

Supporting Information

Thermal Decomposition of Sol-Gel Synthesized Bismuth Citrate

Darren Fynn ^{1,2}, Caren Billing ^{*1,2}, David Gordon Billing ^{1,2}

¹ Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa

² DSI-NRF Centre of Excellence in Strong Materials, University of the Witwatersrand, Johannesburg, South Africa

Corresponding author* email: caren.billing@wits.ac.za

Table S1. List of hkl reflections for the decomposition products derived from the Rietveld refinements of BiCit3-300 (BiOAc[#]), BiCit3-400 (*orth*-Bi₂O₂CO₃), BiCit3-500 (*tetrag*-Bi₂O₂CO₃), BiCit3-600 (α -Bi₂O₃) and BiCit3-700 (γ -Bi₂O₃)

Phase	h	k	l	Multiplicity	d/ Å	2theta/ °	Intensity/ arb. units
BiOCl [#]	0	0	1	2	5.64633	18.23056	0.00668
BiOCl [#]	0	0	2	2	2.82317	36.94419	6.95872
BiOCl [#]	0	0	3	2	1.88211	56.7531	0.39424
BiOCl [#]	0	0	4	2	1.41158	78.64513	2.85329
BiOCl [#]	1	0	1	8	3.19067	32.562	23.34266
BiOCl [#]	1	0	2	8	2.28023	46.19346	0.71178
BiOCl [#]	1	0	3	8	1.69234	63.8162	21.38556
BiOCl [#]	1	0	4	8	1.32601	84.84275	0.03999
BiOCl [#]	1	1	0	4	2.73462	38.18595	18.15333
BiOCl [#]	1	1	1	8	2.46116	42.62397	1.3037
BiOCl [#]	1	1	2	8	1.96423	54.18077	28.54496
BiOCl [#]	1	1	3	8	1.55039	70.47267	0.23233
BiOCl [#]	1	1	4	8	1.25433	90.98016	6.4839
BiOCl [#]	2	0	0	4	1.93367	55.109	17.61918
BiOCl [#]	2	0	1	8	1.82937	58.54543	0.03574
BiOCl [#]	2	0	2	8	1.59534	68.20799	16.15822
BiOCl [#]	2	0	3	8	1.34871	83.09261	0.87234
BiOCl [#]	2	1	1	16	1.65369	65.49161	26.54119
BiOCl [#]	2	1	2	16	1.47478	74.67805	0.77132
BiOCl [#]	2	1	3	16	1.27349	89.23971	26.01539
BiOCl [#]	2	2	0	4	1.36731	81.71866	10.21551
BiOCl [#]	2	2	1	8	1.3289	84.61548	0.03775
BiOCl [#]	2	2	2	8	1.23058	93.25298	10.09503
BiOCl [#]	3	0	1	8	1.25677	90.75383	7.95731
BiOCl [#]	3	0	2	8	1.17265	99.42407	0.27326
BiOCl [#]	3	1	0	8	1.22296	94.01155	13.05158
BiOCl [#]	3	1	1	16	1.19524	96.90088	0.71157
BiOBr [#]	0	0	1	2	5.64746	18.22689	0.16209
BiOBr [#]	0	0	2	2	2.82373	36.93656	6.36725
BiOBr [#]	0	0	3	2	1.88249	56.74076	1.11985
BiOBr [#]	0	0	4	2	1.41186	78.62641	1.8571
BiOBr [#]	1	0	1	8	3.19074	32.56132	10.80811
BiOBr [#]	1	0	2	8	2.28048	46.18819	2.37899
BiOBr [#]	1	0	3	8	1.69259	63.80557	19.00901
BiOBr [#]	1	0	4	8	1.32624	84.82511	0.38282
BiOBr [#]	1	1	0	4	2.73445	38.18849	19.74786
BiOBr [#]	1	1	1	8	2.46113	42.6246	2.42397
BiOBr [#]	1	1	2	8	1.96435	54.17705	26.71206
BiOBr [#]	1	1	3	8	1.55057	70.46338	1.86778
BiOBr [#]	1	1	4	8	1.25451	90.96338	4.5578
BiOBr [#]	2	0	0	4	1.93355	55.11283	19.35587
BiOBr [#]	2	0	1	8	1.8293	58.54777	0.48541
BiOBr [#]	2	0	2	8	1.59537	68.20643	16.8316
BiOBr [#]	2	0	3	8	1.34881	83.08537	2.77436

BiOBr [#]	2	1	1	16	1.65362	65.49466	14.40909
BiOBr [#]	2	1	2	16	1.47479	74.67736	2.91761
BiOBr [#]	2	1	3	16	1.27356	89.23331	26.20847
BiOBr [#]	2	2	0	4	1.36722	81.725	12.61937
BiOBr [#]	2	2	1	8	1.32884	84.62064	0.3743
BiOBr [#]	2	2	2	8	1.23056	93.25467	11.96855
BiOBr [#]	3	0	1	8	1.25671	90.75975	5.07398
BiOBr [#]	3	0	2	8	1.17263	99.42658	1.01185
BiOBr [#]	3	1	0	8	1.22288	94.01941	18.01328
BiOBr [#]	3	1	1	16	1.19518	96.90763	1.67047
BiOI [#]	0	0	1	2	5.6481	18.2248	0.23305
BiOI [#]	0	0	2	2	2.82405	36.93221	5.15588
BiOI [#]	0	0	3	2	1.8827	56.73372	1.4721
BiOI [#]	0	0	4	2	1.41203	78.61574	1.10162
BiOI [#]	1	0	1	8	3.19186	32.54954	2.89194
BiOI [#]	1	0	2	8	2.28102	46.17669	2.80623
BiOI [#]	1	0	3	8	1.6929	63.79268	8.93355
BiOI [#]	1	0	4	8	1.32644	84.80891	1.32461
BiOI [#]	1	1	0	4	2.73571	38.1701	15.83173
BiOI [#]	1	1	1	8	2.46211	42.60684	2.19632
BiOI [#]	1	1	2	8	1.96493	54.1598	20.66918
BiOI [#]	1	1	3	8	1.55092	70.44508	3.18932
BiOI [#]	1	1	4	8	1.25475	90.94155	2.68418
BiOI [#]	2	0	0	4	1.93444	55.0851	15.02947
BiOI [#]	2	0	1	8	1.83008	58.52034	0.64871
BiOI [#]	2	0	2	8	1.59593	68.17913	13.4886
BiOI [#]	2	0	3	8	1.34919	83.05654	3.77638
BiOI [#]	2	1	1	16	1.65434	65.4627	3.99362
BiOI [#]	2	1	2	16	1.47534	74.64517	3.54935
BiOI [#]	2	1	3	16	1.27395	89.199	12.35328
BiOI [#]	2	2	0	4	1.36786	81.67904	9.86945
BiOI [#]	2	2	1	8	1.32943	84.5743	0.48516
BiOI [#]	2	2	2	8	1.23105	93.2065	9.56671
BiOI [#]	3	0	1	8	1.25727	90.70792	1.40799
BiOI [#]	3	0	2	8	1.1731	99.37207	1.24412
BiOI [#]	3	1	0	8	1.22345	93.96242	14.45082
BiOI [#]	3	1	1	16	1.19572	96.84971	1.6269
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	0	2	2	6.85971	14.98531	0.99313
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	0	4	2	3.42985	30.23486	1.87271
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	0	6	2	2.28657	46.05804	4.11733
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	0	8	2	1.71493	62.8788	0.01278
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	0	10	2	1.37194	81.38446	2.47505
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	1	4	3.71387	27.87391	3.35971
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	3	4	2.94878	35.31731	11.98619
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	5	4	2.23601	47.16171	0.73727
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	7	4	1.74736	61.58305	4.90283
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	9	4	1.41772	78.23948	5.28035
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	1	11	4	1.18674	97.83131	0.082

