

Reflex Summary Report for Rietveld Refinement of [C₆N₂H₁₈]BiI₅:

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.11869 ± 0.08427	Yes
b	14.26340 ± 0.07887	Yes
c	8.63905 ± 0.04962	Yes
α	90.00000 ± 0.00000	Yes
β	90.00000 ± 0.00000	Yes
γ	90.00000 ± 2824008413.66867	Yes

Errors are unusually large: This may be due to correlations between refined parameters.

Structure Parameters

Refined Motion Groups: 0
Refined Torsions: 0

Refined Angles: 0
Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	Bi1	0.38917	0.62103	0.50315	No
2	Bi2	0.61083	0.37897	0.00315	No
3	Bi3	0.88917	0.87897	0.50315	No
4	Bi4	0.11083	0.12103	0.00315	No
5	I1	0.48458	0.51909	0.21060	No
6	I2	0.51542	0.48091	0.71060	No
7	I3	0.98458	0.98091	0.21060	No
8	I4	0.01542	0.01909	0.71060	No
9	I5	0.25948	0.45560	0.50969	No
10	I6	0.74052	0.54440	0.00969	No
11	I7	0.75948	0.04440	0.50969	No
12	I8	0.24052	0.95560	0.00969	No
13	I9	0.29912	0.73228	0.26645	No
14	I10	0.70088	0.26772	0.76645	No
15	I11	0.79912	0.76772	0.26645	No
16	I12	0.20088	0.23228	0.76645	No
17	I13	0.30809	0.69835	0.78842	No
18	I14	0.69191	0.30165	0.28842	No
19	I15	0.80809	0.80165	0.78842	No

20	I16	0.19191	0.19835	0.28842	No
21	I17	0.54645	0.76181	0.52133	No
22	I18	0.45355	0.23819	0.02133	No
23	I19	0.04645	0.73819	0.52133	No
24	I20	0.95355	0.26181	0.02133	No
25	N1	0.45000	0.29950	0.42990	No
26	N2	0.55000	0.70050	0.92990	No
27	N3	0.95000	0.20050	0.42990	No
28	N4	0.05000	0.79950	0.92990	No
29	N5	0.19340	0.94140	0.42680	No
30	N6	0.80660	0.05860	0.92680	No
31	N7	0.69340	0.55860	0.42680	No
32	N8	0.30660	0.44140	0.92680	No
33	H1	0.43960	0.27810	0.33200	No
34	H2	0.56040	0.72190	0.83200	No
35	H3	0.93960	0.22190	0.33200	No
36	H4	0.06040	0.77810	0.83200	No
37	H5	0.50570	0.32420	0.43520	No
38	H6	0.49430	0.67580	0.93520	No
39	H7	0.00570	0.17580	0.43520	No
40	H8	0.99430	0.82420	0.93520	No
41	H9	0.40970	0.34510	0.45430	No
42	H10	0.59030	0.65490	0.95430	No
43	H11	0.90970	0.15490	0.45430	No
44	H12	0.09030	0.84510	0.95430	No
45	H13	0.22060	0.90500	0.35380	No
46	H14	0.77940	0.09500	0.85380	No
47	H15	0.72060	0.59500	0.35380	No
48	H16	0.27940	0.40500	0.85380	No
49	H17	0.17940	0.99870	0.38510	No
50	H18	0.82060	0.00130	0.88510	No
51	H19	0.67940	0.50130	0.38510	No
52	H20	0.32060	0.49870	0.88510	No
53	H21	0.14300	0.91200	0.45950	No
54	H22	0.85700	0.08800	0.95950	No
55	H23	0.64300	0.58800	0.45950	No
56	H24	0.35700	0.41200	0.95950	No
57	H25	0.37870	0.20070	0.55210	No

58	H26	0.62130	0.79930	0.05210	No
59	H27	0.87870	0.29930	0.55210	No
60	H28	0.12130	0.70070	0.05210	No
61	H29	0.46340	0.23930	0.64530	No
62	H30	0.53660	0.76070	0.14530	No
63	H31	0.96340	0.26070	0.64530	No
64	H32	0.03660	0.73930	0.14530	No
65	H33	0.47240	0.11130	0.38550	No
66	H34	0.52760	0.88870	0.88550	No
67	H35	0.97240	0.38870	0.38550	No
68	H36	0.02760	0.61130	0.88550	No
69	H37	0.55860	0.15340	0.46910	No
70	H38	0.44140	0.84660	0.96910	No
71	H39	0.05860	0.34660	0.46910	No
72	H40	0.94140	0.65340	0.96910	No
73	H41	0.52810	0.99740	0.55630	No
74	H42	0.47190	0.00260	0.05630	No
75	H43	0.02810	0.50260	0.55630	No
76	H44	0.97190	0.49740	0.05630	No
77	H45	0.52650	0.07110	0.69690	No
78	H46	0.47350	0.92890	0.19690	No
79	H47	0.02650	0.42890	0.69690	No
80	H48	0.97350	0.57110	0.19690	No
81	H49	0.37400	0.06910	0.70420	No
82	H50	0.62600	0.93090	0.20420	No
83	H51	0.87400	0.43090	0.70420	No
84	H52	0.12600	0.56910	0.20420	No
85	H53	0.40970	0.96290	0.71500	No
86	H54	0.59030	0.03710	0.21500	No
87	H55	0.90970	0.53710	0.71500	No
88	H56	0.09030	0.46290	0.21500	No
89	H57	0.33640	0.04580	0.44060	No
90	H58	0.66360	0.95420	0.94060	No
91	H59	0.83640	0.45420	0.44060	No
92	H60	0.16360	0.54580	0.94060	No
93	H61	0.37410	0.93990	0.44850	No
94	H62	0.62590	0.06010	0.94850	No
95	H63	0.87410	0.56010	0.44850	No

96	H64	0.12590	0.43990	0.94850	No
97	H65	0.26160	0.89450	0.61710	No
98	H66	0.73840	0.10550	0.11710	No
99	H67	0.76160	0.60550	0.61710	No
100	H68	0.23840	0.39450	0.11710	No
101	H69	0.22810	0.00160	0.63390	No
102	H70	0.77190	0.99840	0.13390	No
103	H71	0.72810	0.49840	0.63390	No
104	H72	0.27190	0.50160	0.13390	No
105	C1	0.44190	0.21900	0.54200	No
106	C2	0.55810	0.78100	0.04200	No
107	C3	0.94190	0.28100	0.54200	No
108	C4	0.05810	0.71900	0.04200	No
109	C5	0.49640	0.13340	0.48610	No
110	C6	0.50360	0.86660	0.98610	No
111	C7	0.99640	0.36660	0.48610	No
112	C8	0.00360	0.63340	0.98610	No
113	C9	0.49500	0.05130	0.60150	No
114	C10	0.50500	0.94870	0.10150	No
115	C11	0.99500	0.44870	0.60150	No
116	C12	0.00500	0.55130	0.10150	No
117	C13	0.40380	0.01810	0.64510	No
118	C14	0.59620	0.98190	0.14510	No
119	C15	0.90380	0.48190	0.64510	No
120	C16	0.09620	0.51810	0.14510	No
121	C17	0.34450	0.99030	0.50940	No
122	C18	0.65550	0.00970	0.00940	No
123	C19	0.84450	0.50970	0.50940	No
124	C20	0.15550	0.49030	0.00940	No
125	C21	0.25450	0.95520	0.56120	No
126	C22	0.74550	0.04480	0.06120	No
127	C23	0.75450	0.54480	0.56120	No
128	C24	0.24550	0.45520	0.06120	No

Reflex Summary Report for Rietveld Refinement of $0.8[\text{C}_6\text{N}_2\text{H}_{18}]\text{BiI}_5 + 0.2[\text{C}_6\text{N}_2\text{H}_{18}]\text{SbI}_5$:

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.04801 ± 0.09657	Yes
b	14.12300 ± 0.08967	Yes
c	43.08392 ± 0.28274	Yes
α	90.06314 ± 0.81935	Yes
β	89.74369 ± 0.20146	Yes
γ	90.01875 ± 2.01633	Yes

Structure Parameters

Refined Motion Groups: 0 Refined Torsions: 0

Refined Angles: 0 Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C1	0.44190	0.21900	0.10840	No
2	C2	0.44190	0.21900	0.30840	No
3	C3	0.44190	0.21900	0.50840	No
4	C4	0.44190	0.21900	0.70840	No
5	C5	0.44190	0.21900	0.90840	No
6	C6	0.55810	0.78100	0.00840	No
7	C7	0.55810	0.78100	0.20840	No
8	C8	0.55810	0.78100	0.40840	No
9	C9	0.55810	0.78100	0.60840	No
10	C10	0.55810	0.78100	0.80840	No
11	C11	0.94190	0.28100	0.10840	No
12	C12	0.94190	0.28100	0.30840	No
13	C13	0.94190	0.28100	0.50840	No
14	C14	0.94190	0.28100	0.70840	No
15	C15	0.94190	0.28100	0.90840	No
16	C16	0.05810	0.71900	0.00840	No
17	C17	0.05810	0.71900	0.20840	No
18	C18	0.05810	0.71900	0.40840	No
19	C19	0.05810	0.71900	0.60840	No
20	C20	0.05810	0.71900	0.80840	No
21	C21	0.49640	0.13340	0.09722	No
22	C22	0.49640	0.13340	0.29722	No
23	C23	0.49640	0.13340	0.49722	No
24	C24	0.49640	0.13340	0.69722	No

