AM-89-423

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

Johan P. de Villiers, Peter R. Buseck

For deposit: List of postulated cation coordinates

American Mineralogist, 74, 11-12, 1325-1336. pp. 1-6

Bixbyite

No	Atom	x	y	z
1	O	.61970	.67150	.60240
2	O	.88030	.17150	.60240
3	O	.38030	.82850	.60240
4	O	.11970	.32850	.60240
5	O	.83140	.90100	.62440
6	O	.66860	.40100	.62440
7	O	.16860	.59900	.62440
8	O	.33140	.09900	.62440
9	O	.89820	.62270	.66480
10	O	.60180	.12270	.66480
11	O	.10180	.87730	.66480
12	O	.39820	.37730	.66480
13	O	.61780	.90710	.85160
14	O	.88220	.40710	.85160
15	O	.38220	.59290	.85160
16	O	.11780	.09290	.85160
17	O	.67010	.61210	.86360
18	O	.82990	.11210	.86360
19	O	.32990	.88790	.86360
20	O	.17010	.38790	.86360
21	O	.88740	.83610	.90160
22	O	.61260	.33610	.90160
23	O	.11260	.66390	.90160
24	O	.38740	.16390	.90160
25	Mn	.53120	.50060	.75160
26	Mn	.96880	.00060	.75160
27	Mn	.46880	.99940	.75160
28	Mn	.03120	.49940	.75160
29	Mn	.74560	.75960	.74920
30	Mn	.24560	.24040	.74920
31	Mn	.75440	.25960	.74920
32	Mn	.25440	.74040	.74920
33	Mn	.00000	.25000	.43920
34	Mn	.50000	.75000	.43920
35	Mn	.00000	.75000	.56360
36	Mn	.50000	.25000	.56360
37	Mn	.25360	.44335	.50140
38	Mn	.24640	.94335	.50140
39	Mn	.74640	.05665	.50140
40	Mn	.75360	.55665	.50140
41	O	.11970	.17150	.10240
42	O	.38030	.67150	.10240
43	O	.88030	.32850	.10240
44	O	.61970	.82850	.10240
45	O	.33140	.40100	.12440
46	O	.16860	.90100	.12440
47	O	.66860	.09900	.12440
48	O	.83140	.59900	.12440
49	O	.39820	.12270	.16480
50	O	.10180	.62270	.16480
51	O	.60180	.37730	.16480
52	O	.89820	.87730	.16480
53	O	.11780	.40710	.35160
54	O	.38220	.90710	.35160
55	O	.88220	.09290	.35160
56	O	.61780	.59290	.35160
57	O	.17010	.11210	.36360
58	O	.32990	.61210	.36360
59	O	.82990	.38790	.36360
60	O	.67010	.88790	.36360
61	O	.38740	.33610	.40160
62	O	.11260	.83610	.40160
63	O	.61260	.16390	.40160
64	O	.88740	.66390	.40160
65	Mn	.03120	.00060	.25160
66	Mn	.46880	.50060	.25160
67	Mn	.96880	.49940	.25160
68	Mn	.53120	.99940	.25160
69	Mn	.24560	.25960	.24920
70	Mn	.74560	.74040	.24920
71	Mn	.25440	.75960	.24920
72	Mn	.75440	.24040	.24920
73	Mn	.00000	.25000	.93920
74	Mn	.50000	.75000	.93920
75	Mn	.00000	.75000	.06360
76	Mn	.50000	.25000	.06360
77	Mn	.24640	.55665	.00140
78	Mn	.25360	.05665	.00140
79	Mn	.75360	.94335	.00140
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	.65710	.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	.67010	.61210	.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	.61260	.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

Braunite II

