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ARTICLE TYPE

Supplementary Information for

Joint Experimental and Computational ^{17}O Solid State NMR Study of Brownmillerite $Ba_2In_2O_5$

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Table of Contents

1. Additional Figures.

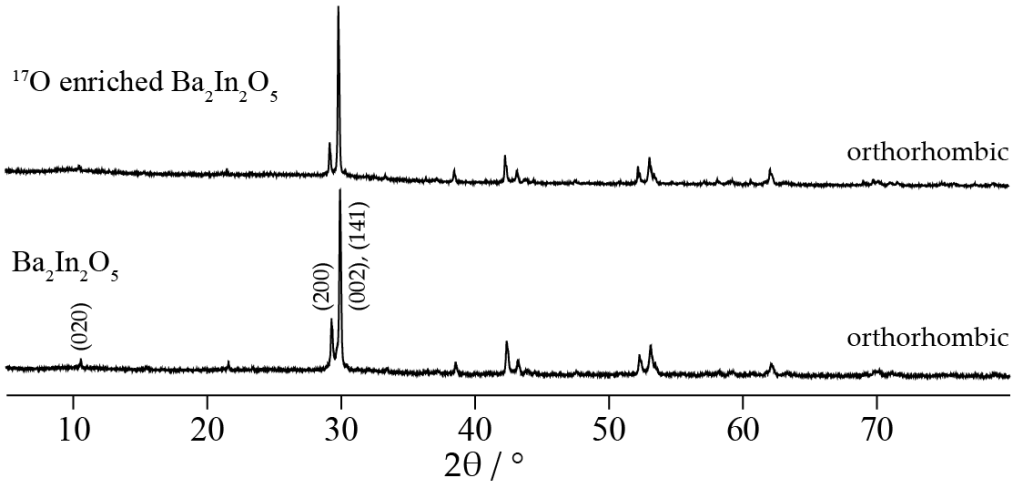

Figure S1. Powder x-ray diffraction patterns of $Ba_2In_2O_5$ and ^{17}O enriched $Ba_2In_2O_5$.

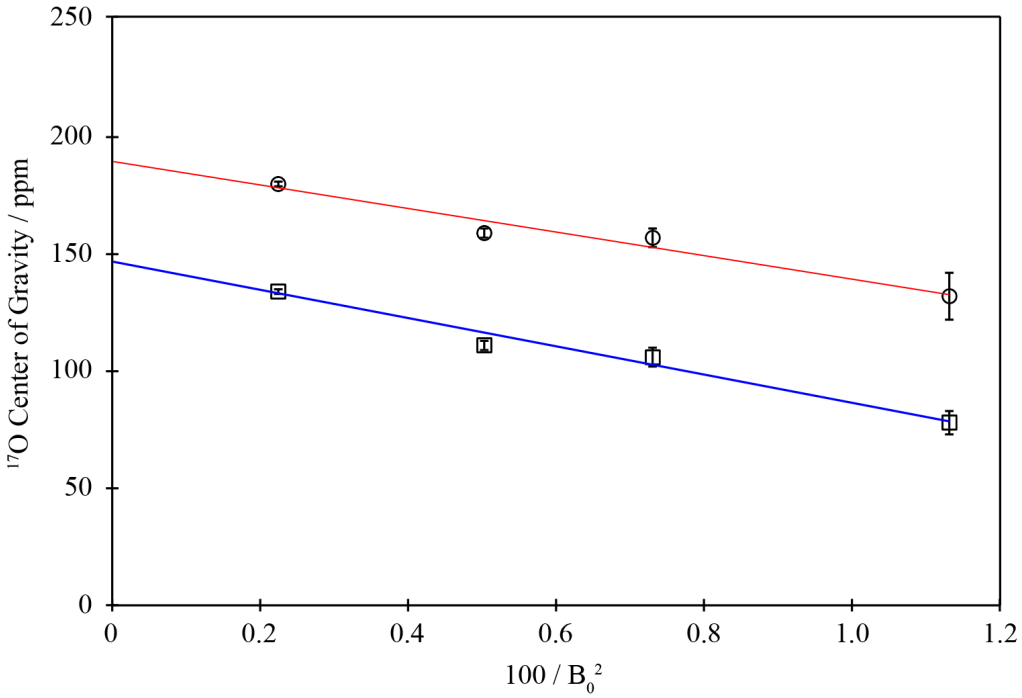

Figure S2. Variable B_0 field dependence of the ^{17}O MAS NMR shifts of the centre of gravity of two ^{17}O signals in $Ba_2In_2O_5$. The straight lines denote least squares fits, yielding isotropic chemical shifts of 189 (8) and 146 (8) ppm for the high and low shift of the ^{17}O sites, respectively.