25	C25	0.49640	0.13340	0.89722	No
26	C26	0.50360	0.86660	0.99722	No
27	C27	0.50360	0.86660	0.19722	No
28	C28	0.50360	0.86660	0.39722	No
29	C29	0.50360	0.86660	0.59722	No
30	C30	0.50360	0.86660	0.79722	No
31	C31	0.99640	0.36660	0.09722	No
32	C32	0.99640	0.36660	0.29722	No
33	C33	0.99640	0.36660	0.49722	No
34	C34	0.99640	0.36660	0.69722	No
35	C35	0.99640	0.36660	0.89722	No
36	C36	0.00360	0.63340	0.99722	No
37	C37	0.00360	0.63340	0.19722	No
38	C38	0.00360	0.63340	0.39722	No
39	C39	0.00360	0.63340	0.59722	No
40	C40	0.00360	0.63340	0.79722	No
41	C41	0.49500	0.05130	0.12030	No
42	C42	0.49500	0.05130	0.32030	No
43	C43	0.49500	0.05130	0.52030	No
44	C44	0.49500	0.05130	0.72030	No
45	C45	0.49500	0.05130	0.92030	No
46	C46	0.50500	0.94870	0.02030	No
47	C47	0.50500	0.94870	0.22030	No
48	C48	0.50500	0.94870	0.42030	No
49	C49	0.50500	0.94870	0.62030	No
50	C50	0.50500	0.94870	0.82030	No
51	C51	0.99500	0.44870	0.12030	No
52	C52	0.99500	0.44870	0.32030	No
53	C53	0.99500	0.44870	0.52030	No
54	C54	0.99500	0.44870	0.72030	No
55	C55	0.99500	0.44870	0.92030	No
56	C56	0.00500	0.55130	0.02030	No
57	C57	0.00500	0.55130	0.22030	No
58	C58	0.00500	0.55130	0.42030	No
59	C59	0.00500	0.55130	0.62030	No
60	C60	0.00500	0.55130	0.82030	No
61	C61	0.40380	0.01810	0.12902	No
62	C62	0.40380	0.01810	0.32902	No

63	C63	0.40380	0.01810	0.52902	No
64	C64	0.40380	0.01810	0.72902	No
65	C65	0.40380	0.01810	0.92902	No
66	C66	0.59620	0.98190	0.02902	No
67	C67	0.59620	0.98190	0.22902	No
68	C68	0.59620	0.98190	0.42902	No
69	C69	0.59620	0.98190	0.62902	No
70	C70	0.59620	0.98190	0.82902	No
71	C71	0.90380	0.48190	0.12902	No
72	C72	0.90380	0.48190	0.32902	No
73	C73	0.90380	0.48190	0.52902	No
74	C74	0.90380	0.48190	0.72902	No
75	C75	0.90380	0.48190	0.92902	No
76	C76	0.09620	0.51810	0.02902	No
77	C77	0.09620	0.51810	0.22902	No
78	C78	0.09620	0.51810	0.42902	No
79	C79	0.09620	0.51810	0.62902	No
80	C80	0.09620	0.51810	0.82902	No
81	C81	0.34450	0.99030	0.10188	No
82	C82	0.34450	0.99030	0.30188	No
83	C83	0.34450	0.99030	0.50188	No
84	C84	0.34450	0.99030	0.70188	No
85	C85	0.34450	0.99030	0.90188	No
86	C86	0.65550	0.00970	0.00188	No
87	C87	0.65550	0.00970	0.20188	No
88	C88	0.65550	0.00970	0.40188	No
89	C89	0.65550	0.00970	0.60188	No
90	C90	0.65550	0.00970	0.80188	No
91	C91	0.84450	0.50970	0.10188	No
92	C92	0.84450	0.50970	0.30188	No
93	C93	0.84450	0.50970	0.50188	No
94	C94	0.84450	0.50970	0.70188	No
95	C95	0.84450	0.50970	0.90188	No
96	C96	0.15550	0.49030	0.00188	No
97	C97	0.15550	0.49030	0.20188	No
98	C98	0.15550	0.49030	0.40188	No
99	C99	0.15550	0.49030	0.60188	No
100	C100	0.15550	0.49030	0.80188	No

101	C101	0.25450	0.95520	0.11224	No
102	C102	0.25450	0.95520	0.31224	No
103	C103	0.25450	0.95520	0.51224	No
104	C104	0.25450	0.95520	0.71224	No
105	C105	0.25450	0.95520	0.91224	No
106	C106	0.74550	0.04480	0.01224	No
107	C107	0.74550	0.04480	0.21224	No
108	C108	0.74550	0.04480	0.41224	No
109	C109	0.74550	0.04480	0.61224	No
110	C110	0.74550	0.04480	0.81224	No
111	C111	0.75450	0.54480	0.11224	No
112	C112	0.75450	0.54480	0.31224	No
113	C113	0.75450	0.54480	0.51224	No
114	C114	0.75450	0.54480	0.71224	No
115	C115	0.75450	0.54480	0.91224	No
116	C116	0.24550	0.45520	0.01224	No
117	C117	0.24550	0.45520	0.21224	No
118	C118	0.24550	0.45520	0.41224	No
119	C119	0.24550	0.45520	0.61224	No
120	C120	0.24550	0.45520	0.81224	No
121	I1	0.48458	0.51909	0.04212	No
122	I2	0.48458	0.51909	0.24212	No
123	I3	0.48458	0.51909	0.44212	No
124	I4	0.48458	0.51909	0.64212	No
125	I5	0.48458	0.51909	0.84212	No
126	I6	0.51542	0.48091	0.94212	No
127	I7	0.51542	0.48091	0.14212	No
128	I8	0.51542	0.48091	0.34212	No
129	I9	0.51542	0.48091	0.54212	No
130	I10	0.51542	0.48091	0.74212	No
131	I11	0.98458	0.98091	0.04212	No
132	I12	0.98458	0.98091	0.24212	No
133	I13	0.98458	0.98091	0.44212	No
134	I14	0.98458	0.98091	0.64212	No
135	I15	0.98458	0.98091	0.84212	No
136	I16	0.01542	0.01909	0.94212	No
137	I17	0.01542	0.01909	0.14212	No
138	I18	0.01542	0.01909	0.34212	No

139	I19	0.01542	0.01909	0.54212	No
140	I20	0.01542	0.01909	0.74212	No
141	I21	0.25948	0.45560	0.10194	No
142	I22	0.25948	0.45560	0.30194	No
143	I23	0.25948	0.45560	0.50194	No
144	I24	0.25948	0.45560	0.70194	No
145	I25	0.25948	0.45560	0.90194	No
146	I26	0.74052	0.54440	0.00194	No
147	I27	0.74052	0.54440	0.20194	No
148	I28	0.74052	0.54440	0.40194	No
149	I29	0.74052	0.54440	0.60194	No
150	I30	0.74052	0.54440	0.80194	No
151	I31	0.75948	0.04440	0.10194	No
152	I32	0.75948	0.04440	0.30194	No
153	I33	0.75948	0.04440	0.50194	No
154	I34	0.75948	0.04440	0.70194	No
155	I35	0.75948	0.04440	0.90194	No
156	I36	0.24052	0.95560	0.00194	No
157	I37	0.24052	0.95560	0.20194	No
158	I38	0.24052	0.95560	0.40194	No
159	I39	0.24052	0.95560	0.60194	No
160	I40	0.24052	0.95560	0.80194	No
161	I41	0.29912	0.73228	0.05329	No
162	I42	0.29912	0.73228	0.25329	No
163	I43	0.29912	0.73228	0.45329	No
164	I44	0.29912	0.73228	0.65329	No
165	I45	0.29912	0.73228	0.85329	No
166	I46	0.70088	0.26772	0.95329	No
167	I47	0.70088	0.26772	0.15329	No
168	I48	0.70088	0.26772	0.35329	No
169	I49	0.70088	0.26772	0.55329	No
170	I50	0.70088	0.26772	0.75329	No
171	I51	0.79912	0.76772	0.05329	No
172	I52	0.79912	0.76772	0.25329	No
173	I53	0.79912	0.76772	0.45329	No
174	I54	0.79912	0.76772	0.65329	No
175	I55	0.79912	0.76772	0.85329	No
176	I56	0.20088	0.23228	0.95329	No

