

Table 1: Third order Gram–Charlier coefficients ( $10^{-4}\text{\AA}^3$ )

	X2			NEUT2
	F	C3	N	N
$c_{111}$	0.132(12)	0.00000	0.00000	0.00000
$c_{112}$	-0.071(14)	-0.08(2)	-0.26(3)	-0.28(10)
$c_{122}$	0.016(10)	0.00000	0.00000	0.00000
$c_{113}$	0.051(14)	-0.22(2)	-0.82(4)	-1.10(11)
$c_{123}$	-0.088(12)	0.00000	0.00000	0.00000
$c_{133}$	-0.021(11)	0.00000	0.00000	0.00000
$c_{222}$	0.002(7)	-0.018(6)	-0.047(8)	0.03(2)
$c_{223}$	0.129(10)	-0.001(10)	-0.020(14)	-0.05(5)
$c_{233}$	0.094(10)	-0.020(10)	-0.155(15)	-0.14(5)
$c_{333}$	0.036(9)	-0.042(7)	-0.074(11)	-0.18(3)

Table 2: Core monopole populations (e) and radial parameters  $\kappa$  ( $\kappa_0 = \kappa_1 = \kappa_2$ ) and  $\alpha_3$  (bohr $^{-1}$ )

	X1	X2
P <sub>core</sub>	1.9335(12)	1.9307(10)
$\kappa(\text{F})$	0.9891(7)	0.9883(7)
$\kappa(\text{N})$	0.9813(14)	0.9805(13)
$\kappa(\text{C1,C2})$	1.0105(13)	1.0102(11)
$\kappa(\text{C3})$	1.015(2)	1.0120(18)
$\alpha_3(\text{N})$	3.30(18)	3.13(13)
$\alpha_3(\text{C1,C2})$	3.279(19)	3.289(17)
$\alpha_3(\text{C3})$	2.87(14)	2.80(13)

## 1 Supplementary Material

Table 3: X1: Valence monopole populations (e) and dipole populations (e $\text{\AA}$ )

	Y00	Y11+	Y11-	Y10
F	7.065(10)	0.012(5)	0.007(6)	0.025(5)
	7.067(9)	-0.079(11)	0.016(13)	-0.042(13)
N	5.19(2)	0.00	-0.015(12)	-0.072(11)
	5.206(19)	0.00	0.099(19)	0.002(17)
C1	4.023(13)	0.00	0.097(12)	-0.054(12)
	4.013(12)	0.00	0.103(11)	-0.065(10)
C2	4.019(11)	-0.250(9)	0.146(9)	-0.108(8)
	4.018(10)	-0.265(8)	0.153(8)	-0.099(7)
C3	4.087(18)	0.00	-0.326(15)	0.179(13)
	4.095(19)	0.00	-0.25(2)	0.222(18)

Table 4: Quadrupole populations ( $e\text{\AA}^2$ ). X1 1st line, and X2 2nd line

	Y22+	Y22-	Y21+	Y21-	Y20
F	-0.032(5)	0.284(10)	-0.211(10)	0.069(11)	0.089(11)
	-0.031(5)	0.283(9)	-0.201(9)	0.068(10)	0.081(10)
N	-0.368(14)	0.00	0.00	-1.23(3)	-0.12(2)
	-0.377(13)	0.00	0.00	-1.28(3)	-0.105(19)
C1	0.518(19)	0.00	0.00	-1.00(3)	-0.68(3)
	0.543(17)	0.00	0.00	-0.96(3)	-0.73(3)
C2	0.120(12)	0.58(3)	-0.40(2)	-1.35(2)	-0.58(2)
	0.130(11)	0.64(2)	-0.42(2)	-1.34(2)	-0.566(19)
C3	-0.78(2)	0.00	0.00	-2.42(4)	-0.19(3)
	-0.76(2)	0.00	0.00	-2.46(4)	-0.16(3)

Table 5: Octopole populations ( $e\text{\AA}^3$ ). X1 1st line, and X2 2nd line

	Y33+	Y33-	Y32+	Y32-	Y31+	Y31-	Y30
N	0.00	-0.32(9)	0.42(16)	0.00	0.00	0.06(3)	0.27(6)
	0.00	-0.35(7)	1.3(2)	0.00	0.00	0.18(4)	0.21(4)
C1	0.00	1.23(4)	-2.18(8)	0.00	0.00	-0.365(19)	0.104(15)
	0.00	1.19(4)	-2.16(7)	0.00	0.00	-0.355(17)	0.099(13)
C2	0.043(16)	-1.58(5)	2.42(8)	-1.42(8)	-0.188(13)	0.339(16)	-0.267(11)
	0.059(14)	-1.53(4)	2.40(7)	-1.36(7)	-0.198(12)	0.326(14)	-0.265(10)
C3	0.00	-0.53(13)	1.6(4)	0.00	0.00	0.17(4)	0.16(4)
	0.00	-0.66(14)	2.2(5)	0.00	0.00	0.19(5)	0.19(5)