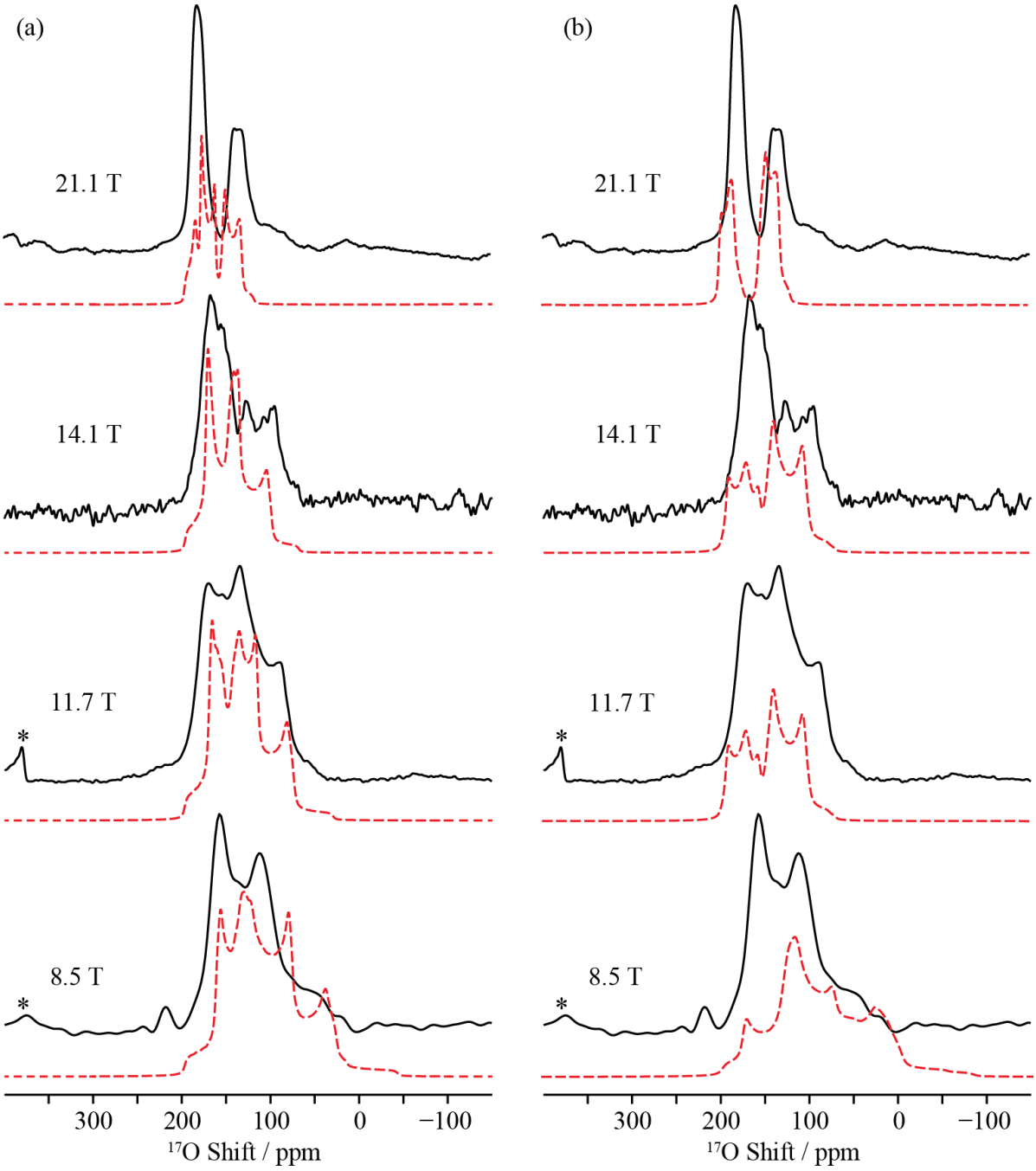

Figure S3. Comparison of the experimental (full lines) ^{17}O MAS NMR spectra of $Ba_2In_2O_5$ and the simulation (red dashed lines) of the GIPAW calculated ^{17}O NMR spectra of computed $Ba_2In_2O_5$ in (a) the ground state ⋯OctTetOctTet′⋯ staggered oxygen vacancy configuration and (b) the first excited state ⋯OctTetOctTet⋯ stacked oxygen vacancy configuration as a function of magnetic field strengths. The asterisks denote the oxygen signal from the ZrO_2 rotor.[1]

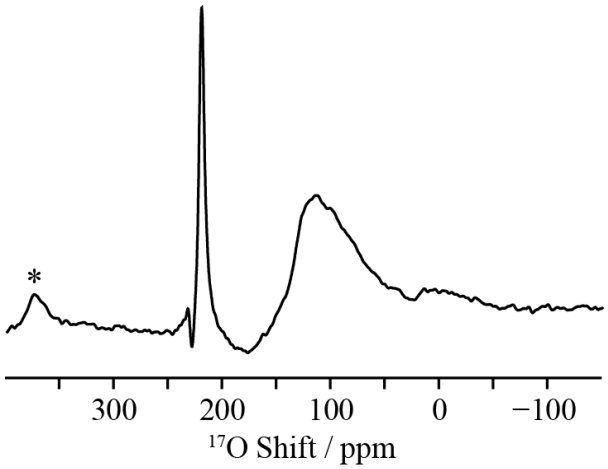

Figure S4. ^{17}O MAS NMR spectrum of ^{17}O enriched $Ba_2In_2O_4(OH)_2$ at 9.4 T obtained using a 3 μs pulse length corresponding to π/2 pulse at a radio frequency field amplitude of 80 kHz as measurement in liquid water. The lineshape distortion of the broad site at ~ 100 ppm arise from the long pulse length used in this experiment.[2] The asterisks denote the oxygen signal from the ZrO_2 rotor.[1]

Examining the In σ–values, it is found that the octahedral sites are approximately 376 ppm more shielded than the tetrahedral**.** The C_Q–values obtained for both In environments are very large, with magnitudes exceeding 200 MHz in each case. ^{115}In studies in literature[3-5] show C_Q values in a range of 20-600 MHz. The C_Q–values for $^{135/137}$Ba sites are substantially lower, in the approximate range from 31 to 33 MHz.[2]

2. List of CIF structural files of all DFT calculated configurations and respective CASTEP GIPAW outputs

Ground state Brownmillerite structures in ⋯OctTetOctTet'⋯ fashion:

#===

CRYSTAL DATA

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O5	0.559148	0.638967	0.521359
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O10	0.133838	0.751039	0.622551
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O12	0.635172	0.250554	0.122923
O13	0.257564	0.992363	0.245803
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O17	0.756871	0.492519	0.746008
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Ba5	0.519175	0.610208	-0.002544
Ba6	0.482281	0.390443	-0.001273
Ba7	0.483296	0.110297	0.997657
Ba8	0.519173	0.890538	-0.001331