177	I57	0.20088	0.23228	0.15329	No
178	I58	0.20088	0.23228	0.35329	No
179	I59	0.20088	0.23228	0.55329	No
180	I60	0.20088	0.23228	0.75329	No
181	I61	0.30809	0.69835	0.15768	No
182	I62	0.30809	0.69835	0.35768	No
183	I63	0.30809	0.69835	0.55768	No
184	I64	0.30809	0.69835	0.75768	No
185	I65	0.30809	0.69835	0.95768	No
186	I66	0.69191	0.30165	0.05768	No
187	I67	0.69191	0.30165	0.25768	No
188	I68	0.69191	0.30165	0.45768	No
189	I69	0.69191	0.30165	0.65768	No
190	I70	0.69191	0.30165	0.85768	No
191	I71	0.80809	0.80165	0.15768	No
192	I72	0.80809	0.80165	0.35768	No
193	I73	0.80809	0.80165	0.55768	No
194	I74	0.80809	0.80165	0.75768	No
195	I75	0.80809	0.80165	0.95768	No
196	I76	0.19191	0.19835	0.05768	No
197	I77	0.19191	0.19835	0.25768	No
198	I78	0.19191	0.19835	0.45768	No
199	I79	0.19191	0.19835	0.65768	No
200	I80	0.19191	0.19835	0.85768	No
201	I81	0.54645	0.76181	0.10427	No
202	I82	0.54645	0.76181	0.30427	No
203	I83	0.54645	0.76181	0.50427	No
204	I84	0.54645	0.76181	0.70427	No
205	I85	0.54645	0.76181	0.90427	No
206	I86	0.45355	0.23819	0.00427	No
207	I87	0.45355	0.23819	0.20427	No
208	I88	0.45355	0.23819	0.40427	No
209	I89	0.45355	0.23819	0.60427	No
210	I90	0.45355	0.23819	0.80427	No
211	I91	0.04645	0.73819	0.10427	No
212	I92	0.04645	0.73819	0.30427	No
213	I93	0.04645	0.73819	0.50427	No
214	I94	0.04645	0.73819	0.70427	No

215	I95	0.04645	0.73819	0.90427	No
216	I96	0.95355	0.26181	0.00427	No
217	I97	0.95355	0.26181	0.20427	No
218	I98	0.95355	0.26181	0.40427	No
219	I99	0.95355	0.26181	0.60427	No
220	I100	0.95355	0.26181	0.80427	No
221	H1	0.43960	0.27810	0.06640	No
222	H2	0.43960	0.27810	0.26640	No
223	H3	0.43960	0.27810	0.46640	No
224	H4	0.43960	0.27810	0.66640	No
225	H5	0.43960	0.27810	0.86640	No
226	H6	0.56040	0.72190	0.96640	No
227	H7	0.56040	0.72190	0.16640	No
228	H8	0.56040	0.72190	0.36640	No
229	H9	0.56040	0.72190	0.56640	No
230	H10	0.56040	0.72190	0.76640	No
231	H11	0.93960	0.22190	0.06640	No
232	H12	0.93960	0.22190	0.26640	No
233	H13	0.93960	0.22190	0.46640	No
234	H14	0.93960	0.22190	0.66640	No
235	H15	0.93960	0.22190	0.86640	No
236	H16	0.06040	0.77810	0.96640	No
237	H17	0.06040	0.77810	0.16640	No
238	H18	0.06040	0.77810	0.36640	No
239	H19	0.06040	0.77810	0.56640	No
240	H20	0.06040	0.77810	0.76640	No
241	H21	0.50570	0.32420	0.08704	No
242	H22	0.50570	0.32420	0.28704	No
243	H23	0.50570	0.32420	0.48704	No
244	H24	0.50570	0.32420	0.68704	No
245	H25	0.50570	0.32420	0.88704	No
246	H26	0.49430	0.67580	0.98704	No
247	H27	0.49430	0.67580	0.18704	No
248	H28	0.49430	0.67580	0.38704	No
249	H29	0.49430	0.67580	0.58704	No
250	H30	0.49430	0.67580	0.78704	No
251	H31	0.00570	0.17580	0.08704	No
252	H32	0.00570	0.17580	0.28704	No

253	H33	0.00570	0.17580	0.48704	No
254	H34	0.00570	0.17580	0.68704	No
255	H35	0.00570	0.17580	0.88704	No
256	H36	0.99430	0.82420	0.98704	No
257	H37	0.99430	0.82420	0.18704	No
258	H38	0.99430	0.82420	0.38704	No
259	H39	0.99430	0.82420	0.58704	No
260	H40	0.99430	0.82420	0.78704	No
261	H41	0.40970	0.34510	0.09086	No
262	H42	0.40970	0.34510	0.29086	No
263	H43	0.40970	0.34510	0.49086	No
264	H44	0.40970	0.34510	0.69086	No
265	H45	0.40970	0.34510	0.89086	No
266	H46	0.59030	0.65490	0.99086	No
267	H47	0.59030	0.65490	0.19086	No
268	H48	0.59030	0.65490	0.39086	No
269	H49	0.59030	0.65490	0.59086	No
270	H50	0.59030	0.65490	0.79086	No
271	H51	0.90970	0.15490	0.09086	No
272	H52	0.90970	0.15490	0.29086	No
273	H53	0.90970	0.15490	0.49086	No
274	H54	0.90970	0.15490	0.69086	No
275	H55	0.90970	0.15490	0.89086	No
276	H56	0.09030	0.84510	0.99086	No
277	H57	0.09030	0.84510	0.19086	No
278	H58	0.09030	0.84510	0.39086	No
279	H59	0.09030	0.84510	0.59086	No
280	H60	0.09030	0.84510	0.79086	No
281	H61	0.22060	0.90500	0.07076	No
282	H62	0.22060	0.90500	0.27076	No
283	H63	0.22060	0.90500	0.47076	No
284	H64	0.22060	0.90500	0.67076	No
285	H65	0.22060	0.90500	0.87076	No
286	H66	0.77940	0.09500	0.97076	No
287	H67	0.77940	0.09500	0.17076	No
288	H68	0.77940	0.09500	0.37076	No
289	H69	0.77940	0.09500	0.57076	No
290	H70	0.77940	0.09500	0.77076	No

291	H71	0.72060	0.59500	0.07076	No
292	H72	0.72060	0.59500	0.27076	No
293	H73	0.72060	0.59500	0.47076	No
294	H74	0.72060	0.59500	0.67076	No
295	H75	0.72060	0.59500	0.87076	No
296	H76	0.27940	0.40500	0.97076	No
297	H77	0.27940	0.40500	0.17076	No
298	H78	0.27940	0.40500	0.37076	No
299	H79	0.27940	0.40500	0.57076	No
300	H80	0.27940	0.40500	0.77076	No
301	H81	0.17940	0.99870	0.07702	No
302	H82	0.17940	0.99870	0.27702	No
303	H83	0.17940	0.99870	0.47702	No
304	H84	0.17940	0.99870	0.67702	No
305	H85	0.17940	0.99870	0.87702	No
306	H86	0.82060	0.00130	0.97702	No
307	H87	0.82060	0.00130	0.17702	No
308	H88	0.82060	0.00130	0.37702	No
309	H89	0.82060	0.00130	0.57702	No
310	H90	0.82060	0.00130	0.77702	No
311	H91	0.67940	0.50130	0.07702	No
312	H92	0.67940	0.50130	0.27702	No
313	H93	0.67940	0.50130	0.47702	No
314	H94	0.67940	0.50130	0.67702	No
315	H95	0.67940	0.50130	0.87702	No
316	H96	0.32060	0.49870	0.97702	No
317	H97	0.32060	0.49870	0.17702	No
318	H98	0.32060	0.49870	0.37702	No
319	H99	0.32060	0.49870	0.57702	No
320	H100	0.32060	0.49870	0.77702	No
321	H101	0.14300	0.91200	0.09190	No
322	H102	0.14300	0.91200	0.29190	No
323	H103	0.14300	0.91200	0.49190	No
324	H104	0.14300	0.91200	0.69190	No
325	H105	0.14300	0.91200	0.89190	No
326	H106	0.85700	0.08800	0.99190	No
327	H107	0.85700	0.08800	0.19190	No
328	H108	0.85700	0.08800	0.39190	No