<i>orth</i> -Bi ₂ O ₂ CO ₃	0	2	0	2	1.92895	55.25518	5.21831
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	2	2	4	1.85693	57.59405	2.1364
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	2	4	4	1.6813	64.28525	3.33107
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	2	6	4	1.47439	74.70127	5.06527
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	2	8	4	1.28165	88.52179	0.01221
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	3	1	4	1.28036	88.63489	1.22174
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	3	3	4	1.23796	92.53285	5.13454
<i>orth</i> -Bi ₂ O ₂ CO ₃	0	3	5	4	1.16443	100.3828	0.25413
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	1	4	3.72913	27.75755	1.90892
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	3	4	2.9564	35.22329	14.04439
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	5	4	2.23933	47.08762	0.58358
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	7	4	1.74894	61.5213	5.10619
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	9	4	1.41856	78.18402	5.0109
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	0	11	4	1.18724	97.77651	0.03612
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	0	4	2.73398	38.19519	10.91203
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	2	8	2.5397	41.24468	2.00148
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	4	8	2.13789	49.46764	11.87082
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	6	8	1.75399	61.32517	16.48184
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	8	8	1.45278	76.00819	0.15774
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	1	10	8	1.22621	93.68595	6.08312
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	2	1	8	1.71331	62.9448	4.87503
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	2	3	8	1.6155	67.24242	13.68552
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	2	5	8	1.46149	75.47505	0.95828
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	2	7	8	1.29567	87.3202	6.48401
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	3	0	4	1.22052	94.25792	4.96455
<i>orth</i> -Bi ₂ O ₂ CO ₃	1	3	2	8	1.20164	96.21469	0.84738
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	0	0	2	1.93751	54.99045	6.57344
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	0	2	4	1.86456	57.33644	1.28526
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	0	4	4	1.68696	64.04396	2.66639
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	0	6	4	1.4782	74.47599	5.342
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	0	8	4	1.28415	88.30453	0.00947
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	1	1	8	1.7178	62.76175	4.22785
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	1	3	8	1.61925	67.06567	14.6034
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	1	5	8	1.46427	75.30672	0.86436
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	1	7	8	1.2976	87.15712	6.49143
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	2	0	4	1.36699	81.74174	6.62731
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	2	2	8	1.34063	83.70616	2.51047
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	2	4	8	1.26985	89.56433	4.39701
<i>orth</i> -Bi ₂ O ₂ CO ₃	2	2	6	8	1.17331	99.34828	7.1136
<i>orth</i> -Bi ₂ O ₂ CO ₃	3	0	1	4	1.28599	88.14604	1.15085
<i>orth</i> -Bi ₂ O ₂ CO ₃	3	0	3	4	1.24304	92.04381	5.29423
<i>orth</i> -Bi ₂ O ₂ CO ₃	3	0	5	4	1.16866	99.88639	0.24305
<i>orth</i> -Bi ₂ O ₂ CO ₃	3	1	0	4	1.22485	93.82248	4.667
<i>orth</i> -Bi ₂ O ₂ CO ₃	3	1	2	8	1.20577	95.77794	1.04207
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	0	0	2	2	7.36691	13.94827	0.38794
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	0	0	4	2	3.68346	28.10874	0.42765
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	0	0	6	2	2.45564	42.72457	0.74602
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	0	0	8	2	1.84173	58.11474	0.00436

<i>tetrag</i> -Bi ₂ O ₂ CO ₃	0	0	10	2	1.47338	74.76114	0.17477
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	1	8	3.72499	27.78898	1.38738
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	3	8	3.03001	34.34066	6.98572
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	5	8	2.34002	44.9476	0.4558
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	7	8	1.84686	57.93807	1.30295
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	9	8	1.50655	72.84573	0.95289
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	0	11	8	1.26507	89.99525	0.00138
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	0	4	2.72241	38.36392	2.85201
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	2	8	2.55362	41.00973	0.32028
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	4	8	2.18934	48.2302	2.11917
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	6	8	1.82344	58.75436	2.57152
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	8	8	1.52545	71.80185	0.11033
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	1	1	10	8	1.29578	87.31024	0.16035
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	0	0	4	1.92503	55.37736	1.86973
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	0	2	8	1.8625	57.406	0.84141
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	0	4	8	1.70609	63.24195	0.61937
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	0	6	8	1.51501	72.37459	0.83435
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	0	8	8	1.33077	84.46874	0.00095
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	1	1	16	1.71016	63.07399	1.02681
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	1	3	16	1.62484	66.80467	3.60422
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	1	5	16	1.48663	73.98303	0.23121
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	1	7	16	1.33271	84.31816	0.67953
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	2	0	4	1.3612	82.16402	0.73193
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	2	2	8	1.33855	83.86615	0.15335
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	2	4	8	1.27681	88.94612	0.10592
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	2	2	6	8	1.19053	97.41403	0.27444
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	3	0	1	8	1.27852	88.79622	0.20575
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	3	0	3	8	1.24166	92.1757	0.50821
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	3	0	5	8	1.17661	98.96952	0.02941
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	3	1	0	8	1.2175	94.56429	0.3806
<i>tetrag</i> -Bi ₂ O ₂ CO ₃	3	1	2	16	1.2012	96.26136	0.05182
α -Bi ₂ O ₃	0	0	2	2	3.45752	29.98722	9.86718
α -Bi ₂ O ₃	0	0	4	2	1.72876	62.31905	0.08319
α -Bi ₂ O ₃	0	1	1	4	5.27742	19.51702	0.2803
α -Bi ₂ O ₃	0	1	2	4	3.18395	32.63268	13.391
α -Bi ₂ O ₃	0	1	3	4	2.21835	47.56013	1.0832
α -Bi ₂ O ₃	0	1	4	4	1.69129	63.86066	1.85428
α -Bi ₂ O ₃	0	1	5	4	1.3636	81.98897	5.86164
α -Bi ₂ O ₃	0	2	0	2	4.0835	25.30673	0.71718
α -Bi ₂ O ₃	0	2	1	4	3.51619	29.47546	0.32166
α -Bi ₂ O ₃	0	2	2	4	2.63871	39.63091	4.55103
α -Bi ₂ O ₃	0	2	3	4	2.0073	52.9264	8.75552
α -Bi ₂ O ₃	0	2	4	4	1.59197	68.37193	16.45715
α -Bi ₂ O ₃	0	2	5	4	1.30992	86.13603	9.06817
α -Bi ₂ O ₃	0	3	1	4	2.53311	41.35702	6.55803
α -Bi ₂ O ₃	0	3	2	4	2.1389	49.44259	0.11344
α -Bi ₂ O ₃	0	3	3	4	1.75914	61.12628	15.75641
α -Bi ₂ O ₃	0	3	4	4	1.45937	75.60411	1.64549

