

AM-89-423

Stacking variations and nonstoichiometry in the bixbyite-braunite polysomatic mineral group

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For deposit: List of postulated cation coordinates

American Mineralogist, 74, 11-12, 1325-1336.

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Bixbyte

No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z
1	O	.61970	.67150	.60240	21	O	.88740	.83610	.90160	41	O	.11970	.17150	.10240	61	O	.38740	.33610	.40160
2	O	.88030	.17150	.60240	22	O	.61260	.33610	.90160	42	O	.38030	.67150	.10240	62	O	.11260	.83610	.40160
3	O	.38030	.82850	.60240	23	O	.11260	.66390	.90160	43	O	.88030	.32850	.10240	63	O	.61260	.16390	.40160
4	O	.11970	.32850	.60240	24	O	.38740	.16390	.90160	44	O	.61970	.82850	.10240	64	O	.88740	.66390	.40160
5	O	.83140	.90100	.62440	25	Mn	.53120	.50060	.75160	45	O	.33140	.40100	.12440	65	Mn	.03120	.00060	.25160
6	O	.66860	.40100	.62440	26	Mn	.96880	.00060	.75160	46	O	.16860	.90100	.12440	66	Mn	.46880	.50060	.25160
7	O	.16860	.59900	.62440	27	Mn	.46880	.99940	.75160	47	O	.66860	.09900	.12440	67	Mn	.96880	.49940	.25160
8	O	.33140	.09900	.62440	28	Mn	.03120	.49940	.75160	48	O	.83140	.59900	.12440	68	Mn	.53120	.99940	.25160
9	O	.89820	.62270	.66480	29	Mn	.74560	.75960	.74920	49	O	.39820	.12270	.16480	69	Mn	.24560	.25960	.24920
10	O	.60160	.12270	.66480	30	Mn	.24560	.24040	.74920	50	O	.10180	.62270	.16480	70	Mn	.74560	.74040	.24920
11	O	.10180	.87730	.66480	31	Mn	.75440	.25960	.74920	51	O	.60180	.37730	.16480	71	Mn	.25440	.75960	.24920
12	O	.39820	.37730	.66480	32	Mn	.25440	.74040	.74920	52	O	.89820	.87730	.16480	72	Mn	.75440	.24040	.24920
13	O	.61780	.90710	.85160	33	Mn	.00000	.25000	.43920	53	O	.11780	.40710	.35160	73	Mn	.00000	.25000	.93920
14	O	.88220	.40710	.85160	34	Mn	.50000	.75000	.43920	54	O	.38220	.90710	.35160	74	Mn	.50000	.75000	.93920
15	O	.38220	.59290	.85160	35	Mn	.00000	.75000	.56360	55	O	.88220	.09290	.35160	75	Mn	.00000	.75000	.06360
16	O	.11780	.09290	.85160	36	Mn	.50000	.25000	.56360	56	O	.61780	.59290	.35160	76	Mn	.50000	.25000	.06360
17	O	.67010	.61210	.86360	37	Mn	.25360	.44335	.50140	57	O	.17010	.11210	.36360	77	Mn	.24640	.55665	.00140
18	O	.82990	.11210	.86360	38	Mn	.24640	.94335	.50140	58	O	.32990	.61210	.36360	78	Mn	.25360	.05665	.00140
19	O	.32990	.88790	.86360	39	Mn	.74640	.05665	.50140	59	O	.82990	.38790	.36360	79	Mn	.75360	.94335	.00140
20	O	.17010	.38790	.86360	40	Mn	.75360	.55665	.50140	60	O	.67010	.88790	.36360	80	Mn	.74640	.44335	.00140