329	H109	0.85700	0.08800	0.59190	No
330	H110	0.85700	0.08800	0.79190	No
331	H111	0.64300	0.58800	0.09190	No
332	H112	0.64300	0.58800	0.29190	No
333	H113	0.64300	0.58800	0.49190	No
334	H114	0.64300	0.58800	0.69190	No
335	H115	0.64300	0.58800	0.89190	No
336	H116	0.35700	0.41200	0.99190	No
337	H117	0.35700	0.41200	0.19190	No
338	H118	0.35700	0.41200	0.39190	No
339	H119	0.35700	0.41200	0.59190	No
340	H120	0.35700	0.41200	0.79190	No
341	H121	0.37870	0.20070	0.11042	No
342	H122	0.37870	0.20070	0.31042	No
343	H123	0.37870	0.20070	0.51042	No
344	H124	0.37870	0.20070	0.71042	No
345	H125	0.37870	0.20070	0.91042	No
346	H126	0.62130	0.79930	0.01042	No
347	H127	0.62130	0.79930	0.21042	No
348	H128	0.62130	0.79930	0.41042	No
349	H129	0.62130	0.79930	0.61042	No
350	H130	0.62130	0.79930	0.81042	No
351	H131	0.87870	0.29930	0.11042	No
352	H132	0.87870	0.29930	0.31042	No
353	H133	0.87870	0.29930	0.51042	No
354	H134	0.87870	0.29930	0.71042	No
355	H135	0.87870	0.29930	0.91042	No
356	H136	0.12130	0.70070	0.01042	No
357	H137	0.12130	0.70070	0.21042	No
358	H138	0.12130	0.70070	0.41042	No
359	H139	0.12130	0.70070	0.61042	No
360	H140	0.12130	0.70070	0.81042	No
361	H141	0.46340	0.23930	0.12906	No
362	H142	0.46340	0.23930	0.32906	No
363	H143	0.46340	0.23930	0.52906	No
364	H144	0.46340	0.23930	0.72906	No
365	H145	0.46340	0.23930	0.92906	No
366	H146	0.53660	0.76070	0.02906	No

367	H147	0.53660	0.76070	0.22906	No
368	H148	0.53660	0.76070	0.42906	No
369	H149	0.53660	0.76070	0.62906	No
370	H150	0.53660	0.76070	0.82906	No
371	H151	0.96340	0.26070	0.12906	No
372	H152	0.96340	0.26070	0.32906	No
373	H153	0.96340	0.26070	0.52906	No
374	H154	0.96340	0.26070	0.72906	No
375	H155	0.96340	0.26070	0.92906	No
376	H156	0.03660	0.73930	0.02906	No
377	H157	0.03660	0.73930	0.22906	No
378	H158	0.03660	0.73930	0.42906	No
379	H159	0.03660	0.73930	0.62906	No
380	H160	0.03660	0.73930	0.82906	No
381	H161	0.47240	0.11130	0.07710	No
382	H162	0.47240	0.11130	0.27710	No
383	H163	0.47240	0.11130	0.47710	No
384	H164	0.47240	0.11130	0.67710	No
385	H165	0.47240	0.11130	0.87710	No
386	H166	0.52760	0.88870	0.97710	No
387	H167	0.52760	0.88870	0.17710	No
388	H168	0.52760	0.88870	0.37710	No
389	H169	0.52760	0.88870	0.57710	No
390	H170	0.52760	0.88870	0.77710	No
391	H171	0.97240	0.38870	0.07710	No
392	H172	0.97240	0.38870	0.27710	No
393	H173	0.97240	0.38870	0.47710	No
394	H174	0.97240	0.38870	0.67710	No
395	H175	0.97240	0.38870	0.87710	No
396	H176	0.02760	0.61130	0.97710	No
397	H177	0.02760	0.61130	0.17710	No
398	H178	0.02760	0.61130	0.37710	No
399	H179	0.02760	0.61130	0.57710	No
400	H180	0.02760	0.61130	0.77710	No
401	H181	0.55860	0.15340	0.09382	No
402	H182	0.55860	0.15340	0.29382	No
403	H183	0.55860	0.15340	0.49382	No
404	H184	0.55860	0.15340	0.69382	No

405	H185	0.55860	0.15340	0.89382	No
406	H186	0.44140	0.84660	0.99382	No
407	H187	0.44140	0.84660	0.19382	No
408	H188	0.44140	0.84660	0.39382	No
409	H189	0.44140	0.84660	0.59382	No
410	H190	0.44140	0.84660	0.79382	No
411	H191	0.05860	0.34660	0.09382	No
412	H192	0.05860	0.34660	0.29382	No
413	H193	0.05860	0.34660	0.49382	No
414	H194	0.05860	0.34660	0.69382	No
415	H195	0.05860	0.34660	0.89382	No
416	H196	0.94140	0.65340	0.99382	No
417	H197	0.94140	0.65340	0.19382	No
418	H198	0.94140	0.65340	0.39382	No
419	H199	0.94140	0.65340	0.59382	No
420	H200	0.94140	0.65340	0.79382	No
421	H201	0.52810	0.99740	0.11126	No
422	H202	0.52810	0.99740	0.31126	No
423	H203	0.52810	0.99740	0.51126	No
424	H204	0.52810	0.99740	0.71126	No
425	H205	0.52810	0.99740	0.91126	No
426	H206	0.47190	0.00260	0.01126	No
427	H207	0.47190	0.00260	0.21126	No
428	H208	0.47190	0.00260	0.41126	No
429	H209	0.47190	0.00260	0.61126	No
430	H210	0.47190	0.00260	0.81126	No
431	H211	0.02810	0.50260	0.11126	No
432	H212	0.02810	0.50260	0.31126	No
433	H213	0.02810	0.50260	0.51126	No
434	H214	0.02810	0.50260	0.71126	No
435	H215	0.02810	0.50260	0.91126	No
436	H216	0.97190	0.49740	0.01126	No
437	H217	0.97190	0.49740	0.21126	No
438	H218	0.97190	0.49740	0.41126	No
439	H219	0.97190	0.49740	0.61126	No
440	H220	0.97190	0.49740	0.81126	No
441	H221	0.52650	0.07110	0.13938	No
442	H222	0.52650	0.07110	0.33938	No

443	H223	0.52650	0.07110	0.53938	No
444	H224	0.52650	0.07110	0.73938	No
445	H225	0.52650	0.07110	0.93938	No
446	H226	0.47350	0.92890	0.03938	No
447	H227	0.47350	0.92890	0.23938	No
448	H228	0.47350	0.92890	0.43938	No
449	H229	0.47350	0.92890	0.63938	No
450	H230	0.47350	0.92890	0.83938	No
451	H231	0.02650	0.42890	0.13938	No
452	H232	0.02650	0.42890	0.33938	No
453	H233	0.02650	0.42890	0.53938	No
454	H234	0.02650	0.42890	0.73938	No
455	H235	0.02650	0.42890	0.93938	No
456	H236	0.97350	0.57110	0.03938	No
457	H237	0.97350	0.57110	0.23938	No
458	H238	0.97350	0.57110	0.43938	No
459	H239	0.97350	0.57110	0.63938	No
460	H240	0.97350	0.57110	0.83938	No
461	H241	0.37400	0.06910	0.14084	No
462	H242	0.37400	0.06910	0.34084	No
463	H243	0.37400	0.06910	0.54084	No
464	H244	0.37400	0.06910	0.74084	No
465	H245	0.37400	0.06910	0.94084	No
466	H246	0.62600	0.93090	0.04084	No
467	H247	0.62600	0.93090	0.24084	No
468	H248	0.62600	0.93090	0.44084	No
469	H249	0.62600	0.93090	0.64084	No
470	H250	0.62600	0.93090	0.84084	No
471	H251	0.87400	0.43090	0.14084	No
472	H252	0.87400	0.43090	0.34084	No
473	H253	0.87400	0.43090	0.54084	No
474	H254	0.87400	0.43090	0.74084	No
475	H255	0.87400	0.43090	0.94084	No
476	H256	0.12600	0.56910	0.04084	No
477	H257	0.12600	0.56910	0.24084	No
478	H258	0.12600	0.56910	0.44084	No
479	H259	0.12600	0.56910	0.64084	No
480	H260	0.12600	0.56910	0.84084	No

481	H261	0.40970	0.96290	0.14300	No
482	H262	0.40970	0.96290	0.34300	No
483	H263	0.40970	0.96290	0.54300	No
484	H264	0.40970	0.96290	0.74300	No
485	H265	0.40970	0.96290	0.94300	No
486	H266	0.59030	0.03710	0.04300	No
487	H267	0.59030	0.03710	0.24300	No
488	H268	0.59030	0.03710	0.44300	No
489	H269	0.59030	0.03710	0.64300	No
490	H270	0.59030	0.03710	0.84300	No
491	H271	0.90970	0.53710	0.14300	No
492	H272	0.90970	0.53710	0.34300	No
493	H273	0.90970	0.53710	0.54300	No
494	H274	0.90970	0.53710	0.74300	No
495	H275	0.90970	0.53710	0.94300	No
496	H276	0.09030	0.46290	0.04300	No
497	H277	0.09030	0.46290	0.24300	No
498	H278	0.09030	0.46290	0.44300	No
499	H279	0.09030	0.46290	0.64300	No
500	H280	0.09030	0.46290	0.84300	No
501	H281	0.33640	0.04580	0.08812	No
502	H282	0.33640	0.04580	0.28812	No
503	H283	0.33640	0.04580	0.48812	No
504	H284	0.33640	0.04580	0.68812	No
505	H285	0.33640	0.04580	0.88812	No
506	H286	0.66360	0.95420	0.98812	No
507	H287	0.66360	0.95420	0.18812	No
508	H288	0.66360	0.95420	0.38812	No
509	H289	0.66360	0.95420	0.58812	No
510	H290	0.66360	0.95420	0.78812	No
511	H291	0.83640	0.45420	0.08812	No
512	H292	0.83640	0.45420	0.28812	No
513	H293	0.83640	0.45420	0.48812	No
514	H294	0.83640	0.45420	0.68812	No
515	H295	0.83640	0.45420	0.88812	No
516	H296	0.16360	0.54580	0.98812	No
517	H297	0.16360	0.54580	0.18812	No
518	H298	0.16360	0.54580	0.38812	No