No	Atom	x	y	z
1	O	.07850	.13030	.22440
2	O	.57850	.86970	.22440
3	O	.92150	.36970	.22440
4	O	.42150	.63030	.22440
5	O	.84900	.91860	.21890
6	O	.34900	.08140	.21890
7	O	.15100	.58140	.21890
8	O	.65100	.41860	.21890
9	O	.12730	.85180	.20880
10	O	.62730	.14820	.20880
11	O	.87270	.64820	.20880
12	O	.37270	.35180	.20880
13	O	.84290	.13220	.16210
14	O	.34290	.86780	.16210
15	O	.15710	.36780	.16210
16	O	.65710	.63220	.16210
17	O	.13790	.07990	.15910
18	O	.63790	.92010	.15910
19	O	.86210	.42010	.15910
20	O	.36210	.57990	.15910
21	O	.91390	.86260	.14960
22	O	.41390	.13740	.14960
23	O	.08610	.63740	.14960
24	O	.58610	.36260	.14960
25	Mn	.24940	.21880	.18710
26	Mn	.74940	.78120	.18710
27	Mn	.75060	.28120	.18710
28	Mn	.25060	.71880	.18710
29	Mn	.99040	.00440	.18770
30	Mn	.50960	.50440	.18770
31	Mn	.49040	.99560	.18770
32	Mn	.00960	.49560	.18770
33	Ca	.00000	.25000	.12500
34	Ca	.50000	.75000	.12500
35	Si	.00000	.75000	.12500
36	Si	.50000	.25000	.12500
37	Mn	.24007	.49007	.12500
38	Mn	.25993	.99007	.12500
39	Mn	.75993	.00993	.12500
40	Mn	.74007	.50993	.12500
41	O	.42150	.36970	.27560
42	O	.92150	.63030	.27560
43	O	.57850	.13030	.27560
44	O	.07850	.86970	.27560
45	O	.65100	.58140	.28110
46	O	.15100	.41860	.28110
47	O	.34900	.91860	.28110
48	O	.84900	.08140	.28110
49	O	.37270	.64820	.29120
50	O	.87270	.35180	.29120
51	O	.62730	.85180	.29120
52	O	.12730	.14820	.29120
53	O	.65710	.36780	.33790
54	O	.15710	.63220	.33790
55	O	.34290	.13220	.33790
56	O	.84290	.86780	.33790
57	O	.36210	.42010	.34090
58	O	.86210	.57990	.34090
59	O	.63790	.07990	.34090
60	O	.13790	.92010	.34090
61	O	.58610	.63740	.35040
62	O	.08610	.36260	.35040
63	O	.41390	.86260	.35040
64	O	.91390	.13740	.35040
65	Mn	.25060	.28120	.31290
66	Mn	.75060	.71880	.31290
67	Mn	.74940	.21880	.31290
68	Mn	.24940	.78120	.31290
69	Mn	.50960	.49560	.31230
70	Mn	.99040	.99560	.31230
71	Mn	.00960	.50440	.31230
72	Mn	.49040	.00440	.31230
73	Mn	.00000	.25000	.26557
74	Mn	.50000	.75000	.26557
75	Mn	.00000	.75000	.23443
76	Mn	.50000	.25000	.23443
77	Mn	.31507	.50000	.25000
78	Mn	.18493	.00000	.25000
79	Mn	.68493	.00000	.25000
80	Mn	.81507	.50000	.25000
81	O	.38030	.32850	.47440
82	O	.11970	.82850	.47440
83	O	.61970	.17150	.47440
84	O	.88030	.67150	.47440
85	O	.16860	.09900	.46890
86	O	.33140	.59900	.46890
87	O	.83140	.40100	.46890
88	O	.66860	.90100	.46890
89	O	.10180	.37730	.45880
90	O	.39820	.87730	.45880
91	O	.89820	.12270	.45880
92	O	.60180	.62270	.45880
93	O	.38220	.09290	.41210
94	O	.11780	.59290	.41210
95	O	.61780	.40710	.41210
96	O	.88220	.90710	.41210
97	O	.32990	.38790	.40910