α -Bi ₂ O ₃	0	3	5	4	1.23302	93.01352	0.04135
α -Bi ₂ O ₃	0	4	0	2	2.04175	51.96598	1.20043
α -Bi ₂ O ₃	0	4	1	4	1.95818	54.3619	34.23254
α -Bi ₂ O ₃	0	4	2	4	1.75809	61.16648	1.46862
α -Bi ₂ O ₃	0	4	3	4	1.52838	71.64297	1.29373
α -Bi ₂ O ₃	0	4	4	4	1.31935	85.37252	1.79537
α -Bi ₂ O ₃	0	5	1	4	1.58966	68.48552	2.9665
α -Bi ₂ O ₃	0	5	2	4	1.47689	74.55347	0.41689
α -Bi ₂ O ₃	0	5	3	4	1.33271	84.31783	2.68369
α -Bi ₂ O ₃	0	5	4	4	1.18727	97.77309	1.82653
α -Bi ₂ O ₃	0	6	0	2	1.36117	82.16672	2.22598
α -Bi ₂ O ₃	0	6	1	4	1.33554	84.09812	1.96913
α -Bi ₂ O ₃	0	6	2	4	1.26655	89.86089	0.00238
α -Bi ₂ O ₃	0	6	3	4	1.17206	99.49148	9.8167
α -Bi ₂ O ₃	1	0	-6	2	1.2295	93.36001	7.50787
α -Bi ₂ O ₃	1	0	-4	2	1.87249	57.07152	20.53577
α -Bi ₂ O ₃	1	0	-2	2	3.62272	28.58994	3.41049
α -Bi ₂ O ₃	1	0	0	2	5.38504	19.12324	0.00024
α -Bi ₂ O ₃	1	0	2	2	2.49942	41.94053	5.94854
α -Bi ₂ O ₃	1	0	4	2	1.48582	74.0299	10.62645
α -Bi ₂ O ₃	1	1	-6	4	1.2158	94.73812	6.15455
α -Bi ₂ O ₃	1	1	-5	4	1.46263	75.40618	1.55633
α -Bi ₂ O ₃	1	1	-4	4	1.82513	58.69458	0.89772
α -Bi ₂ O ₃	1	1	-3	4	2.39195	43.92047	4.52384
α -Bi ₂ O ₃	1	1	-2	4	3.31155	31.34229	9.18375
α -Bi ₂ O ₃	1	1	-1	4	4.49831	22.93972	0.56262
α -Bi ₂ O ₃	1	1	0	4	4.49572	22.95313	0.29854
α -Bi ₂ O ₃	1	1	1	4	3.30844	31.37243	7.97266
α -Bi ₂ O ₃	1	1	2	4	2.39	43.95815	9.90182
α -Bi ₂ O ₃	1	1	3	4	1.82392	58.73741	12.37401
α -Bi ₂ O ₃	1	1	4	4	1.46183	75.4548	0.01959
α -Bi ₂ O ₃	1	1	5	4	1.21523	94.79582	4.11973
α -Bi ₂ O ₃	1	2	-6	4	1.17729	98.89228	0.33768
α -Bi ₂ O ₃	1	2	-5	4	1.39697	79.63087	1.01544
α -Bi ₂ O ₃	1	2	-4	4	1.70207	63.40865	0.25826
α -Bi ₂ O ₃	1	2	-3	4	2.13317	49.58438	0.94387
α -Bi ₂ O ₃	1	2	-2	4	2.70998	38.5468	13.18222
α -Bi ₂ O ₃	1	2	-1	4	3.25477	31.90347	20.96182
α -Bi ₂ O ₃	1	2	0	4	3.25379	31.91336	34.62443
α -Bi ₂ O ₃	1	2	1	4	2.70828	38.57197	13.83311
α -Bi ₂ O ₃	1	2	2	4	2.13179	49.6187	8.45102
α -Bi ₂ O ₃	1	2	3	4	1.70109	63.44957	0.14267
α -Bi ₂ O ₃	1	2	4	4	1.39627	79.6787	0.15058
α -Bi ₂ O ₃	1	2	5	4	1.17678	98.95049	0.70654
α -Bi ₂ O ₃	1	3	-5	4	1.30478	86.55849	2.47193
α -Bi ₂ O ₃	1	3	-4	4	1.54277	70.87292	2.11792
α -Bi ₂ O ₃	1	3	-3	4	1.84202	58.10475	5.53955
α -Bi ₂ O ₃	1	3	-2	4	2.17634	48.53673	1.67393

α -Bi ₂ O ₃	1	3	-1	4	2.42994	43.19904	2.66928
α -Bi ₂ O ₃	1	3	0	4	2.42953	43.20668	2.21623
α -Bi ₂ O ₃	1	3	1	4	2.17546	48.55766	3.68594
α -Bi ₂ O ₃	1	3	2	4	1.84113	58.13553	6.15309
α -Bi ₂ O ₃	1	3	3	4	1.54204	70.91165	0.7
α -Bi ₂ O ₃	1	3	4	4	1.30421	86.60562	3.662
α -Bi ₂ O ₃	1	4	-5	4	1.20183	96.19507	21.15303
α -Bi ₂ O ₃	1	4	-4	4	1.38001	80.80929	0.94233
α -Bi ₂ O ₃	1	4	-3	4	1.58179	68.87373	19.42785
α -Bi ₂ O ₃	1	4	-2	4	1.77871	60.38323	2.33368
α -Bi ₂ O ₃	1	4	-1	4	1.90933	55.87248	0.08898
α -Bi ₂ O ₃	1	4	0	4	1.90913	55.8788	3.36513
α -Bi ₂ O ₃	1	4	1	4	1.77823	60.40127	0.39522
α -Bi ₂ O ₃	1	4	2	4	1.58123	68.90175	1.57832
α -Bi ₂ O ₃	1	4	3	4	1.37949	80.84636	12.40935
α -Bi ₂ O ₃	1	4	4	4	1.20138	96.2424	0.13571
α -Bi ₂ O ₃	1	5	-4	4	1.23089	93.22207	3.30191
α -Bi ₂ O ₃	1	5	-3	4	1.36768	81.69183	5.55517
α -Bi ₂ O ₃	1	5	-2	4	1.48904	73.84307	3.2962
α -Bi ₂ O ₃	1	5	-1	4	1.56319	69.81153	1.39722
α -Bi ₂ O ₃	1	5	0	4	1.56308	69.8171	2.07201
α -Bi ₂ O ₃	1	5	1	4	1.48876	73.8594	5.8306
α -Bi ₂ O ₃	1	5	2	4	1.36732	81.71825	9.01821
α -Bi ₂ O ₃	1	5	3	4	1.23052	93.25872	4.81765
α -Bi ₂ O ₃	1	6	-3	4	1.19564	96.85827	4.95627
α -Bi ₂ O ₃	1	6	-2	4	1.27419	89.17732	0.93632
α -Bi ₂ O ₃	1	6	-1	4	1.31973	85.34255	17.90007
α -Bi ₂ O ₃	1	6	0	4	1.31966	85.3478	6.57246
α -Bi ₂ O ₃	1	6	1	4	1.27402	89.193	13.5215
α -Bi ₂ O ₃	1	6	2	4	1.1954	96.8846	0.07644
α -Bi ₂ O ₃	2	0	-6	2	1.25082	91.30756	0.27128
α -Bi ₂ O ₃	2	0	-4	2	1.81136	59.18497	0.23175
α -Bi ₂ O ₃	2	0	-2	2	2.69475	38.77335	16.20691
α -Bi ₂ O ₃	2	0	0	2	2.69252	38.80673	18.05986
α -Bi ₂ O ₃	2	0	2	2	1.80933	59.25799	1.46284
α -Bi ₂ O ₃	2	0	4	2	1.24971	91.41214	1.5915
α -Bi ₂ O ₃	2	1	-6	4	1.23641	92.68306	1.45669
α -Bi ₂ O ₃	2	1	-5	4	1.46482	75.27391	1.62289
α -Bi ₂ O ₃	2	1	-4	4	1.76839	60.77265	4.97125
α -Bi ₂ O ₃	2	1	-3	4	2.15502	49.0483	4.11836
α -Bi ₂ O ₃	2	1	-2	4	2.55905	40.9189	10.26101
α -Bi ₂ O ₃	2	1	-1	4	2.75342	37.91523	3.0492
α -Bi ₂ O ₃	2	1	0	4	2.55714	40.95082	2.3894
α -Bi ₂ O ₃	2	1	1	4	2.15274	49.10365	1.04958
α -Bi ₂ O ₃	2	1	2	4	1.7665	60.84452	14.54472
α -Bi ₂ O ₃	2	1	3	4	1.46339	75.36038	2.2599
α -Bi ₂ O ₃	2	1	4	4	1.23533	92.78774	0.61137
α -Bi ₂ O ₃	2	2	-6	4	1.19597	96.82209	11.82853