519	H299	0.16360	0.54580	0.58812	No
520	H300	0.16360	0.54580	0.78812	No
521	H301	0.37410	0.93990	0.08970	No
522	H302	0.37410	0.93990	0.28970	No
523	H303	0.37410	0.93990	0.48970	No
524	H304	0.37410	0.93990	0.68970	No
525	H305	0.37410	0.93990	0.88970	No
526	H306	0.62590	0.06010	0.98970	No
527	H307	0.62590	0.06010	0.18970	No
528	H308	0.62590	0.06010	0.38970	No
529	H309	0.62590	0.06010	0.58970	No
530	H310	0.62590	0.06010	0.78970	No
531	H311	0.87410	0.56010	0.08970	No
532	H312	0.87410	0.56010	0.28970	No
533	H313	0.87410	0.56010	0.48970	No
534	H314	0.87410	0.56010	0.68970	No
535	H315	0.87410	0.56010	0.88970	No
536	H316	0.12590	0.43990	0.98970	No
537	H317	0.12590	0.43990	0.18970	No
538	H318	0.12590	0.43990	0.38970	No
539	H319	0.12590	0.43990	0.58970	No
540	H320	0.12590	0.43990	0.78970	No
541	H321	0.26160	0.89450	0.12342	No
542	H322	0.26160	0.89450	0.32342	No
543	H323	0.26160	0.89450	0.52342	No
544	H324	0.26160	0.89450	0.72342	No
545	H325	0.26160	0.89450	0.92342	No
546	H326	0.73840	0.10550	0.02342	No
547	H327	0.73840	0.10550	0.22342	No
548	H328	0.73840	0.10550	0.42342	No
549	H329	0.73840	0.10550	0.62342	No
550	H330	0.73840	0.10550	0.82342	No
551	H331	0.76160	0.60550	0.12342	No
552	H332	0.76160	0.60550	0.32342	No
553	H333	0.76160	0.60550	0.52342	No
554	H334	0.76160	0.60550	0.72342	No
555	H335	0.76160	0.60550	0.92342	No
556	H336	0.23840	0.39450	0.02342	No

557	H337	0.23840	0.39450	0.22342	No
558	H338	0.23840	0.39450	0.42342	No
559	H339	0.23840	0.39450	0.62342	No
560	H340	0.23840	0.39450	0.82342	No
561	H341	0.22810	0.00160	0.12678	No
562	H342	0.22810	0.00160	0.32678	No
563	H343	0.22810	0.00160	0.52678	No
564	H344	0.22810	0.00160	0.72678	No
565	H345	0.22810	0.00160	0.92678	No
566	H346	0.77190	0.99840	0.02678	No
567	H347	0.77190	0.99840	0.22678	No
568	H348	0.77190	0.99840	0.42678	No
569	H349	0.77190	0.99840	0.62678	No
570	H350	0.77190	0.99840	0.82678	No
571	H351	0.72810	0.49840	0.12678	No
572	H352	0.72810	0.49840	0.32678	No
573	H353	0.72810	0.49840	0.52678	No
574	H354	0.72810	0.49840	0.72678	No
575	H355	0.72810	0.49840	0.92678	No
576	H356	0.27190	0.50160	0.02678	No
577	H357	0.27190	0.50160	0.22678	No
578	H358	0.27190	0.50160	0.42678	No
579	H359	0.27190	0.50160	0.62678	No
580	H360	0.27190	0.50160	0.82678	No
581	Bi1	0.38917	0.62103	0.10063	No
582	Bi2	0.38917	0.62103	0.30063	No
583	Bi3	0.38917	0.62103	0.50063	No
584	Bi4	0.38917	0.62103	0.70063	No
585	Bi5	0.38917	0.62103	0.90063	No
586	Bi6	0.61083	0.37897	0.00063	No
587	Bi7	0.61083	0.37897	0.40063	No
588	Bi8	0.61083	0.37897	0.60063	No
589	Bi9	0.88917	0.87897	0.30063	No
590	Bi10	0.88917	0.87897	0.50063	No
591	Bi11	0.88917	0.87897	0.70063	No
592	Bi12	0.88917	0.87897	0.90063	No
593	Bi13	0.11083	0.12103	0.20063	No
594	Bi14	0.11083	0.12103	0.40063	No

595	Bi15	0.11083	0.12103	0.60063	No
596	Bi16	0.11083	0.12103	0.80063	No
597	N1	0.45000	0.29950	0.08598	No
598	N2	0.45000	0.29950	0.28598	No
599	N3	0.45000	0.29950	0.48598	No
600	N4	0.45000	0.29950	0.68598	No
601	N5	0.45000	0.29950	0.88598	No
602	N6	0.55000	0.70050	0.98598	No
603	N7	0.55000	0.70050	0.18598	No
604	N8	0.55000	0.70050	0.38598	No
605	N9	0.55000	0.70050	0.58598	No
606	N10	0.55000	0.70050	0.78598	No
607	N11	0.95000	0.20050	0.08598	No
608	N12	0.95000	0.20050	0.28598	No
609	N13	0.95000	0.20050	0.48598	No
610	N14	0.95000	0.20050	0.68598	No
611	N15	0.95000	0.20050	0.88598	No
612	N16	0.05000	0.79950	0.98598	No
613	N17	0.05000	0.79950	0.18598	No
614	N18	0.05000	0.79950	0.38598	No
615	N19	0.05000	0.79950	0.58598	No
616	N20	0.05000	0.79950	0.78598	No
617	N21	0.19340	0.94140	0.08536	No
618	N22	0.19340	0.94140	0.28536	No
619	N23	0.19340	0.94140	0.48536	No
620	N24	0.19340	0.94140	0.68536	No
621	N25	0.19340	0.94140	0.88536	No
622	N26	0.80660	0.05860	0.98536	No
623	N27	0.80660	0.05860	0.18536	No
624	N28	0.80660	0.05860	0.38536	No
625	N29	0.80660	0.05860	0.58536	No
626	N30	0.80660	0.05860	0.78536	No
627	N31	0.69340	0.55860	0.08536	No
628	N32	0.69340	0.55860	0.28536	No
629	N33	0.69340	0.55860	0.48536	No
630	N34	0.69340	0.55860	0.68536	No
631	N35	0.69340	0.55860	0.88536	No
632	N36	0.30660	0.44140	0.98536	No

633	N37	0.30660	0.44140	0.18536	No
634	N38	0.30660	0.44140	0.38536	No
635	N39	0.30660	0.44140	0.58536	No
636	N40	0.30660	0.44140	0.78536	No
637	Sb1	0.61083	0.37897	0.20063	No
638	Sb2	0.61083	0.37897	0.80063	No
639	Sb3	0.88917	0.87897	0.10063	No
640	Sb4	0.11083	0.12103	0.00063	No

Reflex Summary Report for Rietveld Refinement of 0.6[C₆N₂H₁₈]BiI₅+0.4[C₆N₂H₁₈]SbI₅:

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.06429 ± 0.21994	Yes
b	14.10948 ± 0.20620	Yes
c	43.10452 ± 0.64775	Yes
α	89.87726 ± 0.88933	Yes
β	90.24297 ± 0.46325	Yes
γ	89.99018 ± 3.11252	Yes

Structure Parameters

Refined Motion Groups: 0
Refined Torsions: 0

Refined Angles: 0
Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C1	0.44190	0.21900	0.10840	No
2	C2	0.44190	0.21900	0.30840	No
3	C3	0.44190	0.21900	0.50840	No
4	C4	0.44190	0.21900	0.70840	No
5	C5	0.44190	0.21900	0.90840	No
6	C6	0.55810	0.78100	0.00840	No
7	C7	0.55810	0.78100	0.20840	No
8	C8	0.55810	0.78100	0.40840	No
9	C9	0.55810	0.78100	0.60840	No
10	C10	0.55810	0.78100	0.80840	No
11	C11	0.94190	0.28100	0.10840	No
12	C12	0.94190	0.28100	0.30840	No