Braunite

No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z
1	O	.42150	.36970	.30120	41	O	.61970	.67150	.55120	81	O	.92150	.86970	.80120	121	O	.11970	.17150	.05120
2	O	.92150	.63030	.30120	42	O	.88030	.17150	.55120	82	O	.42150	.13030	.80120	122	O	.38030	.67150	.05120
3	O	.57850	.13030	.30120	43	O	.38030	.82850	.55120	83	O	.07850	.63030	.80120	123	O	.88030	.32850	.05120
4	O	.07850	.86970	.30120	44	O	.11970	.32850	.55120	84	O	.57850	.36970	.80120	124	O	.61970	.82850	.05120
5	O	.65100	.58140	.31220	45	O	.83140	.90100	.56220	85	O	.15100	.08140	.81220	125	O	.33140	.40100	.06220
6	O	.15100	.41860	.31220	46	O	.66860	.40100	.56220	86	O	.65100	.91860	.81220	126	O	.16860	.90100	.06220
7	O	.34900	.91860	.31220	47	O	.16860	.59900	.56220	87	O	.84900	.41860	.81220	127	O	.66860	.09900	.06220
8	O	.84900	.08140	.31220	48	O	.33140	.09900	.56220	88	O	.34900	.58140	.81220	128	O	.83140	.59900	.06220
9	O	.37270	.64820	.33240	49	O	.89820	.62270	.58240	89	O	.87270	.14820	.83240	129	O	.39820	.12270	.08240
10	O	.87270	.35180	.33240	50	O	.60180	.12270	.58240	90	O	.37270	.85180	.83240	130	O	.10180	.62270	.08240
11	O	.62730	.85180	.33240	51	O	.10180	.87730	.58240	91	O	.12730	.35180	.83240	131	O	.60180	.37730	.08240
12	O	.12730	.14820	.33240	52	O	.39820	.37730	.58240	92	O	.62730	.64820	.83240	132	O	.89820	.87730	.08240
13	O	.65710	.36780	.42580	53	O	.61780	.90710	.67580	93	O	.15710	.86780	.92580	133	O	.11780	.40710	.17580
14	O	.15710	.63220	.42580	54	O	.88220	.40710	.67580	94	O	.85710	.13220	.92580	134	O	.38220	.90710	.17580
15	O	.34290	.13220	.42580	55	O	.38220	.59290	.67580	95	O	.84290	.63220	.92580	135	O	.88220	.09290	.17580
16	O	.84290	.86780	.42580	56	O	.11780	.09290	.67580	96	O	.34290	.36780	.92580	136	O	.61780	.59290	.17580
17	O	.36210	.42010	.43180	57	O	.87010	.81210	.68180	97	O	.86210	.92010	.93180	137	O	.17010	.11210	.18180
18	O	.86210	.57990	.43180	58	O	.82990	.11210	.68180	98	O	.36210	.07990	.93180	138	O	.32990	.61210	.18180
19	O	.63790	.07990	.43180	59	O	.32990	.88790	.68180	99	O	.13790	.57990	.93180	139	O	.82990	.38790	.18180
20	O	.13790	.92010	.43180	60	O	.17010	.38790	.68180	100	O	.63790	.42010	.93180	140	O	.67010	.88790	.18180