α -Bi ₂ O ₃	2	2	-5	4	1.39887	79.50075	12.91808
α -Bi ₂ O ₃	2	2	-4	4	1.65577	65.39876	19.93785
α -Bi ₂ O ₃	2	2	-3	4	1.96002	54.30665	5.8462
α -Bi ₂ O ₃	2	2	-2	4	2.24916	46.86955	5.32232
α -Bi ₂ O ₃	2	2	-1	4	2.37772	44.19717	0.13806
α -Bi ₂ O ₃	2	2	0	4	2.24786	46.8982	0.01894
α -Bi ₂ O ₃	2	2	1	4	1.9583	54.35814	0.12472
α -Bi ₂ O ₃	2	2	2	4	1.65422	65.46774	6.58671
α -Bi ₂ O ₃	2	2	3	4	1.39762	79.58582	6.44519
α -Bi ₂ O ₃	2	2	4	4	1.195	96.92741	7.17397
α -Bi ₂ O ₃	2	3	-5	4	1.30634	86.43028	0.69455
α -Bi ₂ O ₃	2	3	-4	4	1.50804	72.76204	0.05805
α -Bi ₂ O ₃	2	3	-3	4	1.72705	62.38763	8.48867
α -Bi ₂ O ₃	2	3	-2	4	1.91515	55.68779	1.69319
α -Bi ₂ O ₃	2	3	-1	4	1.99267	53.3457	0.45257
α -Bi ₂ O ₃	2	3	0	4	1.91435	55.7131	1.01367
α -Bi ₂ O ₃	2	3	1	4	1.72588	62.43482	17.2738
α -Bi ₂ O ₃	2	3	2	4	1.50687	72.82771	1.03451
α -Bi ₂ O ₃	2	3	3	4	1.30532	86.51409	10.66684
α -Bi ₂ O ₃	2	4	-5	4	1.20304	96.06637	0.1343
α -Bi ₂ O ₃	2	4	-4	4	1.35499	82.623	2.13021
α -Bi ₂ O ₃	2	4	-3	4	1.50719	72.80985	4.196
α -Bi ₂ O ₃	2	4	-2	4	1.62738	66.6867	1.82657
α -Bi ₂ O ₃	2	4	-1	4	1.67415	64.59322	33.90076
α -Bi ₂ O ₃	2	4	0	4	1.62689	66.70947	0.42777
α -Bi ₂ O ₃	2	4	1	4	1.50641	72.85362	13.19704
α -Bi ₂ O ₃	2	4	2	4	1.35414	82.68626	0.97616
α -Bi ₂ O ₃	2	4	3	4	1.20225	96.15049	0.82498
α -Bi ₂ O ₃	2	5	-4	4	1.21304	95.02151	0.10943
α -Bi ₂ O ₃	2	5	-3	4	1.31859	85.43347	6.90104
α -Bi ₂ O ₃	2	5	-2	4	1.39683	79.64006	2.77186
α -Bi ₂ O ₃	2	5	-1	4	1.42607	77.69505	1.24448
α -Bi ₂ O ₃	2	5	0	4	1.39652	79.66132	1.0366
α -Bi ₂ O ₃	2	5	1	4	1.31807	85.47543	2.8451
α -Bi ₂ O ₃	2	5	2	4	1.21243	95.08449	0.89939
α -Bi ₂ O ₃	2	6	-2	4	1.21497	94.8231	0.55053
α -Bi ₂ O ₃	2	6	-1	4	1.23406	92.91167	2.01539
α -Bi ₂ O ₃	2	6	0	4	1.21476	94.84409	2.81248
α -Bi ₂ O ₃	3	0	-6	2	1.20757	95.58927	10.93936
α -Bi ₂ O ₃	3	0	-4	2	1.5945	68.24881	13.83312
α -Bi ₂ O ₃	3	0	-2	2	1.93098	55.1923	0.57611
α -Bi ₂ O ₃	3	0	0	2	1.79501	59.77846	0.18627
α -Bi ₂ O ₃	3	0	2	2	1.38698	80.32033	2.09789
α -Bi ₂ O ₃	3	1	-6	4	1.19459	96.97224	2.42079
α -Bi ₂ O ₃	3	1	-5	4	1.36893	81.60111	0.27105
α -Bi ₂ O ₃	3	1	-4	4	1.56495	69.72143	4.7229
α -Bi ₂ O ₃	3	1	-3	4	1.75455	61.30322	0.41259
α -Bi ₂ O ₃	3	1	-2	4	1.87917	56.85005	8.99821

