

ClO₃⁻...ClO₃⁻ interactions in crystalline sodium chlorate

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Table 1. Monopole Populations, Radial Parameters and Net Atomic Charges.

Atom	Pval	Kappa	P00	Kappa'	Net charge
CL(1)	6.349(72)	1.045	0.000	0.994(59)	+0.651(72)
NA(1)	0.190	1.000	0.000	1.000	+0.81008
O(1)	6.487(24)	0.971	0.000	1.489(247)	-0.487(24)

Table 2. Dipole Population Parameters.

Atom	D11+	D11-	D10	Kappa'
CL(1)	0.000	0.000	0.153(43)	0.994
NA(1)	0.000	0.000	-0.218(242)	1.000
O(1)	0.008(17)	-0.025(17)	0.001(16)	1.489

Table 3. Quadrupole Population Parameters.

Atom	Q20	Q21+	Q21-	Q22+	Q22-	Kappa'
CL(1)	0.102(38)	0.000	0.000	0.000	0.000	0.994
NA(1)	-0.002(362)	0.000	0.000	0.000	0.000	1.000
O(1)	-0.082(26)	0.002(21)	-0.011(21)	-0.004(21)	-0.013(22)	1.489

Table 4. Octupole Population Parameters.

Atom	O30	O31+	O31-	O32+	O32-	O33+	O33-	Kappa'
CL(1)	0.320(77)	0.000	0.000	0.000	0.000	0.269(54)	-0.050(42)	0.994
NA(1)	0.308(464)	0.000	0.000	0.000	0.000	-0.135(274)	-0.036(343)	1.000
O(1)	-0.040(15)	0.030(13)	-0.025(12)	0.035(11)	0.016(12)	0.018(15)	0.031(12)	1.489

Table 5. Hexadecapole Population Parameters.

Atom	H40	H41+	H41-	H42+	H42-	H43+	H43-	H44+	H44-	Kappa'
CL(1)	0.104(41)	0.000	0.000	0.000	0.000	-0.128(34)	-0.011(32)	0.000	0.000	0.994
NA(1)	0.186(192)	0.000	0.000	0.000	0.000	-0.076(132)	-0.075(134)	0.000	0.000	1.000
O(1)	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.489

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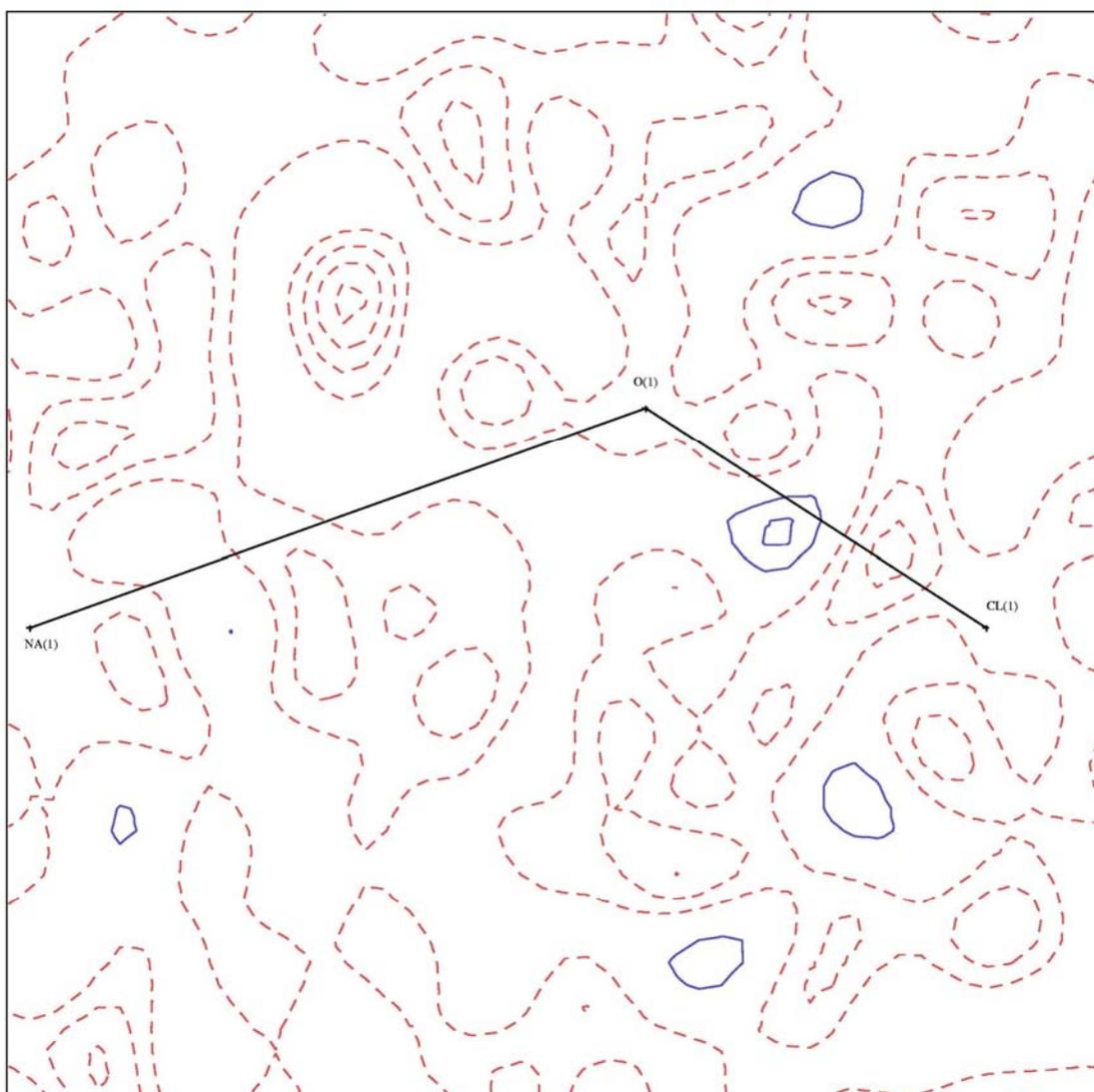