98	O	.17010	.88790	.40910
99	O	.67010	.11210	.40910
100	O	.82990	.61210	.40910
101	O	.11260	.16390	.39960
102	O	.38740	.66390	.39960
103	O	.88740	.33610	.39960
104	O	.61260	.83610	.39960
105	Mn	.46880	.49940	.43710
106	Mn	.03120	.99940	.43710
107	Mn	.53120	.00060	.43710
108	Mn	.96880	.50060	.43710
109	Mn	.25440	.24040	.43770
110	Mn	.75440	.75960	.43770
111	Mn	.24560	.74040	.43770
112	Mn	.74560	.25960	.43770
113	Si	.00000	.25000	.37500
114	Si	.50000	.75000	.37500
115	Ca	.00000	.75000	.37500
116	Ca	.50000	.25000	.37500
117	Mn	.24007	.50993	.37500
118	Mn	.25993	.00993	.37500
119	Mn	.75993	.99007	.37500
120	Mn	.74007	.49007	.37500
121	O	.61970	.67150	.52560
122	O	.88030	.17150	.52560
123	O	.38030	.82850	.52560
124	O	.11970	.32850	.52560
125	O	.83140	.90100	.53110
126	O	.66860	.40100	.53110
127	O	.16860	.59900	.53110
128	O	.33140	.09900	.53110
129	O	.89820	.62270	.54120
130	O	.60180	.12270	.54120
131	O	.10180	.87730	.54120
132	O	.39820	.37730	.54120
133	O	.61780	.90710	.58790
134	O	.88220	.40710	.58790
135	O	.38220	.59290	.58790
136	O	.11780	.09290	.58790
137	O	.67010	.61210	.59090
138	O	.82990	.11210	.59090
139	O	.32990	.88790	.59090
140	O	.17010	.38790	.59090
141	O	.88740	.83610	.60040
142	O	.61260	.33610	.60040
143	O	.11260	.66390	.60040
144	O	.38740	.16390	.60040
145	Mn	.53120	.50060	.56290
146	Mn	.96880	.00060	.56290
147	Mn	.46880	.99940	.56290
148	Mn	.03120	.49940	.56290
149	Mn	.74560	.75960	.56230
150	Mn	.24560	.24040	.56230
151	Mn	.75440	.25960	.56230
152	Mn	.25440	.74040	.56230
153	Mn	.00000	.25000	.48443
154	Mn	.50000	.75000	.48443
155	Mn	.00000	.75000	.51557
156	Mn	.50000	.25000	.51557
157	Mn	.25000	.43493	.50000
158	Mn	.25000	.93493	.50000
159	Mn	.75000	.06507	.50000
160	Mn	.75000	.56507	.50000
161	O	.57850	.63030	.72440
162	O	.07850	.36970	.72440
163	O	.42150	.86970	.72440
164	O	.92150	.13030	.72440
165	O	.34900	.41860	.71890
166	O	.84900	.58140	.71890
167	O	.65100	.08140	.71890
168	O	.15100	.91860	.71890
169	O	.62730	.35180	.70880
170	O	.12730	.64820	.70880
171	O	.37270	.14820	.70880
172	O	.87270	.85180	.70880
173	O	.34290	.63220	.66210
174	O	.84290	.36780	.66210
175	O	.65710	.86780	.66210
176	O	.15710	.13220	.66210
177	O	.63790	.57990	.65910
178	O	.13790	.42010	.65910
179	O	.36210	.92010	.65910
180	O	.86210	.07990	.65910
181	O	.41390	.36260	.64960
182	O	.91390	.63740	.64960
183	O	.58610	.13740	.64960
184	O	.08610	.86260	.64960
185	Mn	.74940	.71880	.68710
186	Mn	.24940	.28120	.68710
187	Mn	.25060	.78120	.68710
188	Mn	.75060	.21880	.68710
189	Mn	.49040	.50440	.68770
190	Mn	.00960	.00440	.68770
191	Mn	.99040	.49560	.68770