α -Bi ₂ O ₃	3	1	-1	4	1.8786	56.86878	3.29859
α -Bi ₂ O ₃	3	1	0	4	1.75317	61.35685	0.48833
α -Bi ₂ O ₃	3	1	1	4	1.56331	69.80501	13.32593
α -Bi ₂ O ₃	3	1	2	4	1.3674	81.71207	2.38912
α -Bi ₂ O ₃	3	1	3	4	1.19328	97.11447	9.08151
α -Bi ₂ O ₃	3	2	-5	4	1.31465	85.75117	0.11318
α -Bi ₂ O ₃	3	2	-4	4	1.48528	74.06128	2.14397
α -Bi ₂ O ₃	3	2	-3	4	1.6444	65.90829	2.34362
α -Bi ₂ O ₃	3	2	-2	4	1.74565	61.65001	18.07016
α -Bi ₂ O ₃	3	2	-1	4	1.74519	61.66783	16.03452
α -Bi ₂ O ₃	3	2	0	4	1.64326	65.95982	15.72887
α -Bi ₂ O ₃	3	2	1	4	1.48388	74.14282	3.42207
α -Bi ₂ O ₃	3	2	2	4	1.31329	85.86125	0.08579
α -Bi ₂ O ₃	3	3	-5	4	1.23696	92.62916	0.00075
α -Bi ₂ O ₃	3	3	-4	4	1.37587	81.10353	0.17926
α -Bi ₂ O ₃	3	3	-3	4	1.49944	73.24745	11.60963
α -Bi ₂ O ₃	3	3	-2	4	1.575	69.21289	0.05974
α -Bi ₂ O ₃	3	3	-1	4	1.57467	69.22966	4.42955
α -Bi ₂ O ₃	3	3	0	4	1.49857	73.29658	3.16193
α -Bi ₂ O ₃	3	3	1	4	1.37476	81.1829	0.64179
α -Bi ₂ O ₃	3	3	2	4	1.23583	92.73907	7.32025
α -Bi ₂ O ₃	3	4	-4	4	1.25669	90.76171	1.06405
α -Bi ₂ O ₃	3	4	-3	4	1.34874	83.09085	5.48363
α -Bi ₂ O ₃	3	4	-2	4	1.40294	79.22497	1.97577
α -Bi ₂ O ₃	3	4	-1	4	1.4027	79.24093	0.43969
α -Bi ₂ O ₃	3	4	0	4	1.34811	83.13824	1.42191
α -Bi ₂ O ₃	3	4	1	4	1.25584	90.84013	0.26753
α -Bi ₂ O ₃	3	5	-3	4	1.20855	95.48768	4.8976
α -Bi ₂ O ₃	3	5	-2	4	1.24708	91.66032	0.02408
α -Bi ₂ O ₃	3	5	-1	4	1.24691	91.67601	0.0782
α -Bi ₂ O ₃	3	5	0	4	1.20809	95.53495	5.34664
α -Bi ₂ O ₃	4	0	-4	2	1.34738	83.19345	0.73558
α -Bi ₂ O ₃	4	0	-2	2	1.46232	75.42479	10.43741
α -Bi ₂ O ₃	4	0	0	2	1.34626	83.27768	8.80288
α -Bi ₂ O ₃	4	1	-5	4	1.22154	94.15404	0.81317
α -Bi ₂ O ₃	4	1	-4	4	1.3294	84.57598	2.925
α -Bi ₂ O ₃	4	1	-3	4	1.40954	78.7811	5.13296
α -Bi ₂ O ₃	4	1	-2	4	1.43943	76.84073	1.23583
α -Bi ₂ O ₃	4	1	-1	4	1.4089	78.82373	5.43652
α -Bi ₂ O ₃	4	1	0	4	1.32833	84.66	5.65607
α -Bi ₂ O ₃	4	1	1	4	1.2203	94.27986	2.08056
α -Bi ₂ O ₃	4	2	-5	4	1.18251	98.30334	11.63105
α -Bi ₂ O ₃	4	2	-4	4	1.27952	88.70788	11.40163
α -Bi ₂ O ₃	4	2	-3	4	1.35049	82.95885	1.35248
α -Bi ₂ O ₃	4	2	-2	4	1.37671	81.04359	0.17964
α -Bi ₂ O ₃	4	2	-1	4	1.34993	83.00099	1.55222
α -Bi ₂ O ₃	4	2	0	4	1.27857	88.79155	0.00298
α -Bi ₂ O ₃	4	2	1	4	1.18138	98.43017	0.00285

α -Bi ₂ O ₃	4	3	-4	4	1.20757	95.59003	1.86038
α -Bi ₂ O ₃	4	3	-3	4	1.26668	89.84974	2.98028
α -Bi ₂ O ₃	4	3	-2	4	1.28823	87.95276	3.86447
α -Bi ₂ O ₃	4	3	-1	4	1.26621	89.89156	2.3367
α -Bi ₂ O ₃	4	3	0	4	1.20676	95.67408	1.50279
α -Bi ₂ O ₃	4	4	-3	4	1.17185	99.51587	6.33318
α -Bi ₂ O ₃	4	4	-2	4	1.18886	97.59789	0.43768
α -Bi ₂ O ₃	4	4	-1	4	1.17148	99.55828	16.90363
α -Bi ₂ O ₃	5	0	-2	2	1.16558	100.2469	0.12182
γ - Bi ₂ O ₃	1	1	0	12	7.19115	14.29095	0.00317
γ - Bi ₂ O ₃	2	0	0	6	5.08491	20.26355	0.01244
γ - Bi ₂ O ₃	2	1	1	24	4.15181	24.88364	0.13123
γ - Bi ₂ O ₃	2	2	0	12	3.59557	28.81044	0.42268
γ - Bi ₂ O ₃	2	2	2	8	2.93577	35.479	1.09517
γ - Bi ₂ O ₃	3	0	1	12	3.21598	32.29874	0.58026
γ - Bi ₂ O ₃	3	1	0	12	3.21598	32.29874	3.35794
γ - Bi ₂ O ₃	3	1	2	24	2.718	38.42862	0.07816
γ - Bi ₂ O ₃	3	2	1	24	2.718	38.42862	4.73222
γ - Bi ₂ O ₃	3	3	0	12	2.39705	43.82216	0.30126
γ - Bi ₂ O ₃	3	3	2	24	2.16821	48.73048	0.64103
γ - Bi ₂ O ₃	4	0	0	6	2.54245	41.19801	0.49489
γ - Bi ₂ O ₃	4	0	2	12	2.27404	46.32656	0.33198
γ - Bi ₂ O ₃	4	1	1	24	2.39705	43.82216	0.01826
γ - Bi ₂ O ₃	4	1	3	24	1.99447	53.29384	1.01935
γ - Bi ₂ O ₃	4	2	0	12	2.27404	46.32656	0.02829
γ - Bi ₂ O ₃	4	2	2	24	2.07591	51.04892	1.21037
γ - Bi ₂ O ₃	4	3	1	24	1.99447	53.29384	0.2517
γ - Bi ₂ O ₃	4	3	3	24	1.74411	61.71028	0.69613
γ - Bi ₂ O ₃	4	4	0	12	1.79779	59.67691	0.00589
γ - Bi ₂ O ₃	4	4	2	24	1.69497	63.70551	0.28643
γ - Bi ₂ O ₃	4	4	4	8	1.46789	75.0893	0.14706
γ - Bi ₂ O ₃	5	0	1	12	1.99447	53.29384	0.08256
γ - Bi ₂ O ₃	5	0	3	12	1.74411	61.71028	4.49772
γ - Bi ₂ O ₃	5	1	0	12	1.99447	53.29384	0.21439
γ - Bi ₂ O ₃	5	1	2	24	1.85675	57.6004	0.21781
γ - Bi ₂ O ₃	5	1	4	24	1.56924	69.50356	0.02835
γ - Bi ₂ O ₃	5	2	1	24	1.85675	57.6004	0.35198
γ - Bi ₂ O ₃	5	2	3	24	1.64976	65.66697	0.0028
γ - Bi ₂ O ₃	5	3	0	12	1.74411	61.71028	0.37777
γ - Bi ₂ O ₃	5	3	2	24	1.64976	65.66697	5.20631
γ - Bi ₂ O ₃	5	3	4	24	1.43823	76.91666	1.14147
γ - Bi ₂ O ₃	5	4	1	24	1.56924	69.50356	0.15719
γ - Bi ₂ O ₃	5	4	3	24	1.43823	76.91666	0.63128
γ - Bi ₂ O ₃	5	5	0	12	1.43823	76.91666	0.06161
γ - Bi ₂ O ₃	5	5	2	24	1.38394	80.53312	0.20408
γ - Bi ₂ O ₃	5	5	4	24	1.25182	91.21443	0.03969
γ - Bi ₂ O ₃	6	0	0	6	1.69497	63.70551	2.16613
γ - Bi ₂ O ₃	6	0	2	12	1.60799	67.59851	0.01668