Figure 1S The residual electron density map in the plane of Na(1), O(1) and Cl(1) atoms. Contours are drawn with 0.05 eÅ⁻³ interval, the non-positive ones (red) are dashed.

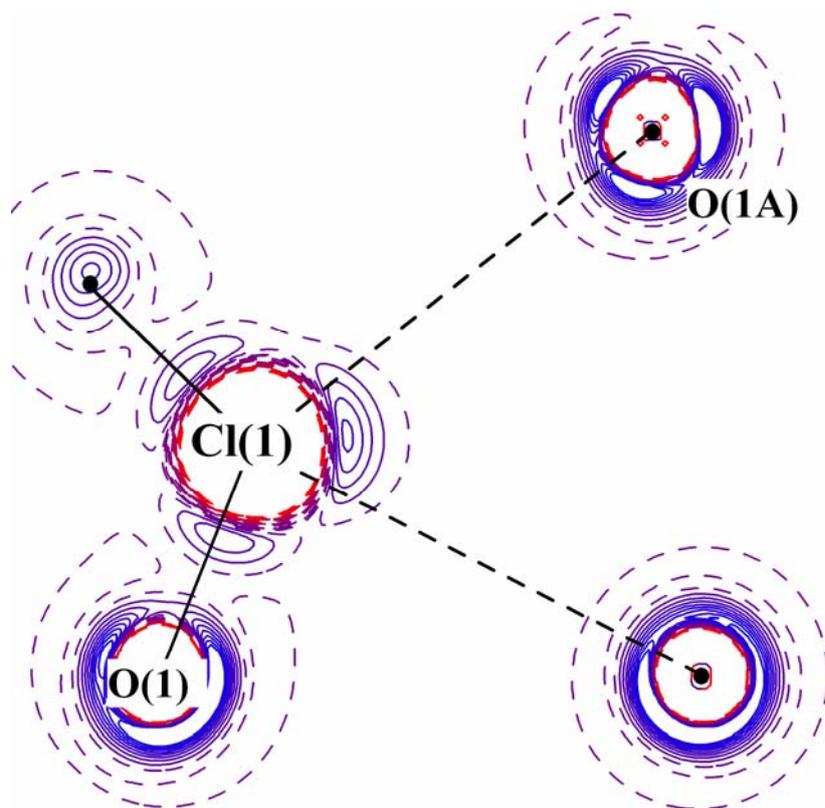


Figure 2S The section of the $-\nabla^2\rho(\mathbf{r})$ distribution in the region of the Cl(1)...O contacts of **1**. Contours are drawn with $10 \text{ e } \text{\AA}^{-5}$ interval, the non-positive contours are dashed.