*	*	0.249(8)	−0.018(11)
C(15)	*	0.009(14)	0.021(14)	*	*	0.300(15)	−0.005(15)

[a] the multipole population coefficients of C(2), C(5) and C(12) were set equal to the corresponding coefficients of C(4), C(6) and C(13) / C(14), respectively (chemically constrained model).

	Li	H(2a)[a]	H(3b)	H(3c)	H(7b)	H(7c)	H(12)[a]
κ’	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]
κ’’	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]	1.20[b]
P_v	0.90(11)	0.888(10)	0.83(3)	0.91(3)	0.82(3)	0.94(3)	0.888(12)
P_{10}		0.099(6)	0.06(2)	0.10(2)	0.11(2)	0.17(2)	0.125(9)

[a] the multipole population coefficients of all methyl group hydrogens, except for H(3b), H(3c), H(7b) and H(7c), were set equal to H(2a) and all aromatic hydrogens equal to H(12) (chemically constrained model).

[b] fixed values.