γ - Bi ₂ O ₃	6	0	4	12	1.4103	78.73058	0.27981
γ - Bi ₂ O ₃	6	1	1	24	1.64976	65.66697	0.13305
γ - Bi ₂ O ₃	6	1	3	24	1.49946	73.24627	0.22611
γ - Bi ₂ O ₃	6	1	5	24	1.29157	87.66762	0.01261
γ - Bi ₂ O ₃	6	2	0	12	1.60799	67.59851	0.00727
γ - Bi ₂ O ₃	6	2	2	24	1.53316	71.38521	0.2822
γ - Bi ₂ O ₃	6	2	4	24	1.359	82.32625	0.11119
γ - Bi ₂ O ₃	6	3	1	24	1.49946	73.24627	2.97484
γ - Bi ₂ O ₃	6	3	3	24	1.38394	80.53312	0.17961
γ - Bi ₂ O ₃	6	3	5	24	1.21553	94.76589	3.39688
γ - Bi ₂ O ₃	6	4	0	12	1.4103	78.73058	0.1249
γ - Bi ₂ O ₃	6	4	2	24	1.359	82.32625	0.06231
γ - Bi ₂ O ₃	6	4	4	24	1.23327	92.98872	0.00236
γ - Bi ₂ O ₃	6	5	1	24	1.29157	87.66762	0.19913
γ - Bi ₂ O ₃	6	5	3	24	1.21553	94.76589	0.16845
γ - Bi ₂ O ₃	6	6	0	12	1.19852	96.54768	1.7034
γ - Bi ₂ O ₃	6	6	2	24	1.16656	100.1322	0.03891
γ - Bi ₂ O ₃	7	0	1	12	1.43823	76.91666	0.00173
γ - Bi ₂ O ₃	7	0	3	12	1.33536	84.11184	0.25611
γ - Bi ₂ O ₃	7	0	5	12	1.18222	98.33584	0.04678
γ - Bi ₂ O ₃	7	1	0	12	1.43823	76.91666	0.30438
γ - Bi ₂ O ₃	7	1	2	24	1.38394	80.53312	0.01806
γ - Bi ₂ O ₃	7	1	4	24	1.25182	91.21443	0.15828
γ - Bi ₂ O ₃	7	2	1	24	1.38394	80.53312	0.34298
γ - Bi ₂ O ₃	7	2	3	24	1.29157	87.66762	0.26112
γ - Bi ₂ O ₃	7	3	0	12	1.33536	84.11184	0.0949
γ - Bi ₂ O ₃	7	3	2	24	1.29157	87.66762	0.25934
γ - Bi ₂ O ₃	7	3	4	24	1.18222	98.33584	0.1026
γ - Bi ₂ O ₃	7	4	1	24	1.25182	91.21443	0.14812
γ - Bi ₂ O ₃	7	4	3	24	1.18222	98.33584	0.03398
γ - Bi ₂ O ₃	7	5	0	12	1.18222	98.33584	0.41163
γ - Bi ₂ O ₃	8	0	0	6	1.27123	89.44129	0.07469
γ - Bi ₂ O ₃	8	0	2	12	1.23327	92.98872	0.14881
γ - Bi ₂ O ₃	8	1	1	24	1.25182	91.21443	0.08697
γ - Bi ₂ O ₃	8	1	3	24	1.18222	98.33584	1.93523
γ - Bi ₂ O ₃	8	2	0	12	1.23327	92.98872	0.08729
γ - Bi ₂ O ₃	8	2	2	24	1.19852	96.54768	2.04507
γ - Bi ₂ O ₃	8	3	1	24	1.18222	98.33584	0.28827

Bismuth oxide halides (BiOCl, BiOBr and BiOI) were used as proxies for BiOAc due to structural similarity [1]

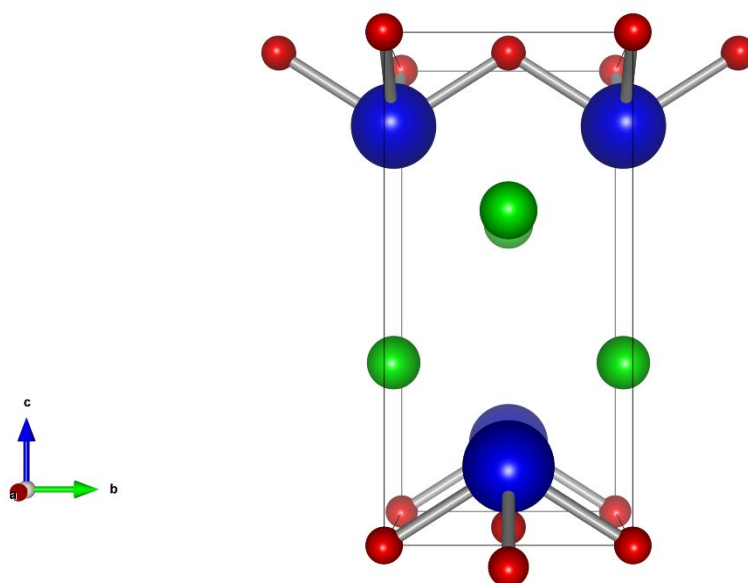


Fig. S2.1. Crystal structure of the bismuth oxide halides (BiOCl, BiOBr and BiOI) which were used as proxies for BiOAc in the Rietveld refinement of BiCit3-300 due to their structural similarity [1]. Bi is shown in blue, O is shown in red, and the halide position is shown in green

Table S2.1. Crystallographic data for BiOCl from the Rietveld refinement of BiCit3-300 using ICSD card no. 24608 as a starting model

Phase: BiOCl

Space group symbol (number): P4/nmm (129)

Z: 2

a/ Å: 3.8673(4)

c/ Å: 5.6463(9)

Volume/ Å³: 84.45(2)

Density/ gcm⁻³: 10.242(3)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi	2c	0	½	0.251(2)	1	2.0(1)
O	2a	0	0	0	1	1
Cl	2c	0	½	0.645	1	1