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	71.98	-65.22	0.90	-6.266E+00	0.13
O	2	76.06	-62.99	0.82	-6.258E+00	0.13
O	3	75.10	-62.56	0.74	-6.260E+00	0.13
O	4	72.02	65.99	1.00	-6.267E+00	0.13
O	5	71.69	-65.77	0.93	-6.261E+00	0.13
O	6	76.67	-61.49	0.73	-6.261E+00	0.13
O	7	75.54	-62.80	0.75	-6.261E+00	0.13
O	8	72.93	-64.98	0.92	-6.263E+00	0.13
O	9	32.22	139.67	0.83	-4.684E+00	0.89
O	10	34.67	136.24	0.86	-4.691E+00	0.89
O	11	29.45	143.30	0.83	-4.709E+00	0.88
O	12	32.03	139.44	0.86	-4.711E+00	0.88
O	13	46.50	-80.24	0.07	-5.739E+00	0.05
O	14	45.61	-80.77	0.07	-5.741E+00	0.05
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O	16	46.26	-80.57	0.11	-5.742E+00	0.05
O	17	47.01	-80.78	0.15	-5.744E+00	0.06
O	18	46.65	-81.37	0.09	-5.736E+00	0.05
O	19	46.66	-80.83	0.08	-5.741E+00	0.06
O	20	46.80	-80.85	0.05	-5.740E+00	0.05
In	1	3070.66	331.56	0.42	-1.967E+02	0.30
In	2	3069.49	334.41	0.42	-1.968E+02	0.28
In	3	3069.69	331.32	0.42	-1.959E+02	0.30
In	4	3069.91	333.45	0.42	-1.957E+02	0.29
In	5	3446.97	44.40	0.58	2.034E+02	0.10
In	6	3447.22	44.74	0.60	2.026E+02	0.10
In	7	3447.40	45.50	0.53	2.029E+02	0.11
In	8	3447.16	44.95	0.50	2.029E+02	0.11
Ba	1	5077.39	274.50	0.23	3.301E+01	0.45
Ba	2	5074.54	265.40	0.24	3.268E+01	0.46
Ba	3	5077.75	269.34	0.24	3.302E+01	0.50
Ba	4	5073.20	270.36	0.23	3.266E+01	0.37
Ba	5	5075.54	274.63	0.23	3.341E+01	0.47
Ba	6	5080.06	273.56	0.24	3.332E+01	0.54
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Ba2         0.982106   0.889339   0.494942
Ba3         0.982045   0.609529   0.498313
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Ba7	0.482043	0.109528	-0.001668
Ba8	0.518886	0.889452	0.994911

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	73.77	65.53	1.00	-6.272E+00	0.12
O	2	74.63	-63.46	0.74	-6.259E+00	0.12
O	3	77.13	-61.54	0.80	-6.267E+00	0.12
O	4	71.88	-65.94	0.91	-6.270E+00	0.13
O	5	73.45	65.58	0.99	-6.273E+00	0.12
O	6	74.43	-63.66	0.74	-6.259E+00	0.12
O	7	77.26	-62.03	0.80	-6.267E+00	0.12
O	8	71.73	-66.16	0.91	-6.270E+00	0.13
O	9	32.20	140.14	0.83	-4.681E+00	0.90
O	10	30.80	141.11	0.85	-4.702E+00	0.88
O	11	32.29	140.17	0.83	-4.682E+00	0.89
O	12	30.85	141.23	0.85	-4.703E+00	0.88
O	13	46.55	-80.50	0.10	-5.739E+00	0.05
O	14	47.06	-80.51	0.07	-5.742E+00	0.05
O	15	46.56	-80.93	0.09	-5.742E+00	0.05
O	16	46.78	-81.43	0.15	-5.743E+00	0.06
O	17	46.38	-80.20	0.10	-5.739E+00	0.05
O	18	47.02	-80.71	0.07	-5.741E+00	0.05
O	19	46.53	-80.86	0.08	-5.742E+00	0.05
O	20	46.64	-80.87	0.15	-5.743E+00	0.06
In	1	3069.99	334.99	0.42	-1.974E+02	0.30
In	2	3069.72	334.37	0.42	-1.960E+02	0.30
In	3	3070.09	334.67	0.42	-1.974E+02	0.30
In	4	3069.57	334.47	0.42	-1.960E+02	0.30
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In	6	3447.67	46.14	0.52	2.051E+02	0.11
In	7	3447.36	45.04	0.58	2.043E+02	0.11
In	8	3447.02	45.52	0.50	2.051E+02	0.11
Ba	1	5073.00	271.46	0.24	3.288E+01	0.37
Ba	2	5075.25	274.00	0.23	3.432E+01	0.51
Ba	3	5079.95	275.05	0.25	3.372E+01	0.51
Ba	4	5080.52	273.91	0.23	3.457E+01	0.46
Ba	5	5073.26	271.32	0.24	3.289E+01	0.37
Ba	6	5075.25	274.16	0.23	3.430E+01	0.51
Ba	7	5079.82	275.18	0.25	3.376E+01	0.51
Ba	8	5080.43	273.74	0.23	3.453E+01	0.46