13	C13	0.94190	0.28100	0.50840	No
14	C14	0.94190	0.28100	0.70840	No
15	C15	0.94190	0.28100	0.90840	No
16	C16	0.05810	0.71900	0.00840	No
17	C17	0.05810	0.71900	0.20840	No
18	C18	0.05810	0.71900	0.40840	No
19	C19	0.05810	0.71900	0.60840	No
20	C20	0.05810	0.71900	0.80840	No
21	C21	0.49640	0.13340	0.09722	No
22	C22	0.49640	0.13340	0.29722	No
23	C23	0.49640	0.13340	0.49722	No
24	C24	0.49640	0.13340	0.69722	No
25	C25	0.49640	0.13340	0.89722	No
26	C26	0.50360	0.86660	0.99722	No
27	C27	0.50360	0.86660	0.19722	No
28	C28	0.50360	0.86660	0.39722	No
29	C29	0.50360	0.86660	0.59722	No
30	C30	0.50360	0.86660	0.79722	No
31	C31	0.99640	0.36660	0.09722	No
32	C32	0.99640	0.36660	0.29722	No
33	C33	0.99640	0.36660	0.49722	No
34	C34	0.99640	0.36660	0.69722	No
35	C35	0.99640	0.36660	0.89722	No
36	C36	0.00360	0.63340	0.99722	No
37	C37	0.00360	0.63340	0.19722	No
38	C38	0.00360	0.63340	0.39722	No
39	C39	0.00360	0.63340	0.59722	No
40	C40	0.00360	0.63340	0.79722	No
41	C41	0.49500	0.05130	0.12030	No
42	C42	0.49500	0.05130	0.32030	No
43	C43	0.49500	0.05130	0.52030	No
44	C44	0.49500	0.05130	0.72030	No
45	C45	0.49500	0.05130	0.92030	No
46	C46	0.50500	0.94870	0.02030	No
47	C47	0.50500	0.94870	0.22030	No
48	C48	0.50500	0.94870	0.42030	No
49	C49	0.50500	0.94870	0.62030	No
50	C50	0.50500	0.94870	0.82030	No

51	C51	0.99500	0.44870	0.12030	No
52	C52	0.99500	0.44870	0.32030	No
53	C53	0.99500	0.44870	0.52030	No
54	C54	0.99500	0.44870	0.72030	No
55	C55	0.99500	0.44870	0.92030	No
56	C56	0.00500	0.55130	0.02030	No
57	C57	0.00500	0.55130	0.22030	No
58	C58	0.00500	0.55130	0.42030	No
59	C59	0.00500	0.55130	0.62030	No
60	C60	0.00500	0.55130	0.82030	No
61	C61	0.40380	0.01810	0.12902	No
62	C62	0.40380	0.01810	0.32902	No
63	C63	0.40380	0.01810	0.52902	No
64	C64	0.40380	0.01810	0.72902	No
65	C65	0.40380	0.01810	0.92902	No
66	C66	0.59620	0.98190	0.02902	No
67	C67	0.59620	0.98190	0.22902	No
68	C68	0.59620	0.98190	0.42902	No
69	C69	0.59620	0.98190	0.62902	No
70	C70	0.59620	0.98190	0.82902	No
71	C71	0.90380	0.48190	0.12902	No
72	C72	0.90380	0.48190	0.32902	No
73	C73	0.90380	0.48190	0.52902	No
74	C74	0.90380	0.48190	0.72902	No
75	C75	0.90380	0.48190	0.92902	No
76	C76	0.09620	0.51810	0.02902	No
77	C77	0.09620	0.51810	0.22902	No
78	C78	0.09620	0.51810	0.42902	No
79	C79	0.09620	0.51810	0.62902	No
80	C80	0.09620	0.51810	0.82902	No
81	C81	0.34450	0.99030	0.10188	No
82	C82	0.34450	0.99030	0.30188	No
83	C83	0.34450	0.99030	0.50188	No
84	C84	0.34450	0.99030	0.70188	No
85	C85	0.34450	0.99030	0.90188	No
86	C86	0.65550	0.00970	0.00188	No
87	C87	0.65550	0.00970	0.20188	No
88	C88	0.65550	0.00970	0.40188	No

89	C89	0.65550	0.00970	0.60188	No
90	C90	0.65550	0.00970	0.80188	No
91	C91	0.84450	0.50970	0.10188	No
92	C92	0.84450	0.50970	0.30188	No
93	C93	0.84450	0.50970	0.50188	No
94	C94	0.84450	0.50970	0.70188	No
95	C95	0.84450	0.50970	0.90188	No
96	C96	0.15550	0.49030	0.00188	No
97	C97	0.15550	0.49030	0.20188	No
98	C98	0.15550	0.49030	0.40188	No
99	C99	0.15550	0.49030	0.60188	No
100	C100	0.15550	0.49030	0.80188	No
101	C101	0.25450	0.95520	0.11224	No
102	C102	0.25450	0.95520	0.31224	No
103	C103	0.25450	0.95520	0.51224	No
104	C104	0.25450	0.95520	0.71224	No
105	C105	0.25450	0.95520	0.91224	No
106	C106	0.74550	0.04480	0.01224	No
107	C107	0.74550	0.04480	0.21224	No
108	C108	0.74550	0.04480	0.41224	No
109	C109	0.74550	0.04480	0.61224	No
110	C110	0.74550	0.04480	0.81224	No
111	C111	0.75450	0.54480	0.11224	No
112	C112	0.75450	0.54480	0.31224	No
113	C113	0.75450	0.54480	0.51224	No
114	C114	0.75450	0.54480	0.71224	No
115	C115	0.75450	0.54480	0.91224	No
116	C116	0.24550	0.45520	0.01224	No
117	C117	0.24550	0.45520	0.21224	No
118	C118	0.24550	0.45520	0.41224	No
119	C119	0.24550	0.45520	0.61224	No
120	C120	0.24550	0.45520	0.81224	No
121	I1	0.48458	0.51909	0.04212	No
122	I2	0.48458	0.51909	0.24212	No
123	I3	0.48458	0.51909	0.44212	No
124	I4	0.48458	0.51909	0.64212	No
125	I5	0.48458	0.51909	0.84212	No
126	I6	0.51542	0.48091	0.94212	No

127	I7	0.51542	0.48091	0.14212	No
128	I8	0.51542	0.48091	0.34212	No
129	I9	0.51542	0.48091	0.54212	No
130	I10	0.51542	0.48091	0.74212	No
131	I11	0.98458	0.98091	0.04212	No
132	I12	0.98458	0.98091	0.24212	No
133	I13	0.98458	0.98091	0.44212	No
134	I14	0.98458	0.98091	0.64212	No
135	I15	0.98458	0.98091	0.84212	No
136	I16	0.01542	0.01909	0.94212	No
137	I17	0.01542	0.01909	0.14212	No
138	I18	0.01542	0.01909	0.34212	No
139	I19	0.01542	0.01909	0.54212	No
140	I20	0.01542	0.01909	0.74212	No
141	I21	0.25948	0.45560	0.10194	No
142	I22	0.25948	0.45560	0.30194	No
143	I23	0.25948	0.45560	0.50194	No
144	I24	0.25948	0.45560	0.70194	No
145	I25	0.25948	0.45560	0.90194	No
146	I26	0.74052	0.54440	0.00194	No
147	I27	0.74052	0.54440	0.20194	No
148	I28	0.74052	0.54440	0.40194	No
149	I29	0.74052	0.54440	0.60194	No
150	I30	0.74052	0.54440	0.80194	No
151	I31	0.75948	0.04440	0.10194	No
152	I32	0.75948	0.04440	0.30194	No
153	I33	0.75948	0.04440	0.50194	No
154	I34	0.75948	0.04440	0.70194	No
155	I35	0.75948	0.04440	0.90194	No
156	I36	0.24052	0.95560	0.00194	No
157	I37	0.24052	0.95560	0.20194	No
158	I38	0.24052	0.95560	0.40194	No
159	I39	0.24052	0.95560	0.60194	No
160	I40	0.24052	0.95560	0.80194	No
161	I41	0.29912	0.73228	0.05329	No
162	I42	0.29912	0.73228	0.25329	No
163	I43	0.29912	0.73228	0.45329	No
164	I44	0.29912	0.73228	0.65329	No

165	I45	0.29912	0.73228	0.85329	No
166	I46	0.70088	0.26772	0.95329	No
167	I47	0.70088	0.26772	0.15329	No
168	I48	0.70088	0.26772	0.35329	No
169	I49	0.70088	0.26772	0.55329	No
170	I50	0.70088	0.26772	0.75329	No
171	I51	0.79912	0.76772	0.05329	No
172	I52	0.79912	0.76772	0.25329	No
173	I53	0.79912	0.76772	0.45329	No
174	I54	0.79912	0.76772	0.65329	No
175	I55	0.79912	0.76772	0.85329	No
176	I56	0.20088	0.23228	0.95329	No
177	I57	0.20088	0.23228	0.15329	No
178	I58	0.20088	0.23228	0.35329	No
179	I59	0.20088	0.23228	0.55329	No
180	I60	0.20088	0.23228	0.75329	No
181	I61	0.30809	0.69835	0.15768	No
182	I62	0.30809	0.69835	0.35768	No
183	I63	0.30809	0.69835	0.55768	No
184	I64	0.30809	0.69835	0.75768	No
185	I65	0.30809	0.69835	0.95768	No
186	I66	0.69191	0.30165	0.05768	No
187	I67	0.69191	0.30165	0.25768	No
188	I68	0.69191	0.30165	0.45768	No
189	I69	0.69191	0.30165	0.65768	No
190	I70	0.69191	0.30165	0.85768	No
191	I71	0.80809	0.80165	0.15768	No
192	I72	0.80809	0.80165	0.35768	No
193	I73	0.80809	0.80165	0.55768	No
194	I74	0.80809	0.80165	0.75768	No
195	I75	0.80809	0.80165	0.95768	No
196	I76	0.19191	0.19835	0.05768	No
197	I77	0.19191	0.19835	0.25768	No
198	I78	0.19191	0.19835	0.45768	No
199	I79	0.19191	0.19835	0.65768	No
200	I80	0.19191	0.19835	0.85768	No
201	I81	0.54645	0.76181	0.10427	No
202	I82	0.54645	0.76181	0.30427	No

