

Supplementary information:

Table S1 Full lists with atomic positions for BCN(r) and BCN(o) structures

a) BCN(r) $a = 10.531895 \text{ \AA}$, $\alpha = 90^\circ$

x	Element	Atom Number	Fractional coordinates of atoms			x
x			u	v	w	x
x	0: 1	1	0. 204946	0. 000000	-0. 000000	x
x	0: 1	2	0. 204946	0. 500000	0. 500000	x
x	0: 1	3	0. 704946	-0. 000000	0. 500000	x
x	0: 1	4	0. 704946	0. 500000	-0. 000000	x
x	0: 1	5	-0. 204946	0. 500000	0. 500000	x
x	0: 1	6	-0. 204946	1. 000000	1. 000000	x
x	0: 1	7	0. 295054	0. 500000	-0. 000000	x
x	0: 1	8	-0. 000000	0. 204946	-0. 000000	x
x	0: 1	9	-0. 000000	0. 704946	0. 500000	x
x	0: 1	10	0. 500000	0. 704946	0. 000000	x
x	0: 1	11	0. 500000	-0. 204946	0. 500000	x
x	0: 1	12	-0. 000000	0. 295054	0. 500000	x
x	0: 1	13	0. 000000	0. 795054	1. 000000	x
x	0: 1	14	0. 500000	1. 204946	0. 500000	x
x	0: 1	15	0. 000000	-0. 000000	0. 204946	x
x	0: 1	16	-0. 000000	0. 500000	0. 704946	x
x	0: 1	17	0. 500000	-0. 000000	0. 704946	x
x	0: 1	18	0. 500000	0. 500000	-0. 204946	x
x	0: 1	19	0. 500000	0. 000000	0. 295054	x
x	0: 1	20	0. 500000	0. 500000	1. 204946	x
x	0: 1	21	0. 750000	0. 454946	0. 750000	x
x	0: 1	22	0. 250000	0. 045054	0. 250000	x
x	0: 1	23	0. 250000	0. 545054	0. 750000	x
x	0: 1	24	0. 750000	0. 545054	0. 250000	x
x	0: 1	25	0. 750000	1. 045054	0. 750000	x
x	0: 1	26	0. 750000	0. 954946	0. 250000	x
x	0: 1	27	0. 954946	0. 250000	0. 750000	x
x	0: 1	28	0. 545054	0. 750000	0. 250000	x
x	0: 1	29	0. 045054	0. 250000	0. 250000	x
x	0: 1	30	0. 045054	0. 750000	0. 750000	x
x	0: 1	31	0. 545054	0. 250000	0. 750000	x
x	0: 1	32	0. 454946	0. 750000	0. 750000	x
x	0: 1	33	0. 454946	1. 250000	1. 250000	x
x	0: 1	34	0. 750000	0. 250000	0. 545054	x
x	0: 1	35	0. 750000	0. 750000	1. 045054	x
x	0: 1	36	0. 250000	0. 750000	0. 954946	x
x	0: 1	37	0. 250000	1. 250000	1. 454946	x
x	0: 1	38	0. 750000	0. 750000	0. 454946	x
x	0: 1	39	0. 250000	0. 250000	0. 045054	x
x	0: 1	40	0. 250000	0. 750000	0. 545054	x
x	0: 1	41	0. 954946	0. 750000	0. 250000	x
x	0: 1	42	0. 250000	0. 954946	0. 750000	x
x	0: 1	43	0. 250000	1. 454946	1. 250000	x
x	0: 1	44	0. 750000	0. 250000	0. 954946	x
x	0: 1	45	0. 500000	0. 295054	0. 000000	x
x	0: 1	46	0. 295054	-0. 000000	0. 500000	x
x	0: 1	47	-0. 000000	0. 500000	0. 295054	x
x	0: 1	48	0. 000000	1. 000000	0. 795054	x
x	0: 1	49	0. 500000	0. 500000	0. 500000	x
x	0: 1	50	-0. 500000	0. 000000	1. 000000	x
x	0: 1	51	-0. 000000	1. 000000	-0. 500000	x
x	0: 1	52	1. 000000	-0. 500000	-0. 000000	x
x	0: 1	53	1. 250000	0. 750000	0. 250000	x
x	0: 1	54	-0. 250000	-0. 250000	-0. 250000	x
x	0: 1	55	0. 750000	0. 250000	1. 250000	x
x	0: 1	56	0. 250000	1. 250000	0. 750000	x
x	Nb: 1	1	0. 125000	0. 125000	0. 125000	x
x	Nb: 1	2	0. 125000	0. 625000	0. 625000	x
x	Nb: 1	3	0. 625000	0. 125000	0. 625000	x
x	Nb: 1	4	0. 625000	0. 625000	0. 125000	x
x	Nb: 1	5	-0. 125000	0. 375000	0. 625000	x
x	Nb: 1	6	-0. 125000	0. 875000	1. 125000	x
x	Nb: 1	7	0. 375000	0. 875000	0. 625000	x
x	Nb: 1	8	0. 375000	0. 625000	-0. 125000	x
x	Nb: 1	9	0. 375000	1. 125000	0. 375000	x
x	Nb: 1	10	0. 875000	0. 625000	0. 375000	x