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Ba4        0.019087   0.390413   0.498913
Ba5        0.519077   0.609805  -0.001055
Ba6        0.482379   0.390326  -0.001020
Ba7        0.482863   0.110033  -0.001534
Ba8        0.519120   0.890423   0.998869
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Chemical Shielding and Electric Field Gradient Tensors							
Nucleus		Shielding tensor			EFG Tensor		
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta	
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O	3	75.62	-61.74	0.77	-6.259E+00	0.13	
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O	5	71.61	-65.28	0.95	-6.262E+00	0.13	
O	6	74.80	-63.20	0.75	-6.252E+00	0.13	
O	7	75.36	-62.27	0.75	-6.260E+00	0.13	
O	8	71.15	-66.48	0.93	-6.257E+00	0.13	
O	9	30.36	141.67	0.84	-4.701E+00	0.89	
O	10	33.23	137.61	0.87	-4.705E+00	0.88	
O	11	30.43	141.79	0.84	-4.700E+00	0.89	
O	12	33.29	137.65	0.87	-4.706E+00	0.88	
O	13	46.94	-80.20	0.09	-5.741E+00	0.05	
O	14	46.61	-80.93	0.05	-5.739E+00	0.05	
O	15	46.26	-80.64	0.05	-5.737E+00	0.05	
O	16	47.05	-80.79	0.08	-5.743E+00	0.05	
O	17	46.99	-80.48	0.08	-5.740E+00	0.05	
O	18	46.59	-81.34	0.05	-5.739E+00	0.05	
O	19	46.47	-80.65	0.05	-5.737E+00	0.05	
O	20	47.15	-80.92	0.08	-5.743E+00	0.05	
In	1	3068.14	333.57	0.42	-1.970E+02	0.29	
In	2	3068.25	335.42	0.42	-1.970E+02	0.27	
In	3	3068.24	332.99	0.42	-1.969E+02	0.29	
In	4	3068.00	335.42	0.42	-1.969E+02	0.27	
In	5	3447.75	44.55	0.55	2.043E+02	0.11	
In	6	3447.99	44.88	0.58	2.039E+02	0.11	
In	7	3447.98	44.73	0.58	2.040E+02	0.11	
In	8	3447.69	44.42	0.55	2.043E+02	0.11	
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Ba	2	5077.88	271.31	0.24	3.293E+01	0.53	
Ba	3	5076.75	267.52	0.24	3.304E+01	0.48	
Ba	4	5076.62	277.20	0.23	3.350E+01	0.47	
Ba	5	5075.77	274.04	0.23	3.324E+01	0.43	
Ba	6	5077.56	270.87	0.24	3.326E+01	0.52	
Ba	7	5076.76	268.22	0.24	3.266E+01	0.49	
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#==

CRYSTAL DATA

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O11         0.367798   0.750076   0.121042
O12         0.630533   0.250073   0.121195
O13         0.253624   0.991646   0.245113
O14         0.744813   0.008551   0.245067
O15         0.744803   0.491620   0.245065
O16         0.253611   0.508516   0.245146
O17         0.753653   0.491603   0.745107
O18         0.244835   0.508522   0.745105
O19         0.244813   0.991650   0.745073
O20         0.753618   0.008571   0.745103
In1         0.933781   0.250077   0.965732
In2         0.064623   0.750078   0.965696
In3         0.433819   0.750077   0.465674
In4         0.564356   0.250078   0.465806
In5        -0.000668   0.000139  -0.000409
In6        -0.000652   0.500037   0.999618
In7         0.499266   0.500110   0.499692
In8         0.499259   1.000064   0.499674
Ba1         1.017828   0.109862   0.498015
Ba2         0.981428   0.890341   0.498423
Ba3         0.981433   0.609719   0.498428
Ba4         0.017891   0.390215   0.498082
Ba5         0.518170   0.609749   0.998448
Ba6         0.481412   0.390330  -0.001588
Ba7         0.481418   0.109727   0.998419
Ba8         0.518176   0.890309  -0.001559