Table S2.2. Crystallographic data for BiOBr from the Rietveld refinement of BiCit3-300 using ICSD card no. 24609 as a starting model

Phase: BiOBr

Space group symbol (number): P4/nmm (129)

Z: 2

a/ Å: 3.8671(6)

c/ Å: 5.647(2)

Volume/ Å³: 84.45(4)

Density/ gcm⁻³: 11.989(5)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi	2c	0	½	0.253(2)	1	1
O	2a	0	0	0	1	1
Br	2c	0	½	0.653	1	1

Table S2.3. Crystallographic data for BiOI from the Rietveld refinement of BiCit3-300 using ICSD card no. 24610 as a starting model

Phase: BiOI

Space group symbol (number): P4/nmm (129)

Z: 2

a/ Å: 3.8689(9)

c/ Å: 5.648(2)

Volume/ Å³: 84.54(5)

Density/ gcm⁻³: 13.823(9)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi	2c	0	½	0.254(2)	1	1
O	2a	0	0	0	1	1
I	2c	0	½	0.668	1	1

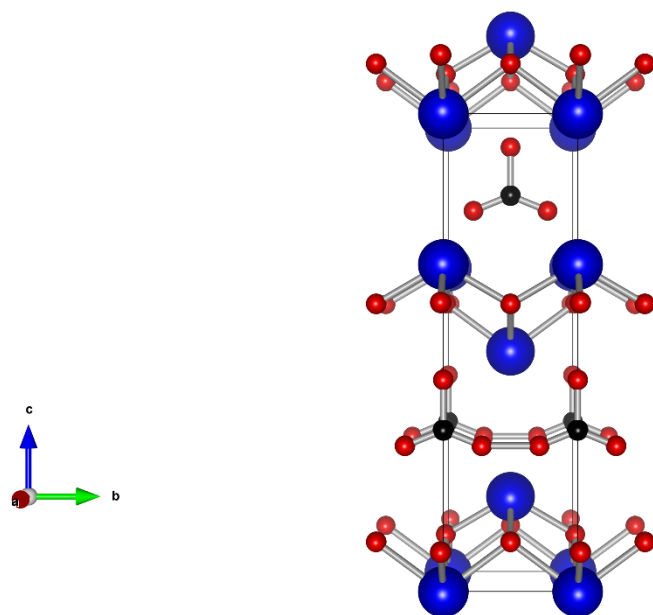


Fig. S3.1. Crystal structure of *orth*-Bi₂O₂CO₃ from the Rietveld refinement of BiCit3-400. Bi is shown in blue, O is shown in red, and C is shown in black

Table S3.1. Crystallographic data for *orth*-Bi₂O₂CO₃[#] from the Rietveld refinement of BiCit3-400 using ICSD card no. 94740 as a starting model

Phase: *orth*-Bi₂O₂CO₃

Space group symbol (number): Imm2 (44)

Z: 2

a/ Å: 3.875(1)^a, 3.874(1)^b, 3.874(2)^c

b/ Å: 3.858(1)^{a,b}, 8.859(2)^c

c/ Å: 13.719(2)^a, 13.724(3)^b, 13.725(3)^c

Volume/ Å³: 205.10(9)^a, 205.1(1)^{b,c}

Density/ gcm⁻³: 8.258(4)^a, 8.257(4)^b, 8.256(6)^c

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi1	2a	0	0	0	1	1.295
Bi2	2a	½	½	0.18433	1	1.35
C	2a	0	0	0.338	1	0.947
O1	2b	0	½	0.104	1	1.5
O2	2b	½	0	0.102	1	1.105
O3	4d	0	0.286	0.305	1	3
O4	2a	0	0	0.443	1	2.132

[#] Crystallographic data is influenced by the use bismuth oxide halides (^a BiOCl, ^b BiOBr or ^c BiOI) as proxies for BiOAc due to their structural similarity [1]

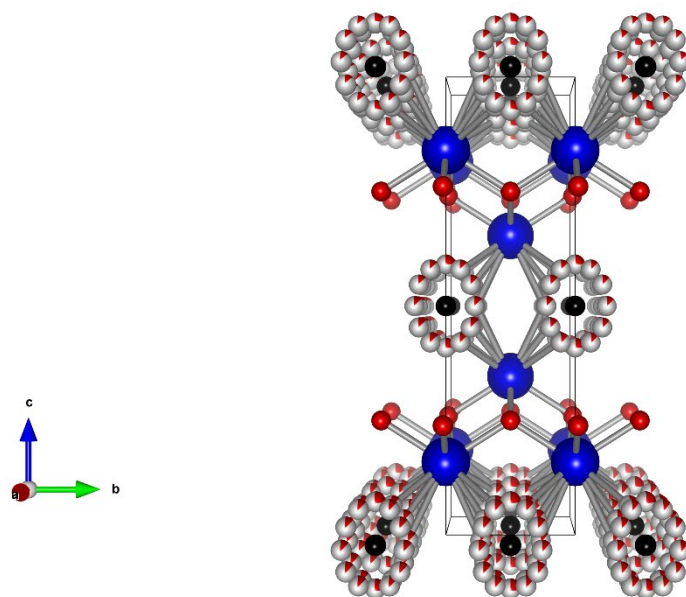


Fig. S3.2. Crystal structure of *tetrag*-Bi₂O₂CO₃ from the Rietveld refinement of BiCit3-500. Bi is shown in blue, O is shown in red, and C is shown in black

Table S3.2. Crystallographic data for *tetrag*-Bi₂O₂CO₃ from the Rietveld refinement of BiCit3-500 using ICSD card no. 36245 as a starting model

Phase: *tetrag*-Bi₂O₂CO₃

Space group symbol (number): I4/mmm (139)

Z: 2

a/ Å: 3.850(1)

c/ Å: 14.734(6)

Volume/ Å³: 218.4(1)

Density/ gcm⁻³: 7.755(5)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi1	4e	0	0	0.16	1	7.2(7)
O1	4d	0	½	¼	1	1
C	2b	0	0	½	1	1
O2	4e	0	0	0.591	¼	1
O3	16m	0.114	0.114	0.579	0.125	1
O4	16m	0.197	0.197	0.546	0.125	1
O5	8h	0.228	0.228	½	0.125	1

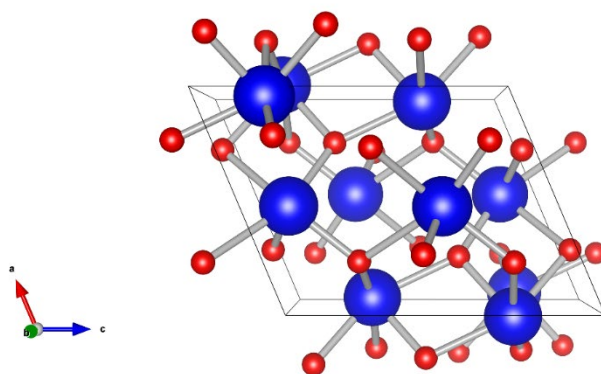


Fig. S4. Crystal structure of α -Bi₂O₃ from the Rietveld refinement of BiCit3-600. Bi is shown in blue, and O is shown in red