21	O	.58610	.63740	.45080	61	O	.88740	.83610	.70080	101	O	.08610	.13740	.95080	141	O	.38740	.33610	.20080
22	O	.08610	.36260	.45080	62	O	.61260	.33610	.70080	102	O	.58610	.86260	.95080	142	O	.11260	.83610	.20080
23	O	.41390	.86260	.45080	63	O	.11260	.66390	.70080	103	O	.91390	.36260	.95080	143	O	.81260	.16390	.20080
24	O	.91390	.13740	.45080	64	O	.38740	.16390	.70080	104	O	.41390	.63740	.95080	144	O	.88740	.66390	.20080
25	Mn	.25060	.28120	.37580	65	Mn	.53120	.50060	.62580	105	Mn	.75060	.78120	.87580	145	Mn	.03120	.00060	.12580
26	Mn	.75060	.71880	.37580	66	Mn	.96880	.00060	.62580	106	Mn	.25060	.21880	.87580	146	Mn	.46880	.50060	.12580
27	Mn	.74940	.21880	.37580	67	Mn	.46880	.99940	.62580	107	Mn	.24940	.71880	.87580	147	Mn	.96880	.49940	.12580
28	Mn	.24940	.78120	.37580	68	Mn	.03120	.49940	.62580	108	Mn	.74940	.28120	.87580	148	Mn	.53120	.99940	.12580
29	Mn	.50960	.49560	.37460	69	Mn	.74560	.75960	.62460	109	Mn	.00960	.99560	.87460	149	Mn	.24560	.25960	.12460
30	Mn	.99040	.99560	.37460	70	Mn	.24560	.24040	.62460	110	Mn	.49040	.49560	.87460	150	Mn	.74560	.74040	.12460
31	Mn	.00960	.50440	.37460	71	Mn	.75440	.25960	.62460	111	Mn	.50960	.00440	.87460	151	Mn	.25440	.75960	.12460
32	Mn	.49040	.00440	.37460	72	Mn	.25440	.74040	.62460	112	Mn	.99040	.50440	.87460	152	Mn	.75440	.24040	.12460
33	Ca	.00000	.25000	.25055	73	Si	.00000	.25000	.50100	113	Ca	.00000	.25000	.75055	153	Si	.00000	.25000	.00100
34	Ca	.50000	.75000	.25055	74	Si	.50000	.75000	.50100	114	Ca	.50000	.75000	.75055	154	Si	.50000	.75000	.00100
35	Si	.00000	.75000	.25100	75	Ca	.00000	.75000	.50055	115	Si	.00000	.75000	.75100	155	Ca	.00000	.75000	.00055
36	Si	.50000	.25000	.25100	76	Ca	.50000	.25000	.50055	116	Si	.50000	.25000	.75100	156	Ca	.50000	.25000	.00055
37	Mn	.29672	.46530	.25070	77	Mn	.21530	.45328	.50070	117	Mn	.20328	.53470	.75070	157	Mn	.28470	.54672	.00070
38	Mn	.20328	.96530	.25070	78	Mn	.28470	.95328	.50070	118	Mn	.29672	.03470	.75070	158	Mn	.21530	.04672	.00070
39	Mn	.70328	.03470	.25070	79	Mn	.78470	.04672	.50070	119	Mn	.79672	.96530	.75070	159	Mn	.71530	.95328	.00070
40	Mn	.79672	.53470	.25070	80	Mn	.71530	.54672	.50070	120	Mn	.70328	.46530	.75070	160	Mn	.78470	.45328	.00070