x	Nb: 1	11	0. 625000	-0. 125000	0. 375000	x
x	Nb: 1	12	0. 625000	0. 375000	0. 875000	x
x	Nb: 1	13	1. 125000	-0. 125000	0. 875000	x
x	Nb: 1	14	0. 875000	1. 125000	0. 875000	x
x	Nb: 1	15	0. 375000	1. 375000	1. 125000	x
x	Nb: 1	16	1. 125000	0. 375000	1. 375000	x
x	Cd: 1	1	0. 625000	0. 625000	0. 625000	x
x	Cd: 1	2	0. 625000	1. 125000	1. 125000	x
x	Cd: 1	3	1. 125000	0. 625000	1. 125000	x
x	Cd: 1	4	1. 125000	1. 125000	0. 625000	x
x	Cd: 1	5	-0. 625000	-0. 125000	1. 125000	x
x	Cd: 1	6	-0. 625000	0. 375000	1. 625000	x
x	Cd: 1	7	-0. 125000	1. 125000	-0. 625000	x
x	Cd: 1	8	-0. 125000	1. 625000	-0. 125000	x
x	Cd: 1	9	1. 125000	-0. 625000	-0. 125000	x
x	Cd: 1	10	1. 625000	-0. 625000	0. 375000	x
x	Cd: 1	11	1. 375000	0. 625000	1. 375000	x
x	Cd: 1	12	0. 875000	1. 375000	0. 125000	x
x	Cd: 1	13	0. 875000	1. 875000	0. 625000	x
x	Cd: 1	14	1. 375000	0. 125000	0. 875000	x
x	Cd: 1	15	0. 125000	0. 875000	1. 375000	x
x	Cd: 1	16	0. 625000	0. 875000	1. 875000	x
x	Cd: 2	1	0. 125000	0. 125000	0. 125000	x
x	Cd: 2	2	0. 125000	0. 625000	0. 625000	x
x	Cd: 2	3	0. 625000	0. 125000	0. 625000	x
x	Cd: 2	4	0. 625000	0. 625000	0. 125000	x
x	Cd: 2	5	-0. 125000	0. 375000	0. 625000	x
x	Cd: 2	6	-0. 125000	0. 875000	1. 125000	x
x	Cd: 2	7	0. 375000	0. 875000	0. 625000	x
x	Cd: 2	8	0. 375000	0. 625000	-0. 125000	x
x	Cd: 2	9	0. 375000	1. 125000	0. 375000	x
x	Cd: 2	10	0. 875000	0. 625000	0. 375000	x
x	Cd: 2	11	0. 625000	-0. 125000	0. 375000	x
x	Cd: 2	12	0. 625000	0. 375000	0. 875000	x
x	Cd: 2	13	1. 125000	-0. 125000	0. 875000	x
x	Cd: 2	14	0. 875000	1. 125000	0. 875000	x
x	Cd: 2	15	0. 375000	1. 375000	1. 125000	x
x	Cd: 2	16	1. 125000	0. 375000	1. 375000	x
x	Bi: 1	1	0. 625000	0. 625000	0. 625000	x
x	Bi: 1	2	0. 625000	1. 125000	1. 125000	x
x	Bi: 1	3	1. 125000	0. 625000	1. 125000	x
x	Bi: 1	4	1. 125000	1. 125000	0. 625000	x
x	Bi: 1	5	-0. 625000	-0. 125000	1. 125000	x
x	Bi: 1	6	-0. 625000	0. 375000	1. 625000	x
x	Bi: 1	7	-0. 125000	1. 125000	-0. 625000	x
x	Bi: 1	8	-0. 125000	1. 625000	-0. 125000	x
x	Bi: 1	9	1. 125000	-0. 625000	-0. 125000	x
x	Bi: 1	10	1. 625000	-0. 625000	0. 375000	x
x	Bi: 1	11	1. 375000	0. 625000	1. 375000	x
x	Bi: 1	12	0. 875000	1. 375000	0. 125000	x
x	Bi: 1	13	0. 875000	1. 875000	0. 625000	x
x	Bi: 1	14	1. 375000	0. 125000	0. 875000	x
x	Bi: 1	15	0. 125000	0. 875000	1. 375000	x
x	Bi: 1	16	0. 625000	0. 875000	1. 875000	x