 ===============================================================================
|          Chemical Shielding and Electric Field Gradient Tensors     |
|-------------------------------------------------------------------------|
|    Nucleus              Shielding tensor           EFG Tensor   |
| Species     Ion    Iso(ppm)  Aniso(ppm)  Asym    Cq(MHz)     Eta  |
|   O         1       75.08     -63.66      0.85  -6.268E+00   0.12 |
|   O         2       74.14     -65.29      0.89  -6.269E+00   0.12 |
|   O         3       74.15     -64.61      0.90  -6.271E+00   0.12 |
```

O	4	74.82	-64.06	0.84	-6.267E+00	0.12
O	5	75.05	-63.85	0.86	-6.270E+00	0.12
O	6	73.94	-64.97	0.90	-6.269E+00	0.12
O	7	74.33	-64.91	0.90	-6.270E+00	0.12
O	8	74.89	-64.26	0.85	-6.268E+00	0.12
O	9	31.18	140.99	0.85	-4.696E+00	0.89
O	10	30.56	142.01	0.84	-4.692E+00	0.89
O	11	31.44	140.98	0.85	-4.694E+00	0.89
O	12	30.67	141.97	0.84	-4.694E+00	0.89
O	13	46.93	-80.20	0.07	-5.740E+00	0.06
O	14	46.88	-80.72	0.08	-5.741E+00	0.06
O	15	47.04	-80.88	0.08	-5.740E+00	0.05
O	16	47.07	-80.63	0.07	-5.740E+00	0.06
O	17	47.06	-80.57	0.07	-5.739E+00	0.06
O	18	47.33	-80.37	0.08	-5.742E+00	0.06
O	19	47.51	-80.32	0.08	-5.741E+00	0.05
O	20	47.23	-80.71	0.07	-5.740E+00	0.06
In	1	3069.35	336.98	0.42	-1.975E+02	0.29
In	2	3069.46	336.48	0.42	-1.974E+02	0.30
In	3	3069.62	336.87	0.42	-1.975E+02	0.30
In	4	3069.10	337.65	0.42	-1.979E+02	0.30
In	5	3447.78	45.22	0.54	2.056E+02	0.11
In	6	3448.27	45.57	0.57	2.057E+02	0.11
In	7	3448.24	45.20	0.57	2.055E+02	0.11
In	8	3447.72	45.21	0.56	2.056E+02	0.11
Ba	1	5077.46	274.35	0.24	3.366E+01	0.48
Ba	2	5077.78	275.96	0.24	3.401E+01	0.47
Ba	3	5077.61	275.34	0.24	3.395E+01	0.46
Ba	4	5077.75	274.93	0.24	3.374E+01	0.49
Ba	5	5077.85	273.76	0.24	3.387E+01	0.47
Ba	6	5077.60	276.11	0.23	3.400E+01	0.47
Ba	7	5077.30	275.46	0.24	3.397E+01	0.46
Ba	8	5077.96	274.42	0.24	3.393E+01	0.48

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CRYSTAL DATA

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_cell_angle_beta                90.001283
_cell_angle_gamma               89.999931
_symmetry_space_group_name_H-M      'P 1  '
_symmetry_Int_Tables_number         1

loop_
_symmetry_equiv_pos_as_xyz
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loop_
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_atom_site_label	_atom_site_fract_x	_atom_site_fract_y	_atom_site_fract_z
O1	0.056584	0.138308	0.01908
O2	0.943845	0.862081	1.019029
O3	0.943802	0.638304	0.019148
O4	0.056545	0.362087	1.018969
O5	0.556614	0.638307	0.5191
O6	0.443851	0.362084	0.518963
O7	0.443797	0.138309	0.519081
O8	0.556571	0.862074	0.519056
O9	0.868858	0.250174	0.621272
O10	0.131591	0.750161	0.621354
O11	0.368838	0.750169	0.12134
O12	0.631596	0.250167	0.121281
O13	0.254588	0.99174	0.245298
O14	0.745776	0.008624	0.245321
O15	0.745784	0.491738	0.245279
O16	0.254622	0.508633	0.245271
O17	0.754614	0.491755	0.745256
O18	0.245783	0.508632	0.745301
O19	0.245769	0.991748	0.74529
O20	0.754602	0.00863	0.745299
In1	0.934794	0.250176	0.965898
In2	0.065604	0.75017	0.965959
In3	0.434788	0.750169	0.465965
In4	0.565622	0.250173	0.465902
In5	1.000147	1.000182	-0.000158
In6	0.000181	0.500201	-0.000172
In7	0.500161	0.500186	0.499828
In8	0.500177	1.000194	0.499844
Ba1	0.018415	0.109773	0.498481
Ba2	0.981676	0.890349	0.498468
Ba3	0.981685	0.609778	0.498485
Ba4	0.018434	0.39036	0.49846
Ba5	0.518422	0.609772	-0.001517
Ba6	0.481672	0.390351	-0.001534
Ba7	0.481684	0.109778	-0.001513
Ba8	0.518431	0.890355	-0.001533

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	75.00	-64.17	0.89	-6.271E+00	0.12
O	2	74.62	-64.48	0.87	-6.266E+00	0.12
O	3	75.06	-63.64	0.89	-6.270E+00	0.12
O	4	74.36	-64.67	0.88	-6.267E+00	0.12
O	5	74.66	-64.11	0.90	-6.270E+00	0.12
O	6	74.51	-64.61	0.87	-6.266E+00	0.12
O	7	75.07	-64.18	0.88	-6.270E+00	0.12
O	8	74.27	-64.92	0.88	-6.266E+00	0.12
O	9	31.00	141.65	0.84	-4.694E+00	0.89
O	10	31.24	141.29	0.84	-4.694E+00	0.89
O	11	31.09	141.68	0.84	-4.693E+00	0.89
O	12	31.28	141.42	0.84	-4.694E+00	0.89