203	I83	0.54645	0.76181	0.50427	No
204	I84	0.54645	0.76181	0.70427	No
205	I85	0.54645	0.76181	0.90427	No
206	I86	0.45355	0.23819	0.00427	No
207	I87	0.45355	0.23819	0.20427	No
208	I88	0.45355	0.23819	0.40427	No
209	I89	0.45355	0.23819	0.60427	No
210	I90	0.45355	0.23819	0.80427	No
211	I91	0.04645	0.73819	0.10427	No
212	I92	0.04645	0.73819	0.30427	No
213	I93	0.04645	0.73819	0.50427	No
214	I94	0.04645	0.73819	0.70427	No
215	I95	0.04645	0.73819	0.90427	No
216	I96	0.95355	0.26181	0.00427	No
217	I97	0.95355	0.26181	0.20427	No
218	I98	0.95355	0.26181	0.40427	No
219	I99	0.95355	0.26181	0.60427	No
220	I100	0.95355	0.26181	0.80427	No
221	H1	0.43960	0.27810	0.06640	No
222	H2	0.43960	0.27810	0.26640	No
223	H3	0.43960	0.27810	0.46640	No
224	H4	0.43960	0.27810	0.66640	No
225	H5	0.43960	0.27810	0.86640	No
226	H6	0.56040	0.72190	0.96640	No
227	H7	0.56040	0.72190	0.16640	No
228	H8	0.56040	0.72190	0.36640	No
229	H9	0.56040	0.72190	0.56640	No
230	H10	0.56040	0.72190	0.76640	No
231	H11	0.93960	0.22190	0.06640	No
232	H12	0.93960	0.22190	0.26640	No
233	H13	0.93960	0.22190	0.46640	No
234	H14	0.93960	0.22190	0.66640	No
235	H15	0.93960	0.22190	0.86640	No
236	H16	0.06040	0.77810	0.96640	No
237	H17	0.06040	0.77810	0.16640	No
238	H18	0.06040	0.77810	0.36640	No
239	H19	0.06040	0.77810	0.56640	No
240	H20	0.06040	0.77810	0.76640	No

241	H21	0.50570	0.32420	0.08704	No
242	H22	0.50570	0.32420	0.28704	No
243	H23	0.50570	0.32420	0.48704	No
244	H24	0.50570	0.32420	0.68704	No
245	H25	0.50570	0.32420	0.88704	No
246	H26	0.49430	0.67580	0.98704	No
247	H27	0.49430	0.67580	0.18704	No
248	H28	0.49430	0.67580	0.38704	No
249	H29	0.49430	0.67580	0.58704	No
250	H30	0.49430	0.67580	0.78704	No
251	H31	0.00570	0.17580	0.08704	No
252	H32	0.00570	0.17580	0.28704	No
253	H33	0.00570	0.17580	0.48704	No
254	H34	0.00570	0.17580	0.68704	No
255	H35	0.00570	0.17580	0.88704	No
256	H36	0.99430	0.82420	0.98704	No
257	H37	0.99430	0.82420	0.18704	No
258	H38	0.99430	0.82420	0.38704	No
259	H39	0.99430	0.82420	0.58704	No
260	H40	0.99430	0.82420	0.78704	No
261	H41	0.40970	0.34510	0.09086	No
262	H42	0.40970	0.34510	0.29086	No
263	H43	0.40970	0.34510	0.49086	No
264	H44	0.40970	0.34510	0.69086	No
265	H45	0.40970	0.34510	0.89086	No
266	H46	0.59030	0.65490	0.99086	No
267	H47	0.59030	0.65490	0.19086	No
268	H48	0.59030	0.65490	0.39086	No
269	H49	0.59030	0.65490	0.59086	No
270	H50	0.59030	0.65490	0.79086	No
271	H51	0.90970	0.15490	0.09086	No
272	H52	0.90970	0.15490	0.29086	No
273	H53	0.90970	0.15490	0.49086	No
274	H54	0.90970	0.15490	0.69086	No
275	H55	0.90970	0.15490	0.89086	No
276	H56	0.09030	0.84510	0.99086	No
277	H57	0.09030	0.84510	0.19086	No
278	H58	0.09030	0.84510	0.39086	No

279	H59	0.09030	0.84510	0.59086	No
280	H60	0.09030	0.84510	0.79086	No
281	H61	0.22060	0.90500	0.07076	No
282	H62	0.22060	0.90500	0.27076	No
283	H63	0.22060	0.90500	0.47076	No
284	H64	0.22060	0.90500	0.67076	No
285	H65	0.22060	0.90500	0.87076	No
286	H66	0.77940	0.09500	0.97076	No
287	H67	0.77940	0.09500	0.17076	No
288	H68	0.77940	0.09500	0.37076	No
289	H69	0.77940	0.09500	0.57076	No
290	H70	0.77940	0.09500	0.77076	No
291	H71	0.72060	0.59500	0.07076	No
292	H72	0.72060	0.59500	0.27076	No
293	H73	0.72060	0.59500	0.47076	No
294	H74	0.72060	0.59500	0.67076	No
295	H75	0.72060	0.59500	0.87076	No
296	H76	0.27940	0.40500	0.97076	No
297	H77	0.27940	0.40500	0.17076	No
298	H78	0.27940	0.40500	0.37076	No
299	H79	0.27940	0.40500	0.57076	No
300	H80	0.27940	0.40500	0.77076	No
301	H81	0.17940	0.99870	0.07702	No
302	H82	0.17940	0.99870	0.27702	No
303	H83	0.17940	0.99870	0.47702	No
304	H84	0.17940	0.99870	0.67702	No
305	H85	0.17940	0.99870	0.87702	No
306	H86	0.82060	0.00130	0.97702	No
307	H87	0.82060	0.00130	0.17702	No
308	H88	0.82060	0.00130	0.37702	No
309	H89	0.82060	0.00130	0.57702	No
310	H90	0.82060	0.00130	0.77702	No
311	H91	0.67940	0.50130	0.07702	No
312	H92	0.67940	0.50130	0.27702	No
313	H93	0.67940	0.50130	0.47702	No
314	H94	0.67940	0.50130	0.67702	No
315	H95	0.67940	0.50130	0.87702	No
316	H96	0.32060	0.49870	0.97702	No

317	H97	0.32060	0.49870	0.17702	No
318	H98	0.32060	0.49870	0.37702	No
319	H99	0.32060	0.49870	0.57702	No
320	H100	0.32060	0.49870	0.77702	No
321	H101	0.14300	0.91200	0.09190	No
322	H102	0.14300	0.91200	0.29190	No
323	H103	0.14300	0.91200	0.49190	No
324	H104	0.14300	0.91200	0.69190	No
325	H105	0.14300	0.91200	0.89190	No
326	H106	0.85700	0.08800	0.99190	No
327	H107	0.85700	0.08800	0.19190	No
328	H108	0.85700	0.08800	0.39190	No
329	H109	0.85700	0.08800	0.59190	No
330	H110	0.85700	0.08800	0.79190	No
331	H111	0.64300	0.58800	0.09190	No
332	H112	0.64300	0.58800	0.29190	No
333	H113	0.64300	0.58800	0.49190	No
334	H114	0.64300	0.58800	0.69190	No
335	H115	0.64300	0.58800	0.89190	No
336	H116	0.35700	0.41200	0.99190	No
337	H117	0.35700	0.41200	0.19190	No
338	H118	0.35700	0.41200	0.39190	No
339	H119	0.35700	0.41200	0.59190	No
340	H120	0.35700	0.41200	0.79190	No
341	H121	0.37870	0.20070	0.11042	No
342	H122	0.37870	0.20070	0.31042	No
343	H123	0.37870	0.20070	0.51042	No
344	H124	0.37870	0.20070	0.71042	No
345	H125	0.37870	0.20070	0.91042	No
346	H126	0.62130	0.79930	0.01042	No
347	H127	0.62130	0.79930	0.21042	No
348	H128	0.62130	0.79930	0.41042	No
349	H129	0.62130	0.79930	0.61042	No
350	H130	0.62130	0.79930	0.81042	No
351	H131	0.87870	0.29930	0.11042	No
352	H132	0.87870	0.29930	0.31042	No
353	H133	0.87870	0.29930	0.51042	No
354	H134	0.87870	0.29930	0.71042	No