Polysome B A' B

No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z
1	O	.42150	.36970	.40160	31	Mn	.00960	.50440	.49947	61	O	.91390	.86260	.73227	91	O	.80180	.37730	.10987
2	O	.92150	.63030	.40160	32	Mn	.49040	.00440	.49947	62	O	.41390	.13740	.73227	92	O	.89820	.87730	.10987
3	O	.57850	.13030	.40160	33	Ca	.00000	.25000	.33407	63	O	.08610	.63740	.73227	93	O	.11780	.40710	.23440
4	O	.07850	.86970	.40160	34	Ca	.50000	.75000	.33407	64	O	.58610	.36260	.73227	94	O	.38220	.90710	.23440
5	O	.65100	.58140	.41627	35	Si	.00000	.75000	.33467	65	Mn	.24940	.21880	.83227	95	O	.88220	.09290	.23440
6	O	.15100	.41860	.41627	36	Si	.50000	.25000	.33467	66	Mn	.74940	.78120	.83227	96	O	.61780	.59290	.23440
7	O	.34900	.91860	.41627	37	Mn	.29672	.46530	.33427	67	Mn	.75060	.28120	.83227	97	O	.17010	.11210	.24240
8	O	.84900	.08140	.41627	38	Mn	.20328	.96530	.33427	68	Mn	.25060	.71880	.83227	98	O	.32990	.61210	.24240
9	O	.37270	.64820	.44320	39	Mn	.70328	.03470	.33427	69	Mn	.99040	.00440	.83387	99	O	.82990	.38790	.24240
10	O	.87270	.35180	.44320	40	Mn	.79672	.53470	.33427	70	Mn	.50960	.50440	.83387	100	O	.67010	.88790	.24240
11	O	.62730	.85180	.44320	41	O	.07850	.13030	.93173	71	Mn	.49040	.99560	.83387	101	O	.38740	.33610	.26773
12	O	.12730	.14820	.44320	42	O	.57850	.86970	.93173	72	Mn	.00960	.49560	.83387	102	O	.11260	.83610	.26773
13	O	.65710	.36780	.56773	43	O	.92150	.36970	.93173	73	Mn	.00000	.25000	.70809	103	O	.61260	.16390	.26773
14	O	.15710	.63220	.56773	44	O	.42150	.63030	.93173	74	Mn	.50000	.75000	.70809	104	O	.88740	.86390	.26773
15	O	.34290	.13220	.56773	45	O	.84900	.91860	.91707	75	Mn	.00000	.75000	.62524	105	Mn	.03120	.00060	.16773
16	O	.84290	.86780	.56773	46	O	.34900	.08140	.91707	76	Mn	.50000	.25000	.62524	106	Mn	.46880	.50060	.16773
17	O	.36210	.42010	.57573	47	O	.15100	.58140	.91707	77	Mn	.20177	.50000	.66667	107	Mn	.96880	.49940	.16773
18	O	.86210	.57990	.57573	48	O	.65100	.41860	.91707	78	Mn	.29823	.00000	.66667	108	Mn	.53120	.99940	.16773
19	O	.63790	.07990	.57573	49	O	.12730	.85180	.89013	79	Mn	.79823	.00000	.66667	109	Mn	.24560	.25960	.16613
20	O	.13790	.92010	.57573	50	O	.62730	.14820	.89013	80	Mn	.70177	.50000	.66667	110	Mn	.74560	.74040	.16613
21	O	.58610	.63740	.60107	51	O	.87270	.64820	.89013	81	O	.11970	.17150	.06827	111	Mn	.25440	.75960	.16613
22	O	.08610	.36260	.60107	52	O	.37270	.35180	.89013	82	O	.38030	.67150	.06827	112	Mn	.75440	.24040	.16613
23	O	.41390	.86260	.60107	53	O	.84290	.13220	.76560	83	O	.88030	.32850	.06827	113	Si	.00000	.25000	.00000
24	O	.91390	.13740	.60107	54	O	.34290	.86780	.76560	84	O	.61970	.82850	.06827	114	Si	.50000	.75000	.00000
25	Mn	.25060	.28120	.50107	55	O	.15710	.36780	.76560	85	O	.33140	.40100	.08293	115	Ca	.00000	.75000	.00000
26	Mn	.75060	.71880	.50107	56	O	.65710	.63220	.76560	86	O	.16860	.90100	.08293	116	Ca	.50000	.25000	.00000
27	Mn	.74940	.21880	.50107	57	O	.13790	.07990	.75760	87	O	.66860	.09900	.08293	117	Mn	.29312	.54312	.00000
28	Mn	.24940	.78120	.50107	58	O	.63790	.92010	.75760	88	O	.83140	.59900	.08293	118	Mn	.20688	.04312	.00000
29	Mn	.50960	.49560	.48947	59	O	.86210	.42010	.75760	89	O	.39820	.12270	.10987	119	Mn	.70688	.95688	.00000
30	Mn	.99040	.99560	.48947	60	O	.36210	.57990	.75760	90	O	.10180	.62270	.10987	120	Mn	.79312	.45688	.00000

Polysome B A' B A' A'