	O	13	46.91	-80.60	0.08	-5.740E+00	0.05	
	O	14	46.91	-80.53	0.08	-5.741E+00	0.05	
	O	15	46.95	-80.73	0.08	-5.739E+00	0.05	
	O	16	46.86	-80.68	0.08	-5.741E+00	0.05	
	O	17	47.10	-80.86	0.08	-5.740E+00	0.05	
	O	18	46.97	-80.89	0.08	-5.741E+00	0.05	
	O	19	47.01	-80.81	0.08	-5.740E+00	0.05	
	O	20	47.07	-80.66	0.08	-5.741E+00	0.05	
	In	1	3069.20	336.51	0.42	-1.974E+02	0.30	
	In	2	3069.28	336.49	0.42	-1.974E+02	0.30	
	In	3	3069.26	336.10	0.42	-1.974E+02	0.30	
	In	4	3069.13	336.61	0.42	-1.974E+02	0.30	
	In	5	3447.34	45.04	0.52	2.053E+02	0.11	
	In	6	3447.88	45.41	0.55	2.053E+02	0.11	
	In	7	3447.84	45.21	0.55	2.053E+02	0.11	
	In	8	3447.28	44.92	0.53	2.054E+02	0.11	
	Ba	1	5077.30	274.10	0.24	3.382E+01	0.46	
	Ba	2	5078.03	275.31	0.24	3.393E+01	0.48	
	Ba	3	5077.46	273.55	0.24	3.378E+01	0.46	
	Ba	4	5077.93	275.97	0.24	3.395E+01	0.48	
	Ba	5	5077.46	273.97	0.24	3.383E+01	0.46	
	Ba	6	5078.04	275.40	0.24	3.393E+01	0.49	
	Ba	7	5077.35	273.72	0.24	3.381E+01	0.46	
	Ba	8	5077.94	275.70	0.24	3.393E+01	0.48	

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Excited state structures (Brownmillerite type with stacked Vac channels in ⋯OctTetOctTet⋯ fashion):

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CRYSTAL DATA

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_cell_length_b 17.075117
_cell_length_c 6.044900
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_cell_angle_beta 89.986622
_cell_angle_gamma 90.009552
_symmetry_space_group_name_H-M 'P 1 '
_symmetry_Int_Tables_number 1

loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'

loop_

_atom_site_label	_atom_site_fract_x	_atom_site_fract_y	_atom_site_fract_z
O1	0.046148	0.138062	0.022218
O2	1.044206	0.862731	1.021505
O3	1.044549	0.638332	1.021881
O4	0.045575	0.362048	1.022313
O5	0.457996	0.638263	0.521451
O6	0.457709	0.362022	0.522093
O7	0.457407	0.138098	0.523346
O8	0.458305	0.862759	0.521354
O9	0.880155	0.250335	0.617799
O10	0.622436	0.750504	0.116503
O11	0.879965	0.750468	0.616546
O12	0.624674	0.249385	0.118557
O13	0.258539	1.000434	0.245410
O14	0.751376	0.000757	0.252114
O15	0.752120	0.499968	0.252511
O16	0.259338	0.499849	0.244773
O17	0.750777	0.499949	0.752226
O18	0.243444	0.500119	0.745061
O19	0.243230	1.000347	0.745130
O20	0.750849	0.000663	0.751968
In1	0.932066	0.249943	0.965203
In2	0.571795	0.750434	0.464400
In3	0.930417	0.750439	0.964505
In4	0.572206	0.249939	0.466022
In5	0.998329	1.000419	0.002031
In6	0.998587	0.500191	0.002019
In7	0.503731	0.500093	0.502012
In8	0.503546	0.000443	0.502099
Ba1	0.018796	0.108210	0.499195
Ba2	1.018809	0.892150	0.499096
Ba3	1.018833	0.608209	0.499174
Ba4	0.018748	0.392144	0.499103
Ba5	0.481871	0.607980	-0.000805
Ba6	0.481305	0.389053	-0.001036
Ba7	0.481867	0.108149	0.999170
Ba8	0.481707	0.892088	-0.000896

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	76.03	-67.99	0.60	-6.202E+00	0.14
O	2	74.22	-69.61	0.53	-6.198E+00	0.14
O	3	74.62	-67.21	0.53	-6.217E+00	0.14
O	4	71.59	-73.48	0.61	-6.183E+00	0.14
O	5	75.23	-65.98	0.49	-6.220E+00	0.14
O	6	74.10	-70.27	0.39	-6.183E+00	0.14
O	7	76.77	-66.19	0.46	-6.198E+00	0.14
O	8	75.62	-68.67	0.46	-6.203E+00	0.14
O	9	29.96	143.69	0.75	-4.546E+00	0.99
O	10	30.09	143.30	0.74	-4.556E+00	0.99
O	11	28.28	145.61	0.73	-4.559E+00	0.98
O	12	25.89	149.02	0.76	-4.589E+00	0.97

O	13	21.18	-73.77	0.09	-5.756E+00	0.01
O	14	79.91	-96.71	0.15	-5.718E+00	0.08
O	15	80.83	-95.15	0.15	-5.739E+00	0.10
O	16	23.16	-72.58	0.14	-5.773E+00	0.02
O	17	80.97	-95.74	0.16	-5.733E+00	0.09
O	18	22.41	-72.95	0.12	-5.782E+00	0.01
O	19	21.69	-73.44	0.09	-5.759E+00	0.02
O	20	79.90	-96.69	0.15	-5.713E+00	0.08
In	1	3073.78	331.39	0.35	-2.058E+02	0.44
In	2	3079.93	326.07	0.34	-2.028E+02	0.47
In	3	3079.83	322.03	0.34	-2.011E+02	0.48
In	4	3074.06	330.48	0.35	-2.042E+02	0.44
In	5	3444.58	-26.39	0.97	2.218E+02	0.10
In	6	3449.75	-30.36	0.82	2.282E+02	0.10
In	7	3450.77	29.37	0.91	2.267E+02	0.10
In	8	3445.05	26.25	0.91	2.208E+02	0.10
Ba	1	5087.40	302.01	0.35	-3.765E+01	0.24
Ba	2	5089.77	306.40	0.36	-3.987E+01	0.19
Ba	3	5089.82	300.44	0.37	-3.730E+01	0.23
Ba	4	5087.16	305.29	0.36	-3.861E+01	0.22