192	Mn	.50960	.99560	.68770
193	Ca	.00000	.25000	.62500
194	Ca	.50000	.75000	.62500
195	Si	.00000	.75000	.62500
196	Si	.50000	.25000	.62500
197	Mn	.25993	.50993	.62500
198	Mn	.24007	.00993	.62500
199	Mn	.74007	.99007	.62500
200	Mn	.75993	.49007	.62500
201	O	.92150	.86970	.77560
202	O	.42150	.13030	.77560
203	O	.07850	.63030	.77560
204	O	.57850	.36970	.77560
205	O	.15100	.08140	.78110
206	O	.65100	.91860	.78110
207	O	.84900	.41860	.78110
208	O	.34900	.58140	.78110
209	O	.87270	.14820	.79120
210	O	.37270	.85180	.79120
211	O	.12730	.35180	.79120
212	O	.62730	.64820	.79120
213	O	.15710	.86780	.83790
214	O	.65710	.13220	.83790
215	O	.84290	.63220	.83790
216	O	.34290	.36780	.83790
217	O	.86210	.92010	.84090
218	O	.36210	.07990	.84090
219	O	.13790	.57990	.84090
220	O	.63790	.42010	.84090
221	O	.08610	.13740	.85040
222	O	.58610	.86260	.85040
223	O	.91390	.36260	.85040
224	O	.41390	.63740	.85040
225	Mn	.75060	.78120	.81290
226	Mn	.25060	.21880	.81290
227	Mn	.24940	.71880	.81290
228	Mn	.74940	.28120	.81290
229	Mn	.00960	.99560	.81230
230	Mn	.49040	.49560	.81230
231	Mn	.50960	.00440	.81230
232	Mn	.99040	.50440	.81230
233	Mn	.00000	.25000	.76557
234	Mn	.50000	.75000	.76557
235	Mn	.00000	.75000	.73443
236	Mn	.50000	.25000	.73443
237	Mn	.18493	.50000	.75000
238	Mn	.31507	.00000	.75000
239	Mn	.81507	.00000	.75000
240	Mn	.68493	.50000	.75000
241	O	.88030	.82850	.97440
242	O	.61970	.32850	.97440
243	O	.11970	.67150	.97440
244	O	.38030	.17150	.97440
245	O	.66860	.59900	.96890
246	O	.83140	.09900	.96890
247	O	.33140	.90100	.96890
248	O	.16860	.40100	.96890
249	O	.60180	.87730	.95880
250	O	.89820	.37730	.95880
251	O	.39820	.62270	.95880
252	O	.10180	.12270	.95880
253	O	.88220	.59290	.91210
254	O	.61780	.09290	.91210
255	O	.11780	.90710	.91210
256	O	.38220	.40710	.91210
257	O	.82990	.88790	.90910
258	O	.67010	.38790	.90910
259	O	.17010	.61210	.90910
260	O	.32990	.11210	.90910
261	O	.61260	.66390	.89960
262	O	.88740	.16390	.89960
263	O	.38740	.83610	.89960
264	O	.11260	.33610	.89960
265	Mn	.96880	.99940	.93710
266	Mn	.53120	.49940	.93710
267	Mn	.03120	.50060	.93710
268	Mn	.46880	.00060	.93710
269	Mn	.75440	.74040	.93770
270	Mn	.25440	.25960	.93770
271	Mn	.74560	.24040	.93770
272	Mn	.24560	.75960	.93770
273	Si	.00000	.25000	.87500
274	Si	.50000	.75000	.87500
275	Ca	.00000	.75000	.87500
276	Ca	.50000	.25000	.87500
277	Mn	.25993	.49007	.87500
278	Mn	.24007	.99007	.87500
279	Mn	.74007	.00993	.87500
280	Mn	.75993	.50993	.87500
281	O	.11970	.17150	.02560
282	O	.38030	.67150	.02560
283	O	.88030	.32850	.02560
284	O	.61970	.82850	.02560
285	O	.33140	.40100	.03110
