



STRUCTURAL SCIENCE  
CRYSTAL ENGINEERING  
MATERIALS

**Volume 71 (2015)**

**Supporting information for article:**

**Crystal behavior of potassium bromate under compression**

**David Santamaría-Pérez, Raquel Chulia-Jordan, Placida Rodríguez-Hernández and Alfonso Muñoz**

**Table S1** Experimental lattice parameters and unit-cell volumes at different pressures as obtained from XRD measurements

Pressure (GPa)	Unit-cell volume (Å <sup>3</sup> )	<i>a</i> axis (Å)	$\alpha$ angle (°)
1E-4	85.10(14)	4.409(3)	85.97(4)
0.25	83.8(4)	4.385(7)	86.26(9)
0.59	82.9(4)	4.368(7)	86.42(9)
0.97	81.4(5)	4.341(8)	86.59(10)
1.54	80.0(4)	4.315(7)	86.77(9)
1.82	79.2(4)	4.301(7)	86.90(9)
1.98	78.9(5)	4.294(8)	86.88(10)
2.32	77.9(5)	4.276(8)	86.98(11)
2.8	77.1(4)	4.261(7)	87.14(10)
2.86	76.9(5)	4.257(8)	87.09(12)
3.36	76.0(5)	4.241(8)	87.20(12)
3.8	75.2(5)	4.226(9)	87.28(14)
4.5	74.2(5)	4.206(9)	87.41(13)
5.4	72.9(6)	4.180(12)	87.56(14)
6.16	71.9(6)	4.161(10)	87.7(2)
6.8	70.9(7)	4.143(12)	87.8(2)
7.6	70.2(7)	4.128(13)	87.8(2)
8.4	69.5(8)	4.114(14)	87.9(2)
9.3	68.7(8)	4.098(14)	88.0(2)
10.0	68.1(9)	4.085(15)	88.1(2)
10.8	67.4(9)	4.07(2)	88.1(2)
12.45	66.5(10)	4.05(2)	88.2(2)
14.7	65.3(10)	4.03(2)	88.4(3)

**Table S2** Theoretically calculated structural parameters and unit-cell volumes of KBrO<sub>3</sub> as a function of pressure

Pressure (GPa)	Unit-cell volume(Å <sup>3</sup> )	<i>a</i> axis (Å)	$\alpha$ angle (°)	<i>x</i> (K atom)	<i>x</i> (Br atom)	<i>x</i> (O atom)	<i>z</i> (O atom)
-0.16	84	4.3967	84.8005	0.98131	0.47535	0.54022	0.09287
0.31	82	4.3579	85.3827	0.98515	0.47586	0.53908	0.0908
0.872	80	4.3200	85.7907	0.98897	0.47617	0.53830	0.08822
1.568	78	4.2818	86.1805	0.99252	0.47664	0.53756	0.08568
2.411	76	4.2434	86.5081	0.99539	0.47726	0.53711	0.08307
3.436	74	4.2045	86.8449	0.99891	0.47784	0.53643	0.08035
4.676	72	4.1653	87.1035	0.00160	0.47851	0.53616	0.07753
6.148	70	4.1256	87.3463	0.00423	0.47929	0.53589	0.07465
7.943	68	4.0853	87.5472	0.00637	0.48018	0.53584	0.07172
10.088	66	4.0443	87.7358	0.00855	0.48114	0.53579	0.0687
12.69	64	4.0026	87.9082	0.01036	0.48225	0.53584	0.06569
15.791	62	3.9601	88.0682	0.01237	0.48340	0.53584	0.06251
17.575	61	3.9385	88.1455	0.01328	0.48404	0.53586	0.06091
19.535	60	3.9167	88.2211	0.01416	0.48471	0.53590	0.05930
29.547	56	3.8271	88.5216	0.01744	0.48783	0.53595	0.05281
40.086	53	3.7571	88.7559	0.01964	0.49073	0.53583	0.04792
49.078	51	3.7091	88.9237	0.02104	0.49303	0.53559	0.04471
60.147	49	3.6598	89.0818	0.02233	0.49563	0.53523	0.04153
81.781	46	3.5832	89.3875	0.02386	0.50063	0.53415	0.03718
90.717	45	3.557	89.4857	0.0243	0.50258	0.53365	0.03578
100.54	44	3.5304	89.5898	0.02482	0.50493	0.53301	0.03418
111.108	43	3.5035	89.6958	0.02532	0.50842	0.53211	0.03199
123.473	42	3.4761	89.8044	0.02565	0.51183	0.53104	0.03041
137.388	41	3.4482	89.9117	0.02585	0.51635	0.52949	0.02877
153.175	40	3.42	89.997	0.02603	0.52471	0.5265	0.02623
162.224	39.5	3.4056	90.0048	0.02604	0.52598	0.52601	0.02592
171.795	39	3.3912	90.0022	0.02599	0.52603	0.52597	0.026
241.794	36	3.3019	90.0017	0.02599	0.52603	0.52598	0.02599