Ba	5	5094.10	294.68	0.38	-3.860E+01	0.22
Ba	6	5097.53	315.22	0.36	-4.271E+01	0.25
Ba	7	5082.39	303.19	0.36	-3.807E+01	0.24
Ba	8	5089.97	304.64	0.37	-3.969E+01	0.21

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CRYSTAL DATA

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_cell_angle_gamma 89.974265
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loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'

loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
O1 0.045223 0.138279 1.020756
O2 1.042364 0.862358 1.016792
O3 1.042488 0.637560 1.017426
O4 0.045479 0.361842 0.019147
O5 0.457936 0.637580 0.517302

O6	0.455472	0.361867	0.520450
O7	0.455163	0.138282	0.519409
O8	0.458095	0.862362	0.517798
O9	0.877102	0.249122	0.616997
O10	0.620444	0.749976	0.111833
O11	0.879660	0.749826	0.612004
O12	0.623546	0.251004	0.116990
O13	0.258158	1.000560	0.243011
O14	0.750816	0.000993	0.250133
O15	0.750198	0.498967	0.249494
O16	0.257263	0.499588	0.243078
O17	0.749759	0.499044	0.749552
O18	0.242247	0.499439	0.742558
O19	0.243201	1.000448	0.743512
O20	0.750257	0.001086	0.749967
In1	0.930866	0.250044	0.964219
In2	0.571230	0.749955	0.460267
In3	0.928951	0.749924	0.960546
In4	0.569754	0.250064	0.464216
In5	-0.002185	0.000343	0.000363
In6	0.997428	0.499609	-0.000353
In7	0.502601	0.499687	0.499720
In8	0.502982	1.000446	0.499942
Ba1	0.018418	0.107925	0.498665
Ba2	0.018709	0.892002	0.498630
Ba3	1.018431	0.607183	0.496575
Ba4	0.019018	0.388940	0.498510
Ba5	0.481519	0.607444	-0.003367
Ba6	0.481711	0.392049	-0.001419
Ba7	0.481113	0.111114	0.998575
Ba8	0.481720	0.892817	-0.003216

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	73.97	-72.01	0.60	-6.181E+00	0.13
O	2	76.11	-67.43	0.51	-6.228E+00	0.13
O	3	74.85	-66.44	0.51	-6.229E+00	0.13
O	4	75.74	-70.60	0.51	-6.182E+00	0.14
O	5	75.73	-66.30	0.48	-6.230E+00	0.13
O	6	74.36	-72.00	0.58	-6.180E+00	0.13
O	7	76.00	-70.39	0.49	-6.186E+00	0.14
O	8	74.30	-67.81	0.51	-6.224E+00	0.13
O	9	26.03	149.57	0.77	-4.569E+00	0.98
O	10	30.50	142.73	0.72	-4.545E+00	0.99
O	11	28.50	145.41	0.71	-4.552E+00	0.99
O	12	26.27	149.32	0.77	-4.568E+00	0.98
O	13	23.65	-72.20	0.12	-5.770E+00	0.02
O	14	81.70	-95.67	0.16	-5.726E+00	0.09
O	15	80.71	-96.52	0.17	-5.722E+00	0.09
O	16	21.75	-73.27	0.15	-5.772E+00	0.01
O	17	80.92	-95.93	0.16	-5.723E+00	0.09
O	18	23.12	-72.76	0.11	-5.765E+00	0.02
O	19	21.24	-73.08	0.15	-5.775E+00	0.01
O	20	80.49	-96.65	0.17	-5.726E+00	0.09
In	1	3069.14	338.74	0.36	-2.083E+02	0.42

	In	2	3084.42	319.71	0.33	-1.998E+02 0.50	
	In	3	3084.10	320.52	0.33	-2.000E+02 0.51	
	In	4	3068.95	339.25	0.36	-2.084E+02 0.41	
	In	5	3447.82	-28.02	0.97	2.268E+02 0.09	
	In	6	3448.13	29.26	0.92	2.256E+02 0.10	
	In	7	3447.77	-28.67	0.93	2.254E+02 0.09	
	In	8	3448.57	29.11	0.91	2.268E+02 0.10	
	Ba	1	5080.09	307.22	0.33	-3.839E+01 0.25	
	Ba	2	5092.91	303.78	0.35	-3.971E+01 0.21	
	Ba	3	5093.99	296.91	0.36	-4.007E+01 0.18	
	Ba	4	5094.92	316.84	0.32	-4.234E+01 0.25	
	Ba	5	5091.31	298.83	0.36	-3.816E+01 0.22	
	Ba	6	5079.37	308.19	0.33	-3.849E+01 0.25	
	Ba	7	5095.13	315.28	0.33	-4.214E+01 0.26	
	Ba	8	5094.81	296.15	0.36	-3.986E+01 0.17	

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CRYSTAL DATA

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_cell_length_b                 17.068291
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_symmetry_Int_Tables_number         1

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O2      1.045091        0.861721        0.024575
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O4      0.047241        0.362164        1.026506
O5      0.458977        0.637211        0.524170
O6      0.456315        0.362202        0.526435
O7      0.456867        0.138628        0.525631
O8      0.458574        0.861769        0.524482
O9      0.878542        0.250730        0.621996
O10     0.623068        0.749489        0.118863
O11     0.880700        0.749497        0.618795
O12     0.625136        0.250721        0.122069
O13     0.260201        1.000491        0.245844
```