No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z	No	Atom	x	y	z
1	O	.42150	.36970	.24096	51	O	.87270	.64820	.53408	101	O	.38740	.33610	.76064	151	Mn	.74560	.24040	.90032
2	O	.92150	.63030	.24096	52	O	.37270	.35180	.53408	102	O	.11260	.83610	.76064	152	Mn	.24560	.75960	.90032
3	O	.57850	.13030	.24096	53	O	.84290	.13220	.45936	103	O	.61260	.16390	.76064	153	Mn	.00000	.25000	.77515
4	O	.07850	.86970	.24096	54	O	.34290	.86780	.45936	104	O	.88740	.66390	.76064	154	Mn	.50000	.75000	.77515
5	O	.65100	.58140	.24976	55	O	.15710	.36780	.45936	105	Mn	.03120	.00060	.70064	155	Mn	.00000	.75000	.82485
6	O	.15100	.41860	.24976	56	O	.85710	.63220	.45936	106	Mn	.46880	.50060	.70064	156	Mn	.50000	.25000	.82485
7	O	.34900	.91860	.24976	57	O	.13790	.07990	.45456	107	Mn	.96880	.49940	.70064	157	Mn	.25000	.45177	.80000
8	O	.84900	.08140	.24976	58	O	.83790	.92010	.45456	108	Mn	.53120	.99940	.70064	158	Mn	.25000	.95177	.80000
9	O	.37270	.64820	.26592	59	O	.86210	.42010	.45456	109	Mn	.24560	.25960	.69968	159	Mn	.75000	.04823	.80000
10	O	.87270	.35180	.26592	60	O	.36210	.57990	.45456	110	Mn	.74560	.74040	.69968	160	Mn	.75000	.54823	.80000
11	O	.62730	.85180	.26592	61	O	.91390	.86260	.43936	111	Mn	.25440	.75960	.69968	161	O	.92150	.86970	.04096
12	O	.12730	.14820	.26592	62	O	.41390	.13740	.43936	112	Mn	.75440	.24040	.69968	162	O	.42150	.13030	.04096
13	O	.65710	.36780	.34064	63	O	.08610	.63740	.43936	113	Si	.00000	.25000	.60000	163	O	.07850	.63030	.04096
14	O	.15710	.63220	.34064	64	O	.58610	.36260	.43936	114	Si	.50000	.75000	.60000	164	O	.57850	.36970	.04096
15	O	.34290	.13220	.34064	65	Mn	.24940	.21880	.49936	115	Ca	.00000	.75000	.60000	165	O	.15100	.08140	.04976
16	O	.84290	.86780	.34064	66	Mn	.74940	.78120	.49936	116	Ca	.50000	.25000	.60000	166	O	.65100	.91860	.04976
17	O	.36210	.42010	.34544	67	Mn	.75060	.28120	.49936	117	Mn	.29312	.54312	.60000	167	O	.84900	.41860	.04976
18	O	.86210	.57990	.34544	68	Mn	.25060	.71880	.49936	118	Mn	.20688	.04312	.60000	168	O	.34900	.58140	.04976
19	O	.63790	.07990	.34544	69	Mn	.99040	.00440	.50032	119	Mn	.70688	.95688	.60000	169	O	.87270	.14820	.06592
20	O	.13790	.92010	.34544	70	Mn	.50960	.50440	.50032	120	Mn	.79312	.45688	.60000	170	O	.37270	.85180	.06592
21	O	.58610	.63740	.36064	71	Mn	.49040	.99560	.50032	121	O	.88030	.82850	.95904	171	O	.12730	.35180	.06592
22	O	.08610	.36260	.36064	72	Mn	.00960	.49560	.50032	122	O	.61970	.32850	.95904	172	O	.62730	.64820	.06592
23	O	.41390	.86260	.36064	73	Mn	.00000	.25000	.42485	123	O	.11970	.67150	.95904	173	O	.15710	.86780	.14064
24	O	.91390	.13740	.36064	74	Mn	.50000	.75000	.42485	124	O	.38030	.17150	.95904	174	O	.65710	.13220	.14064
25	Mn	.25060	.28120	.30064	75	Mn	.00000	.75000	.37515	125	O	.66880	.59900	.95024	175	O	.84290	.63220	.14064