b) BCN(o) a = 10.86614 Å, $\alpha = 90,33179^\circ$

x	Element	Atom Number	Fractional coordinates of atoms			x
x			u	v	w	x
x	0	1	-0. 193941	0. 135862	-0. 368210	x
x	0	2	-0. 138283	-0. 380930	0. 105948	x
x	0	3	0. 348270	-0. 369316	-0. 353104	x
x	0	4	0. 298984	0. 110140	0. 122042	x
x	0	5	0. 445711	-0. 378513	0. 120396	x
x	0	6	0. 403428	0. 137819	-0. 399391	x
x	0	7	-0. 107771	0. 135373	0. 123032	x
x	0	8	-0. 354728	-0. 384803	-0. 044079	x
x	0	9	0. 134270	-0. 374178	0. 124791	x
x	0	10	-0. 368210	-0. 193941	0. 135862	x
x	0	11	0. 105948	-0. 138283	-0. 380930	x
x	0	12	-0. 353104	0. 348270	-0. 369316	x
x	0	13	0. 122042	0. 298984	0. 110140	x

x	0	14	0.120396	0.445711	-0.378513	x
x	0	15	-0.399391	0.403428	0.137819	x
x	0	16	0.123032	-0.107771	0.135373	x
x	0	17	-0.044079	-0.354728	-0.384803	x
x	0	18	0.124791	0.134270	-0.374178	x
x	0	19	0.135862	-0.368210	-0.193941	x
x	0	20	-0.380930	0.105948	-0.138283	x
x	0	21	-0.369316	-0.353104	0.348270	x
x	0	22	0.110140	0.122042	0.298984	x
x	0	23	-0.378513	0.120396	0.445711	x
x	0	24	0.137819	-0.399391	0.403428	x
x	0	25	0.135373	0.123032	-0.107771	x
x	0	26	-0.384803	-0.044079	-0.354728	x
x	0	27	-0.374178	0.124791	0.134270	x
x	0	28	-0.135862	0.193941	0.368210	x
x	0	29	0.380930	0.138283	-0.105948	x
x	0	30	0.369316	-0.348270	0.353104	x
x	0	31	-0.110140	-0.298984	-0.122042	x
x	0	32	0.378513	-0.445711	-0.120396	x
x	0	33	-0.137819	-0.403428	0.399391	x
x	0	34	-0.135373	0.107771	-0.123032	x
x	0	35	0.384803	0.354728	0.044079	x
x	0	36	0.374178	-0.134270	-0.124791	x
x	0	37	0.193941	0.368210	-0.135862	x
x	0	38	0.138283	-0.105948	0.380930	x
x	0	39	-0.348270	0.353104	0.369316	x
x	0	40	-0.298984	-0.122042	-0.110140	x
x	0	41	-0.445711	-0.120396	0.378513	x
x	0	42	-0.403428	0.399391	-0.137819	x
x	0	43	0.107771	-0.123032	-0.135373	x
x	0	44	0.354728	0.044079	0.384803	x
x	0	45	-0.134270	-0.124791	0.374178	x
x	0	46	0.368210	-0.135862	0.193941	x
x	0	47	-0.105948	0.380930	0.138283	x
x	0	48	0.353104	0.369316	-0.348270	x
x	0	49	-0.122042	-0.110140	-0.298984	x
x	0	50	-0.120396	0.378513	-0.445711	x
x	0	51	0.399391	-0.137819	-0.403428	x
x	0	52	-0.123032	-0.135373	0.107771	x
x	0	53	0.044079	0.384803	0.354728	x
x	0	54	-0.124791	0.374178	-0.134270	x
x	0	55	-0.380547	-0.380547	-0.380547	x
x	0	56	0.380547	0.380547	0.380547	x
x	Nb	1	-0.247552	0.007542	-0.243054	x
x	Nb	2	-0.243054	-0.247552	0.007542	x
x	Nb	3	0.007542	-0.243054	-0.247552	x
x	Nb	4	-0.007542	0.247552	0.243054	x
x	Nb	5	0.247552	0.243054	-0.007542	x
x	Nb	6	0.243054	-0.007542	0.247552	x
x	Nb	7	0.252240	-0.500000	-0.252240	x
x	Nb	8	-0.252240	0.252240	-0.500000	x
x	Nb	9	-0.500000	-0.252240	0.252240	x
x	Nb	10	0.506430	-0.506430	0.000000	x
x	Nb	11	0.000000	0.506430	-0.506430	x
x	Nb	12	-0.506430	0.000000	0.506430	x
x	Cd	1	-0.246410	0.000000	0.246410	x
x	Cd	2	0.246410	-0.246410	0.000000	x
x	Cd	3	0.000000	0.246410	-0.246410	x
x	Cd	4	0.500000	-0.500000	0.500000	x
x	Cd	5	-0.247014	-0.500000	0.247014	x
x	Cd	6	0.247014	-0.247014	-0.500000	x
x	Cd	7	-0.500000	0.247014	-0.247014	x
x	Cd	8	0.000000	0.000000	0.000000	x
x	Bi	1	0.251798	-0.474942	0.272563	x
x	Bi	2	0.272563	0.251798	-0.474942	x
x	Bi	3	-0.474942	0.272563	0.251798	x
x	Bi	4	0.474942	-0.251798	-0.272563	x
x	Bi	5	-0.251798	-0.272563	0.474942	x
x	Bi	6	-0.272563	0.474942	-0.251798	x
x	Bi	7	0.227154	0.000000	-0.227154	x
x	Bi	8	-0.227154	0.227154	0.000000	x
x	Bi	9	-0.000000	-0.227154	0.227154	x
x	Bi	10	0.018905	-0.018905	0.500000	x
x	Bi	11	0.500000	0.018905	-0.018905	x
x	Bi	12	-0.018905	0.500000	0.018905	x