O14	0.753063	0.000684	0.254766
O15	0.752075	0.499120	0.253920
O16	0.259520	0.499687	0.246553
O17	0.750984	0.499121	0.753714
O18	0.243127	0.499689	0.746440
O19	0.242545	1.000490	0.745786
O20	0.750103	0.000690	0.754504
In1	0.932211	0.250585	0.968812
In2	0.572440	0.749600	0.466618
In3	0.930984	0.749595	0.966608
In4	0.571119	0.250583	0.468816
In5	-0.001185	1.000255	0.003442
In6	0.998728	0.499663	0.003483
In7	0.503835	0.499662	0.503482
In8	0.503788	0.000262	0.503448
Ba1	0.019227	0.110911	0.499295
Ba2	1.018895	0.892127	0.499545
Ba3	1.018934	0.607878	0.499454
Ba4	0.018849	0.391952	0.499535
Ba5	0.481846	0.607955	-0.000529
Ba6	0.481935	0.391875	-0.000448
Ba7	0.481522	0.110989	-0.000676
Ba8	0.481886	0.892049	-0.000442

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	69.53	-76.00	0.53	-6.155E+00	0.14
O	2	72.37	-67.35	0.54	-6.214E+00	0.14
O	3	73.14	-69.82	0.51	-6.190E+00	0.14
O	4	75.15	-68.00	0.57	-6.179E+00	0.15
O	5	74.71	-67.98	0.41	-6.197E+00	0.14
O	6	76.62	-66.27	0.47	-6.186E+00	0.15
O	7	70.92	-73.85	0.44	-6.162E+00	0.14
O	8	74.16	-65.89	0.43	-6.222E+00	0.14
O	9	26.56	147.59	0.77	-4.579E+00	0.97
O	10	30.62	141.63	0.75	-4.563E+00	0.98
O	11	28.90	143.93	0.73	-4.558E+00	0.98
O	12	28.34	145.25	0.79	-4.583E+00	0.97
O	13	24.07	-72.03	0.06	-5.789E+00	0.01
O	14	81.37	-95.03	0.12	-5.752E+00	0.11
O	15	79.37	-97.45	0.14	-5.711E+00	0.08
O	16	21.68	-74.04	0.07	-5.749E+00	0.02
O	17	79.83	-97.12	0.14	-5.712E+00	0.08
O	18	21.46	-74.25	0.09	-5.746E+00	0.02
O	19	23.85	-72.17	0.07	-5.786E+00	0.01
O	20	81.95	-94.63	0.12	-5.752E+00	0.10
In	1	3068.18	333.54	0.37	-2.067E+02	0.41
In	2	3080.37	323.28	0.34	-2.016E+02	0.47
In	3	3079.97	319.67	0.34	-2.006E+02	0.48
In	4	3068.81	336.38	0.37	-2.077E+02	0.40
In	5	3453.49	-32.19	0.87	2.325E+02	0.10
In	6	3444.21	-27.69	0.92	2.202E+02	0.11
In	7	3444.94	26.61	0.93	2.186E+02	0.11
In	8	3453.96	30.32	0.97	2.308E+02	0.11
Ba	1	5093.44	316.51	0.38	-4.123E+01	0.24

```
|   Ba      2    5094.43    296.02     0.40  -3.760E+01   0.21 |
|   Ba      3    5089.16    306.77     0.39  -3.955E+01   0.18 |
|   Ba      4    5080.62    305.79     0.36  -3.728E+01   0.25 |
|   Ba      5    5089.85    303.55     0.40  -3.926E+01   0.22 |
|   Ba      6    5081.48    302.19     0.38  -3.692E+01   0.28 |
|   Ba      7    5094.20    313.42     0.39  -4.101E+01   0.28 |
|   Ba      8    5095.29    292.59     0.41  -3.719E+01   0.24 |
 ================================================================================


#===============================================================================

# CRYSTAL DATA

#-------------------------------------------------------------------------------



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_cell_angle_gamma                        90.009894
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_symmetry_Int_Tables_number            1

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O2         1.041685          0.862323          0.027518
O3         1.041788          0.637688          0.027700
O4         0.044486          0.361067          0.030411
O5         0.455509          0.637710          0.527826
O6         0.452005          0.361107          0.529470
O7         0.451977          0.137958          0.530373
O8         0.455596          0.862247          0.527892
O9         0.873136          0.249878          0.626784
O10        0.619930          0.750037          0.121770
O11        0.877420          0.750006          0.621759
O12        0.622057          0.248943          0.126035
O13        0.257691          1.000192          0.247805
O14        0.749918          0.000995          0.256241
O15        0.750849          0.498624          0.256975
O16        0.258580          0.499165          0.247179
O17        0.746752          0.498536          0.757149
O18        0.239485          0.499079          0.747425
O19        0.239435          1.000450          0.747488
O20        0.747159          0.000890          0.756490
In1        0.929047          0.249470          0.972764
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In2	0.569538	0.749961	0.469323
In3	0.928061	0.749971	0.969249
In4	0.566716	0.249476	0.472003
In5	-0.003635	1.000250	1.005167
In6	0.996584	0.499291	0.005240
In7	0.501415	0.499318	0.505183
In8	0.501262	0.000157	0.505147
Ba1	0.018585	0.110962	0.499755
Ba2	1.018150	0.892150	0.499962
Ba3	1.018266	0.607783	0.499963
Ba4	1.018457	0.388964	0.499777
Ba5	0.481169	0.607716	-0.000040
Ba6	0.480884	0.388910	-0.000225
Ba7	0.481293	0.107898	-0.000046
Ba8	0.481117	0.891933	-0.000078

Chemical Shielding and Electric Field Gradient Tensors

Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
O	1	73.77	-69.62	0.41	-6.153E+00	0.15
O	2	72.87	-66.97	0.43	-6.201E+00	0.15
O	3	72.16	-66.75	0.42	-6.208E+00	0.15
O	4	70.63	-72.76	0.43	-6.145E+00	0.15
O	5	70.89	-68.25	0.48	-6.202E+00	0.15
O	6	69.35	-74.66	0.55	-6.149E+00	0.15
O	7	70.92	-72.75	0.61	-6.153E+00	0.15
O	8	72.32	-68.71	0.46	-6.196E+00	0.15
O	9	25.32	147.78	0.82	-4.616E+00	0.95
O	10	29.69	141.87	0.74	-4.565E+00	0.98
O	11	31.45	139.28	0.75	-4.565E+00	0.98
O	12	29.27	143.47	0.81	-4.576E+00	0.97
O	13	22.32	-73.81	0.11	-5.762E+00	0.02
O	14	80.38	-96.83	0.14	-5.726E+00	0.09
O	15	80.95	-94.93	0.11	-5.747E+00	0.10
O	16	24.23	-72.46	0.06	-5.778E+00	0.01
O	17	81.06	-95.56	0.11	-5.752E+00	0.10
O	18	24.06	-73.01	0.05	-5.776E+00	0.01
O	19	23.10	-73.24	0.11	-5.753E+00	0.02
O	20	79.86	-96.64	0.14	-5.734E+00	0.09
In	1	3061.78	337.94	0.38	-2.082E+02	0.37
In	2	3079.23	316.18	0.34	-1.992E+02	0.48
In	3	3079.43	319.73	0.34	-2.009E+02	0.47
In	4	3062.17	337.40	0.39	-2.097E+02	0.38
In	5	3447.06	29.40	0.88	2.224E+02	0.12
In	6	3452.13	-31.67	0.98	2.288E+02	0.12
In	7	3451.67	-33.39	0.89	2.298E+02	0.12
In	8	3446.01	-30.14	0.85	2.240E+02	0.12
Ba	1	5088.27	316.66	0.39	-4.041E+01	0.32
Ba	2	5093.79	296.45	0.43	-3.837E+01	0.22
Ba	3	5095.42	295.33	0.44	-3.745E+01	0.25
Ba	4	5086.36	315.37	0.41	-3.975E+01	0.31
Ba	5	5095.00	297.26	0.44	-3.777E+01	0.21
Ba	6	5091.64	313.69	0.40	-3.938E+01	0.29
Ba	7	5078.50	305.48	0.40	-3.613E+01	0.27
Ba	8	5089.37	302.32	0.43	-3.718E+01	0.23

3. References for supplementary information

1. K. J. D. MacKenzie and M. E. Smith, *Multinuclear Solid State NMR of Inorganic Materials*, Pergamon Press, 2002.
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4. K. Yamada, K. Kumano and T. Okuda, *Solid State Ionics*, 2005, **176**, 823-829.
5. T. J. Bastow and G. W. West, *J. Phys.: Condens. Matter*, 2003, **15**, 8389-8406.