

**Table S-1. Cell constants for ClC<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub>**

Temp. <sup>a</sup> (K)	type <sup>b</sup>	a (Å)	b (Å)	c (Å)	β (°)	V (Å <sup>3</sup> )
297	film	8.01(4)	7.06(2)	12.47(4)	92.4(3)	704(4)
297	prelim	8.023(2)	7.072(2)	12.435(5)	92.58(3)	704.8(4)
297	prelim	8.016(3)	7.074(2)	12.449(4)	92.58(3)	705.2(4)
273	prelim	7.969(10)	7.050(7)	12.384(10)	92.67(7)	695.0(15)
"	final	7.973(2)	7.055(2)	12.393(3)	92.67(5)	696.4(3)
273	final	7.973(2)	7.058(2)	12.389(3)	92.68(1)	696.4(3)
223	prelim	7.934(2)	7.059(3)	12.373(4)	92.97(3)	692.0(5)
"	final	7.930(1)	7.053(1)	12.359(1)	92.95(1)	690.4(1)
223.0	prelim	7.941(2)	7.065(2)	12.377(3)	93.04(2)	693.4(2)
198.0	prelim	7.920(2)	7.063(2)	12.355(4)	93.11(3)	690.0(3)
174	prelim	7.891(2)	7.055(2)	12.337(7)	93.37(5)	685.6(4)
174	prelim	7.893(2)	7.052(2)	12.322(4)	93.28(3)	684.7(3)
"	final	7.891(1)	7.051(1)	12.329(1)	93.33(1)	684.8(2)
174	prelim	7.886(2)	7.052(2)	12.342(5)	93.29(4)	685.2(4)
"	final	7.896(1)	7.052(1)	12.338(1)	93.32(1)	685.8(1)
173.0	prelim	7.904(3)	7.062(2)	12.331(4)	93.24(3)	687.2(4)
148.0	prelim	7.876(2)	7.062(1)	12.308(3)	93.37(2)	683.3(2)
124	prelim	7.845(2)	7.061(3)	12.281(3)	93.41(2)	679.0(4)
"	final	7.864(1)	7.070(1)	12.304(1)	93.44(1)	682.8(4)
123.0	prelim	7.856(2)	7.062(2)	12.289(4)	93.53(2)	680.5(3)
98.0	prelim	7.840(2)	7.062(2)	12.269(5)	93.61(3)	678.0(4)
"	final	7.832(1)	7.053(1)	12.258(2)	93.61(1)	675.7(2)

**Table S-1. Cell constants for  $\text{ClC}_6\text{H}_3\text{N}_2\text{O}_2$  (cont.)**

- a temperatures quoted to the nearest degree were established with a Siemens LT-2 controller; those quoted to 0.1 degree with an Oxford Cryostream
- b film - original film values (Britton & Noland, 1962)  
prelim - from the preliminary matrix, usually 40-60 indexed reflections  
final - from the complete data set, 1000-3000 reflections
- in each case the *final* values are for the same crystal as the preceding *prelim*

**Table S-2. Cell constants for BrC<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub>**

Temp. <sup>a</sup> (K)	type <sup>b</sup>	a (Å)	b (Å)	c (Å)	β (°)	V (Å <sup>3</sup> )
300.0	prelim	7.959(3)	7.290(3)	12.549(5)	90.11(2)	728.1(4)
297	film <sup>c</sup>	7.98(4)	7.29(4)	12.62(7)	90.2(4)	734(5)
297	film <sup>d</sup>	7.79(1)	7.35(1)	12.67(2)	90.0(1)	725(2)
297	prelim <sup>e</sup>	7.953(2)	7.296(2)	12.546(5)	90.18(4)	728.0(4)
297	prelim <sup>e</sup>	7.956(2)	7.296(2)	12.548(5)	90.15(4)	728.3(5)
297	prelim	7.951(2)	7.290(3)	12.548(4)	90.05(2)	727.3(4)
"	final	7.958(1)	7.299(1)	12.560(1)	90.12(1)	729.6(1)
290.0	prelim <sup>e</sup>	7.948(2)	7.295(3)	12.542(6)	90.12(2)	727.2(4)
290.0	prelim <sup>e</sup>	7.944(2)	7.296(3)	12.543(2)	90.13(2)	727.0(3)
285.0	prelim	7.935(2)	7.297(3)	12.534(5)	90.12(2)	725.7(4)
284.0	prelim	7.932(3)	7.303(4)	12.523(7)	90.04(3)	725.4(4)
283.0	prelim	7.933(2)	7.297(3)	12.526(5)	90.10(2)	725.1(4)
282.0	prelim	7.918(2)	7.305(3)	12.524(4)	90.03(2)	724.4(3)
281.5 <sup>f</sup>	prelim	7.900(3)	7.351(3)	12.511(4)	90.19(3)	726.5(4)
281.0	prelim	7.891(2)	7.346(2)	12.480(3)	90.29(2)	723.5(3)
280.0	prelim <sup>e</sup>	7.880(2)	7.358(2)	12.473(2)	90.35(2)	723.2(4)
280.0	prelim <sup>e</sup>	7.862(2)	7.364(2)	12.421(3)	90.39(3)	719.2(3)
260.0	prelim	7.835(2)	7.393(2)	12.405(2)	90.51(1)	718.6(3)
240.0	prelim	7.810(2)	7.407(2)	12.371(3)	90.45(2)	715.6(3)
223	prelim	7.779(2)	7.406(2)	12.355(2)	90.31(2)	711.8(3)
220.0	prelim	7.790(2)	7.411(2)	12.351(2)	90.39(2)	713.0(3)
200.0	prelim	7.767(2)	7.410(2)	12.329(2)	90.30(2)	709.7(3)
180.0	prelim	7.750(2)	7.410(2)	12.314(2)	90.19(2)	707.2(3)

**Table S-2. Cell constants for BrC<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>2</sub> (cont.)**

173	prelim	7.787(2)	7.350(3)	12.406(2)	90.40(2)	710.0(5)
"	final	7.797(1)	7.359(1)	12.420(2)	90.39(1)	712.6(1)
173.0	prelim	7.742(2)	7.410(2)	12.309(3)	90.16(2)	706.2(3)
173	prelim	7.777(2)	7.335(2)	12.386(2)	90.25(2)	706.6(5)
150.0	prelim	7.727(2)	7.408(2)	12.294(3)	90.06(2)	703.7(3)
130.0	prelim	7.714(2)	7.407(2)	12.283(3)	90.05(2)	701.9(3)
115.5	prelim	7.704(2)	7.406(2)	12.272(3)	90.10(2)	700.2(3)

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- b film - original film values  
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 final - from the complete data set, 1000-3000 reflections  
 in each case the *final* values are for the same crystal as the preceding *prelim*
- c Britton & Noland, 1962
- d Britton, Hardgrove, Hegstrom, & Nelson, 1972
- e these values are for the same crystal before and after a transformation to the other form
- f At this and lower temperatures the values have been obtained by transforming the true cell constants by the matrix  $0.5, 0, 0.5 / 0, 1, 0 / 0.5, 0, -0.5$