286	O	.16860	.90100	.03110
287	O	.66860	.09900	.03110
288	O	.83140	.59900	.03110
289	O	.39820	.12270	.04120
290	O	.10180	.62270	.04120
291	O	.60180	.37730	.04120
292	O	.89820	.87730	.04120
293	O	.11780	.40710	.08790
294	O	.38220	.90710	.08790
295	O	.88220	.09290	.08790
296	O	.61780	.59290	.08790
297	O	.17010	.11210	.09090
298	O	.32990	.61210	.09090
299	O	.82990	.38790	.09090
300	O	.67010	.88790	.09090
301	O	.38740	.33610	.10040
302	O	.11260	.83610	.10040
303	O	.61260	.16390	.10040
304	O	.88740	.66390	.10040
305	Mn	.03120	.00060	.06290
306	Mn	.46880	.50060	.06290
307	Mn	.96880	.49940	.06290
308	Mn	.53120	.99940	.06290
309	Mn	.24560	.25960	.06230
310	Mn	.74560	.74040	.06230
311	Mn	.25440	.75960	.06230
312	Mn	.75440	.24040	.06230
313	Mn	.00000	.25000	.98443
314	Mn	.50000	.75000	.98443
315	Mn	.00000	.75000	.01557
316	Mn	.50000	.25000	.01557
317	Mn	.25000	.56507	.00000
318	Mn	.25000	.06507	.00000
319	Mn	.75000	.93493	.00000
320	Mn	.75000	.43493	.00000

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	.60180	.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	.66390	.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	.49947	59	O	.86210	.42010	.75760	89	O	.39820	.12270	.10987	119	Mn	.70688	.95688	.00000
30	Mn	.99040	.99560	.49947	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	.65710	.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	.63790	.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	.66860	.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	.99940	.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

Polysome B A' B A' A' B A' B

No	Atom	x	y	z
1	O	.42150	.36970	.15060
2	O	.92150	.63030	.15060
3	O	.57850	.13030	.15060
4	O	.07850	.86970	.15060
5	O	.65100	.58140	.15610
6	O	.15100	.41860	.15610
7	O	.34900	.91860	.15610
8	O	.84900	.08140	.15610
9	O	.37270	.64820	.16620
10	O	.87270	.35180	.16620
11	O	.62730	.85180	.16620
12	O	.12730	.14820	.16620
13	O	.65710	.36780	.21290
14	O	.15710	.63220	.21290
15	O	.34290	.13220	.21290
16	O	.84290	.86780	.21290
17	O	.36210	.42010	.21590
18	O	.86210	.57990	.21590
19	O	.63790	.07990	.21590
20	O	.13790	.92010	.21590
21	O	.58610	.63740	.22540
22	O	.08610	.36260	.22540
23	O	.41390	.86260	.22540
24	O	.91390	.13740	.22540
25	Mn	.25060	.28120	.18790
26	Mn	.75060	.71880	.18790
27	Mn	.74940	.21880	.18790
28	Mn	.24940	.78120	.18790
29	Mn	.50960	.49560	.18730
30	Mn	.99040	.99560	.18730
31	Mn	.00960	.50440	.18730
32	Mn	.49040	.00440	.18730
33	Ca	.00000	.25000	.12528
34	Ca	.50000	.75000	.12528
35	Si	.00000	.75000	.12550
36	Si	.50000	.25000	.12550
37	Mn	.29672	.46530	.12535