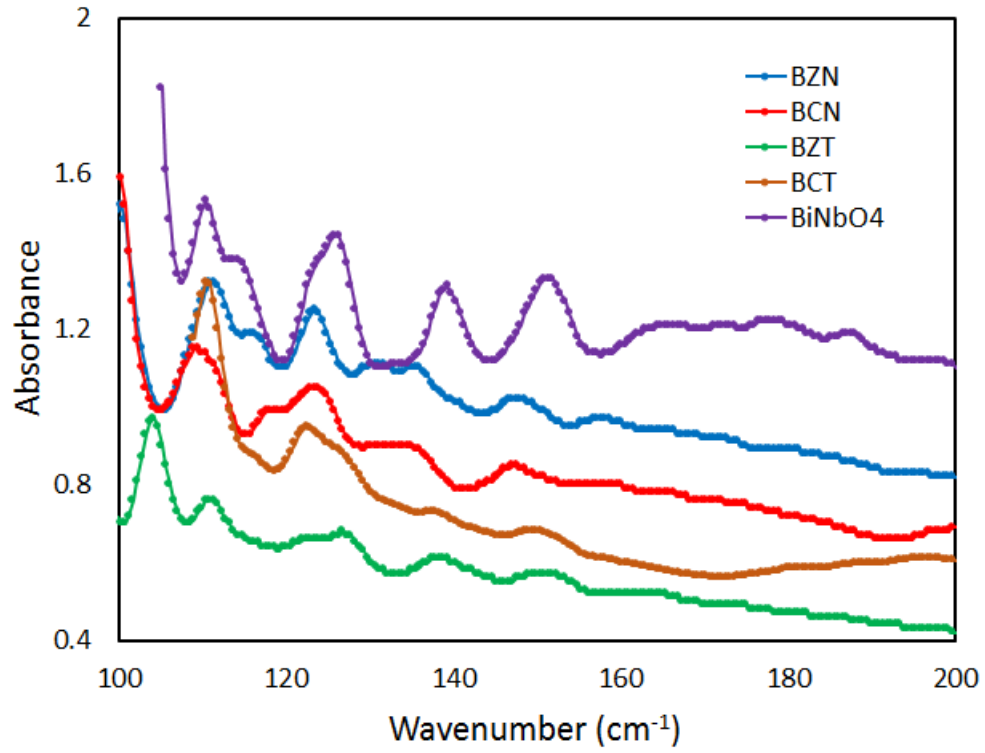


Fig. S1 FTIR (ATR) spectra of BZN, BZT, BCN and BCT samples. The spectra of orthorhombic BiNbO₄ is also shown for comparison.