26	Mn	.75060	.71880	.30064	76	Mn	.50000	.25000	.37515	126	O	.83140	.09900	.95024	176	O	.34290	.36780	.14064
27	Mn	.74940	.21880	.30064	77	Mn	.20177	.50000	.40000	127	O	.33140	.90100	.95024	177	O	.86210	.92010	.14544
28	Mn	.24940	.78120	.30064	78	Mn	.29823	.00000	.40000	128	O	.16860	.40100	.95024	178	O	.36210	.07990	.14544
29	Mn	.50960	.49560	.29968	79	Mn	.79823	.00000	.40000	129	O	.60180	.87730	.93408	179	O	.13790	.57990	.14544
30	Mn	.99040	.99560	.29968	80	Mn	.70177	.50000	.40000	130	O	.89820	.37730	.93408	180	O	.63790	.42010	.14544
31	Mn	.00960	.50440	.29968	81	O	.11970	.17150	.64096	131	O	.39820	.62270	.93408	181	O	.08610	.13740	.16064
32	Mn	.49040	.00440	.29968	82	O	.38030	.67150	.64096	132	O	.10180	.12270	.93408	182	O	.58610	.86260	.16064
33	Ca	.00000	.25000	.20044	83	O	.88030	.32850	.64096	133	O	.88220	.59290	.85936	183	O	.91390	.36260	.16064
34	Ca	.50000	.75000	.20044	84	O	.61970	.82850	.64096	134	O	.61780	.09290	.85936	184	O	.41390	.63740	.16064
35	Si	.00000	.75000	.20080	85	O	.33140	.40100	.64976	135	O	.11780	.90710	.85936	185	Mn	.75060	.78120	.10064
36	Si	.50000	.25000	.20080	86	O	.16860	.90100	.64976	136	O	.38220	.40710	.85936	186	Mn	.25060	.21880	.10064
37	Mn	.29672	.46530	.20056	87	O	.66860	.09900	.64976	137	O	.82990	.88790	.85456	187	Mn	.24940	.71880	.10064
38	Mn	.20328	.96530	.20056	88	O	.83140	.59900	.64976	138	O	.67010	.38790	.85456	188	Mn	.74940	.28120	.10064
39	Mn	.70328	.03470	.20056	89	O	.39820	.12270	.66592	139	O	.17010	.61210	.85456	189	Mn	.00960	.99560	.09968
40	Mn	.79672	.53470	.20056	90	O	.10180	.62270	.66592	140	O	.32990	.11210	.85456	190	Mn	.49040	.49560	.09968
41	O	.07850	.13030	.55904	91	O	.60180	.37730	.66592	141	O	.61260	.66390	.83936	191	Mn	.50960	.00440	.09968
42	O	.57850	.86970	.55904	92	O	.89820	.87730	.66592	142	O	.88740	.16390	.83936	192	Mn	.99040	.50440	.09968
43	O	.92150	.36970	.55904	93	O	.11780	.40710	.74064	143	O	.38740	.83610	.83936	193	Ca	.00000	.25000	.00000
44	O	.42150	.63030	.55904	94	O	.38220	.90710	.74064	144	O	.11260	.33610	.83936	194	Ca	.50000	.75000	.00000
45	O	.84900	.91860	.55024	95	O	.88220	.09290	.74064	145	Mn	.96880	.49940	.89936	195	Si	.00000	.75000	.00000
46	O	.34900	.08140	.55024	96	O	.61780	.59290	.74064	146	Mn	.53120	.49940	.89936	196	Si	.50000	.25000	.00000
47	O	.15100	.58140	.55024	97	O	.17010	.11210	.74544	147	Mn	.03120	.50060	.89936	197	Mn	.20688	.54312	.00000
48	O	.65100	.41860	.55024	98	O	.32990	.61210	.74544	148	Mn	.46880	.00060	.89936	198	Mn	.29312	.04312	.00000
49	O	.12730	.85180	.53408	99	O	.82990	.38790	.74544	149	Mn	.75440	.74040	.90032	199	Mn	.79312	.95688	.00000
50	O	.62730	.14820	.53408	100	O	.67010	.88790	.74544	150	Mn	.25440	.25960	.90032	200	Mn	.70688	.45688	.00000