38	Mn	.20328	.96530	.12535
39	Mn	.70328	.03470	.12535
40	Mn	.79672	.53470	.12535
41	O	.07850	.13030	.34940
42	O	.57850	.86970	.34940
43	O	.92150	.36970	.34940
44	O	.42150	.63030	.34940
45	O	.84900	.91860	.34390
46	O	.34900	.08140	.34390
47	O	.15100	.58140	.34390
48	O	.65100	.41860	.34390
49	O	.12730	.85180	.33380
50	O	.62730	.14820	.33380
51	O	.87270	.64820	.33380
52	O	.37270	.35180	.33380
53	O	.84290	.13220	.28710
54	O	.34290	.86780	.28710
55	O	.15710	.36780	.28710
56	O	.65710	.63220	.28710
57	O	.13790	.07990	.28410
58	O	.63790	.92010	.28410
59	O	.86210	.42010	.28410
60	O	.36210	.57990	.28410
61	O	.91390	.86260	.27460
62	O	.41390	.13740	.27460
63	O	.08610	.63740	.27460
64	O	.58610	.36260	.27460
65	Mn	.24940	.21880	.31210
66	Mn	.74940	.78120	.31210
67	Mn	.75060	.28120	.31210
68	Mn	.25060	.71880	.31210
69	Mn	.99040	.00440	.31270
70	Mn	.50960	.50440	.31270
71	Mn	.49040	.99560	.31270
72	Mn	.00960	.49560	.31270
73	Mn	.00000	.25000	.26553
74	Mn	.50000	.75000	.26553
75	Mn	.00000	.75000	.23447
76	Mn	.50000	.25000	.23447
77	Mn	.20177	.50000	.25000
78	Mn	.29823	.00000	.25000
79	Mn	.79823	.00000	.25000
80	Mn	.70177	.50000	.25000
81	O	.11970	.17150	.40060
82	O	.38030	.67150	.40060
83	O	.88030	.32850	.40060
84	O	.61970	.82850	.40060
85	O	.33140	.40100	.40610
86	O	.16860	.90100	.40610
87	O	.66860	.09900	.40610
88	O	.83140	.59900	.40610
89	O	.39820	.12270	.41620
90	O	.10180	.62270	.41620
91	O	.60180	.37730	.41620
92	O	.89820	.87730	.41620
93	O	.11780	.40710	.46290
94	O	.38220	.90710	.46290
95	O	.88220	.09290	.46290
96	O	.61780	.59290	.46290
97	O	.17010	.11210	.46590
98	O	.32990	.61210	.46590
99	O	.82990	.38790	.46590
100	O	.67010	.88790	.46590
101	O	.38740	.33610	.47540
102	O	.11260	.83610	.47540
103	O	.61260	.16390	.47540
104	O	.88740	.66390	.47540
105	Mn	.03120	.00060	.43790
106	Mn	.46880	.50060	.43790
107	Mn	.96880	.49940	.43790
108	Mn	.53120	.99940	.43790
109	Mn	.24560	.25960	.43730
110	Mn	.74560	.74040	.43730
111	Mn	.25440	.75960	.43730
112	Mn	.75440	.24040	.43730
113	Si	.00000	.25000	.37500
114	Si	.50000	.75000	.37500
115	Ca	.00000	.75000	.37500
116	Ca	.50000	.25000	.37500
117	Mn	.29312	.54312	.37500
118	Mn	.20688	.04312	.37500
119	Mn	.70688	.95688	.37500
120	Mn	.79312	.45688	.37500
121	O	.88030	.82850	.59940
122	O	.61970	.32850	.59940
123	O	.11970	.67150	.59940
124	O	.38030	.17150	.59940
125	O	.66860	.59900	.59390
126	O	.83140	.09900	.59390
127	O	.33140	.90100	.59390
128	O	.16860	.40100	.59390
129	O	.60180	.87730	.58380
130	O	.89820	.37730	.58380
131	O	.39820	.62270	.58380
132	O	.10180	.12270	.58380
133	O	.88220	.59290	.53710