Table S4. Crystallographic data for α -Bi₂O₃ from the Rietveld refinement of BiCit3-600 using ICSD card no. 2374 as a starting model

Phase: α -Bi₂O₃

Space group symbol (number): P2₁/c (14)

Z: 4

a/ Å: 5.84929(9)

b/ Å: 8.1670(1)

c/ Å: 7.5112(1)

Volume/ Å³: 330.340(9)

Density/ gcm⁻³: 9.3691(2)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi1	4e	0.5263(5)	0.1833(4)	0.3621(2)	1	0.73(7)
Bi2	4e	0.0411(4)	0.0446(3)	0.7774(3)	1	0.41(7)
O1	4e	0.7783	0.3037	0.708	1	1
O2	4e	0.2337	0.0467	0.1266	1	1
O3	4e	0.2658	0.0294	0.5115	1	1

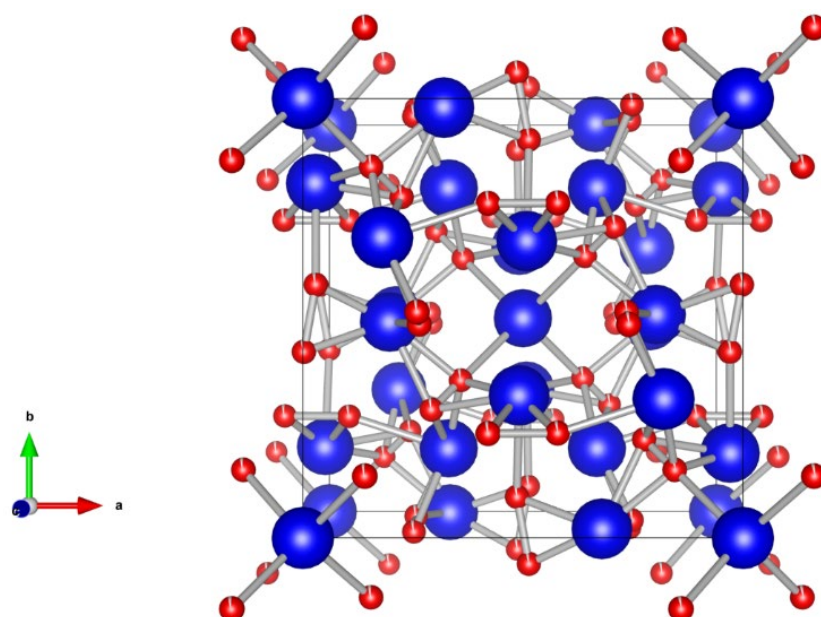


Fig. S5. Crystal structure of γ -Bi₂O₃ from the Rietveld refinement of BiCit3-700. Bi is shown in blue, and O is shown in red

Table S5. Crystallographic data for γ -Bi₂O₃ from the Rietveld refinement of BiCit3-700 using ICSD card no. 2376 as a starting model

Phase: γ -Bi₂O₃

Space group symbol (number): I23 (197)

Z: 13

a/ Å: 10.1698(7)

Volume/ Å³: 1051.8(2)

Density/ gcm⁻³: 9.563(2)

Atom	Wyckoff position	x	y	z	Occupancy	B _{iso} / Å ²
Bi1	24f	0.820(2)	0.684(2)	1.009(3)	1	2.3(4)
Bi2	2a	0	0	0	1	2.3(4)
O1	24f	0.921	0.738	0.514	0.975	1
O2	8c	0.716	0.716	0.716	0.975	1
O3	8c	0.148	0.148	0.148	0.975	1

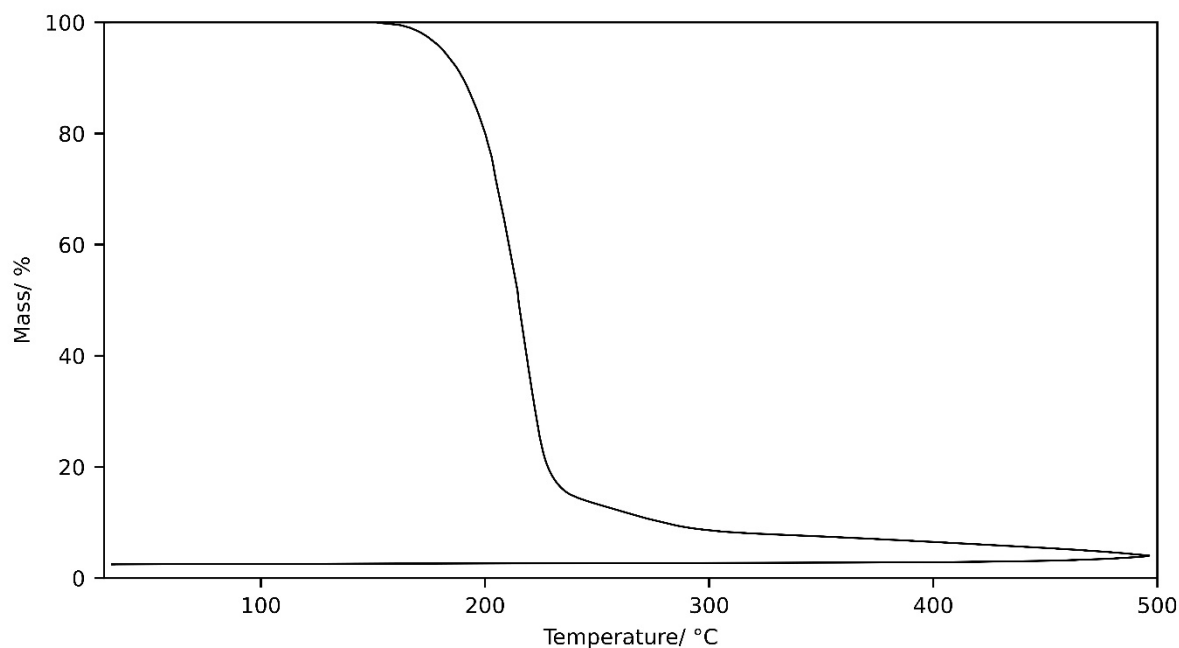


Fig. S6. TG curve for citric acid.

The thermal decomposition of citric acid is incomplete below 500 °C, because, as seen in Fig. S6, the sample mass is always greater than 0% throughout heating and cooling. This aligns well with previous literature regarding citric acid thermal decomposition [2,3].

References

1. Aurivillius B, Gloor U. X-Ray Studies on Bismuth Oxide Acetate $\text{CH}_3\text{COO}\cdot\text{OBi}$ and Related Compounds. *Acta Chem Scand.* 1955; 9: 1213–1218.
2. Wiecinska P. Thermal Degradation of Organic Additives Used in Colloidal Shaping of Ceramics Investigated by the Coupled DTA/TG/MS Analysis. *J Therm Anal Calorim.* 2016; 123: 1419–1430. <https://doi.org/10.1007/s10973-015-5075-1>.
3. Barbooti MM, Al-Sammerrai DA. Thermal Decomposition of Citric Acid. *Thermochim Acta.* 1986; 98: 119–126. [https://doi.org/10.1016/0040-6031\(86\)87081-2](https://doi.org/10.1016/0040-6031(86)87081-2).