134	O	.61780	.09290	.53710
135	O	.11780	.90710	.53710
136	O	.38220	.40710	.53710
137	O	.82990	.88790	.53410
138	O	.67010	.38790	.53410
139	O	.17010	.61210	.53410
140	O	.32990	.11210	.53410
141	O	.61260	.66390	.52460
142	O	.88740	.16390	.52460
143	O	.38740	.83610	.52460
144	O	.11260	.33610	.52460
145	Mn	.96880	.99940	.56210
146	Mn	.53120	.49940	.56210
147	Mn	.03120	.50060	.56210
148	Mn	.46880	.00060	.56210
149	Mn	.75440	.74040	.56270
150	Mn	.25440	.25960	.56270
151	Mn	.74560	.24040	.56270
152	Mn	.24560	.75960	.56270
153	Mn	.00000	.25000	.48447
154	Mn	.50000	.75000	.48447
155	Mn	.00000	.75000	.51553
156	Mn	.50000	.25000	.51553
157	Mn	.25000	.45177	.50000
158	Mn	.25000	.95177	.50000
159	Mn	.75000	.04823	.50000
160	Mn	.75000	.54823	.50000
161	O	.38030	.32850	.72440
162	O	.11970	.82850	.72440
163	O	.61970	.17150	.72440
164	O	.88030	.67150	.72440
165	O	.16860	.09900	.71890
166	O	.33140	.59900	.71890
167	O	.83140	.40100	.71890
168	O	.66860	.90100	.71890
169	O	.10180	.37730	.70880
170	O	.39820	.87730	.70880
171	O	.89820	.12270	.70880
172	O	.60180	.62270	.70880
173	O	.38220	.09290	.66210
174	O	.11780	.59290	.66210
175	O	.61780	.40710	.66210
176	O	.88220	.90710	.66210
177	O	.32990	.38790	.65910
178	O	.17010	.88790	.65910
179	O	.67010	.11210	.65910
180	O	.82990	.61210	.65910
181	O	.11260	.16390	.64960
182	O	.38740	.66390	.64960
183	O	.88740	.33610	.64960
184	O	.61260	.83610	.64960
185	Mn	.46880	.49940	.68710
186	Mn	.03120	.99940	.68710
187	Mn	.53120	.00060	.68710
188	Mn	.96880	.50060	.68710
189	Mn	.25440	.24040	.68770
190	Mn	.75440	.75960	.68770
191	Mn	.24560	.74040	.68770
192	Mn	.74560	.25960	.68770
193	Mn	.00000	.25000	.60910
194	Mn	.50000	.75000	.60910
195	Mn	.00000	.75000	.64020
196	Mn	.50000	.25000	.64020
197	Mn	.25360	.55665	.62465
198	Mn	.24640	.05665	.62465
199	Mn	.74640	.94335	.62465
200	Mn	.75360	.44335	.62465
201	O	.42150	.36970	.77560
202	O	.92150	.63030	.77560
203	O	.57850	.13030	.77560
204	O	.07850	.86970	.77560
205	O	.65100	.58140	.78110
206	O	.15100	.41860	.78110
207	O	.34900	.91860	.78110
208	O	.84900	.08140	.78110
209	O	.37270	.64820	.79120
210	O	.87270	.35180	.79120
211	O	.62730	.85180	.79120
212	O	.12730	.14820	.79120
213	O	.65710	.36780	.83790
214	O	.15710	.63220	.83790
215	O	.34290	.13220	.83790
216	O	.84290	.86780	.83790
217	O	.36210	.42010	.84090
218	O	.86210	.57990	.84090
219	O	.63790	.07990	.84090
220	O	.13790	.92010	.84090
221	O	.58610	.63740	.85040
222	O	.08610	.36260	.85040
223	O	.41390	.86260	.85040
224	O	.91390	.13740	.85040
225	Mn	.25060	.28120	.81290
226	Mn	.75060	.71880	.81290
227	Mn	.74940	.21880	.81290
228	Mn	.24940	.78120	.81290
229	Mn	.50960	.49560	.81230
230	Mn	.99040	.99560	.81230
231	Mn	.00960	.50440	.81230
232	Mn	.49040	.00440	.81230
233	Ca	.00000	.25000	.75000
234	Ca	.50000	.75000	.75000
235	Si	.00000	.75000	.75000
236	Si	.50000	.25000	.75000
237	Mn	.29312	.45688	.75000
238	Mn	.20688	.95688	.75000
239	Mn	.70688	.04312	.75000
240	Mn	.79312	.54312	.75000
241	O	.07850	.13030	.97440
242	O	.57850	.86970	.97440
243	O	.92150	.36970	.97440
244	O	.42150	.63030	.97440
245	O	.84900	.91860	.96890
246	O	.34900	.08140	.96890
247	O	.15100	.58140	.96890
248	O	.65100	.41860	.96890
249	O	.12730	.85180	.95880
250	O	.62730	.14820	.95880
251	O	.87270	.64820	.95880
252	O	.37270	.35180	.95880
253	O	.84290	.13220	.91210
254	O	.34290	.86780	.91210
255	O	.15710	.36780	.91210
256	O	.65710	.63220	.91210
257	O	.13790	.07990	.90910
258	O	.63790	.92010	.90910
259	O	.86210	.42010	.90910
260	O	.36210	.57990	.90910
261	O	.91390	.86260	.89960
262	O	.41390	.13740	.89960
263	O	.08610	.63740	.89960
264	O	.58610	.36260	.89960
265	Mn	.24940	.21880	.93710
266	Mn	.74940	.78120	.93710
267	Mn	.75060	.28120	.93710
268	Mn	.25060	.71880	.93710
269	Mn	.99040	.00440	.93770
270	Mn	.50960	.50440	.93770
271	Mn	.49040	.99560	.93770
272	Mn	.00960	.49560	.93770
273	Mn	.00000	.25000	.89053
274	Mn	.50000	.75000	.89053
275	Mn	.00000	.75000	.85947
276	Mn	.50000	.25000	.85947
277	Mn	.20177	.50000	.87500
278	Mn	.29823	.00000	.87500
279	Mn	.79823	.00000	.87500
280	Mn	.70177	.50000	.87500
281	O	.11970	.17150	.02560
282	O	.38030	.67150	.02560
283	O	.88030	.32850	.02560
284	O	.61970	.82850	.02560
285	O	.33140	.40100	.03110
286	O	.16860	.90100	.03110
287	O	.66860	.09900	.03110
288	O	.83140	.59900	.03110
289	O	.39820	.12270	.04120
290	O	.10180	.62270	.04120
291	O	.60180	.37730	.04120
292	O	.89820	.87730	.04120
293	O	.11780	.40710	.08790
294	O	.38220	.90710	.08790
295	O	.88220	.09290	.08790
296	O	.61780	.59290	.08790
297	O	.17010	.11210	.09090
298	O	.32990	.61210	.09090
299	O	.82990	.38790	.09090
300	O	.67010	.88790	.09090
301	O	.38740	.33610	.10040
302	O	.11260	.83610	.10040
303	O	.61260	.16390	.10040
304	O	.88740	.66390	.10040
305	Mn	.03120	.00060	.06290
306	Mn	.46880	.50060	.06290
307	Mn	.96880	.49940	.06290
308	Mn	.53120	.99940	.06290
309	Mn	.24560	.25960	.06230
310	Mn	.74560	.74040	.06230
311	Mn	.25440	.75960	.06230
312	Mn	.75440	.24040	.06230
313	Si	.00000	.25000	.00000
314	Si	.50000	.75000	.00000
315	Ca	.00000	.75000	.00000
316	Ca	.50000	.25000	.00000
317	Mn	.29312	.54312	.00000
318	Mn	.20688	.04312	.00000
319	Mn	.70688	.95688	.00000
320	Mn	.79312	.45688	.00000