355	H135	0.87870	0.29930	0.91042	No
356	H136	0.12130	0.70070	0.01042	No
357	H137	0.12130	0.70070	0.21042	No
358	H138	0.12130	0.70070	0.41042	No
359	H139	0.12130	0.70070	0.61042	No
360	H140	0.12130	0.70070	0.81042	No
361	H141	0.46340	0.23930	0.12906	No
362	H142	0.46340	0.23930	0.32906	No
363	H143	0.46340	0.23930	0.52906	No
364	H144	0.46340	0.23930	0.72906	No
365	H145	0.46340	0.23930	0.92906	No
366	H146	0.53660	0.76070	0.02906	No
367	H147	0.53660	0.76070	0.22906	No
368	H148	0.53660	0.76070	0.42906	No
369	H149	0.53660	0.76070	0.62906	No
370	H150	0.53660	0.76070	0.82906	No
371	H151	0.96340	0.26070	0.12906	No
372	H152	0.96340	0.26070	0.32906	No
373	H153	0.96340	0.26070	0.52906	No
374	H154	0.96340	0.26070	0.72906	No
375	H155	0.96340	0.26070	0.92906	No
376	H156	0.03660	0.73930	0.02906	No
377	H157	0.03660	0.73930	0.22906	No
378	H158	0.03660	0.73930	0.42906	No
379	H159	0.03660	0.73930	0.62906	No
380	H160	0.03660	0.73930	0.82906	No
381	H161	0.47240	0.11130	0.07710	No
382	H162	0.47240	0.11130	0.27710	No
383	H163	0.47240	0.11130	0.47710	No
384	H164	0.47240	0.11130	0.67710	No
385	H165	0.47240	0.11130	0.87710	No
386	H166	0.52760	0.88870	0.97710	No
387	H167	0.52760	0.88870	0.17710	No
388	H168	0.52760	0.88870	0.37710	No
389	H169	0.52760	0.88870	0.57710	No
390	H170	0.52760	0.88870	0.77710	No
391	H171	0.97240	0.38870	0.07710	No
392	H172	0.97240	0.38870	0.27710	No

393	H173	0.97240	0.38870	0.47710	No
394	H174	0.97240	0.38870	0.67710	No
395	H175	0.97240	0.38870	0.87710	No
396	H176	0.02760	0.61130	0.97710	No
397	H177	0.02760	0.61130	0.17710	No
398	H178	0.02760	0.61130	0.37710	No
399	H179	0.02760	0.61130	0.57710	No
400	H180	0.02760	0.61130	0.77710	No
401	H181	0.55860	0.15340	0.09382	No
402	H182	0.55860	0.15340	0.29382	No
403	H183	0.55860	0.15340	0.49382	No
404	H184	0.55860	0.15340	0.69382	No
405	H185	0.55860	0.15340	0.89382	No
406	H186	0.44140	0.84660	0.99382	No
407	H187	0.44140	0.84660	0.19382	No
408	H188	0.44140	0.84660	0.39382	No
409	H189	0.44140	0.84660	0.59382	No
410	H190	0.44140	0.84660	0.79382	No
411	H191	0.05860	0.34660	0.09382	No
412	H192	0.05860	0.34660	0.29382	No
413	H193	0.05860	0.34660	0.49382	No
414	H194	0.05860	0.34660	0.69382	No
415	H195	0.05860	0.34660	0.89382	No
416	H196	0.94140	0.65340	0.99382	No
417	H197	0.94140	0.65340	0.19382	No
418	H198	0.94140	0.65340	0.39382	No
419	H199	0.94140	0.65340	0.59382	No
420	H200	0.94140	0.65340	0.79382	No
421	H201	0.52810	0.99740	0.11126	No
422	H202	0.52810	0.99740	0.31126	No
423	H203	0.52810	0.99740	0.51126	No
424	H204	0.52810	0.99740	0.71126	No
425	H205	0.52810	0.99740	0.91126	No
426	H206	0.47190	0.00260	0.01126	No
427	H207	0.47190	0.00260	0.21126	No
428	H208	0.47190	0.00260	0.41126	No
429	H209	0.47190	0.00260	0.61126	No
430	H210	0.47190	0.00260	0.81126	No

431	H211	0.02810	0.50260	0.11126	No
432	H212	0.02810	0.50260	0.31126	No
433	H213	0.02810	0.50260	0.51126	No
434	H214	0.02810	0.50260	0.71126	No
435	H215	0.02810	0.50260	0.91126	No
436	H216	0.97190	0.49740	0.01126	No
437	H217	0.97190	0.49740	0.21126	No
438	H218	0.97190	0.49740	0.41126	No
439	H219	0.97190	0.49740	0.61126	No
440	H220	0.97190	0.49740	0.81126	No
441	H221	0.52650	0.07110	0.13938	No
442	H222	0.52650	0.07110	0.33938	No
443	H223	0.52650	0.07110	0.53938	No
444	H224	0.52650	0.07110	0.73938	No
445	H225	0.52650	0.07110	0.93938	No
446	H226	0.47350	0.92890	0.03938	No
447	H227	0.47350	0.92890	0.23938	No
448	H228	0.47350	0.92890	0.43938	No
449	H229	0.47350	0.92890	0.63938	No
450	H230	0.47350	0.92890	0.83938	No
451	H231	0.02650	0.42890	0.13938	No
452	H232	0.02650	0.42890	0.33938	No
453	H233	0.02650	0.42890	0.53938	No
454	H234	0.02650	0.42890	0.73938	No
455	H235	0.02650	0.42890	0.93938	No
456	H236	0.97350	0.57110	0.03938	No
457	H237	0.97350	0.57110	0.23938	No
458	H238	0.97350	0.57110	0.43938	No
459	H239	0.97350	0.57110	0.63938	No
460	H240	0.97350	0.57110	0.83938	No
461	H241	0.37400	0.06910	0.14084	No
462	H242	0.37400	0.06910	0.34084	No
463	H243	0.37400	0.06910	0.54084	No
464	H244	0.37400	0.06910	0.74084	No
465	H245	0.37400	0.06910	0.94084	No
466	H246	0.62600	0.93090	0.04084	No
467	H247	0.62600	0.93090	0.24084	No
468	H248	0.62600	0.93090	0.44084	No

469	H249	0.62600	0.93090	0.64084	No
470	H250	0.62600	0.93090	0.84084	No
471	H251	0.87400	0.43090	0.14084	No
472	H252	0.87400	0.43090	0.34084	No
473	H253	0.87400	0.43090	0.54084	No
474	H254	0.87400	0.43090	0.74084	No
475	H255	0.87400	0.43090	0.94084	No
476	H256	0.12600	0.56910	0.04084	No
477	H257	0.12600	0.56910	0.24084	No
478	H258	0.12600	0.56910	0.44084	No
479	H259	0.12600	0.56910	0.64084	No
480	H260	0.12600	0.56910	0.84084	No
481	H261	0.40970	0.96290	0.14300	No
482	H262	0.40970	0.96290	0.34300	No
483	H263	0.40970	0.96290	0.54300	No
484	H264	0.40970	0.96290	0.74300	No
485	H265	0.40970	0.96290	0.94300	No
486	H266	0.59030	0.03710	0.04300	No
487	H267	0.59030	0.03710	0.24300	No
488	H268	0.59030	0.03710	0.44300	No
489	H269	0.59030	0.03710	0.64300	No
490	H270	0.59030	0.03710	0.84300	No
491	H271	0.90970	0.53710	0.14300	No
492	H272	0.90970	0.53710	0.34300	No
493	H273	0.90970	0.53710	0.54300	No
494	H274	0.90970	0.53710	0.74300	No
495	H275	0.90970	0.53710	0.94300	No
496	H276	0.09030	0.46290	0.04300	No
497	H277	0.09030	0.46290	0.24300	No
498	H278	0.09030	0.46290	0.44300	No
499	H279	0.09030	0.46290	0.64300	No
500	H280	0.09030	0.46290	0.84300	No
501	H281	0.33640	0.04580	0.08812	No
502	H282	0.33640	0.04580	0.28812	No
503	H283	0.33640	0.04580	0.48812	No
504	H284	0.33640	0.04580	0.68812	No
505	H285	0.33640	0.04580	0.88812	No
506	H286	0.66360	0.95420	0.98812	No

507	H287	0.66360	0.95420	0.18812	No
508	H288	0.66360	0.95420	0.38812	No
509	H289	0.66360	0.95420	0.58812	No
510	H290	0.66360	0.95420	0.78812	No
511	H291	0.83640	0.45420	0.08812	No
512	H292	0.83640	0.45420	0.28812	No
513	H293	0.83640	0.45420	0.48812	No
514	H294	0.83640	0.45420	0.68812	No
515	H295	0.83640	0.45420	0.88812	No
516	H296	0.16360	0.54580	0.98812	No
517	H297	0.16360	0.54580	0.18812	No
518	H298	0.16360	0.54580	0.38812	No
519	H299	0.16360	0.54580	0.58812	No
520	H300	0.16360	0.54580	0.78812	No
521	H301	0.37410	0.93990	0.08970	No
522	H302	0.37410	0.93990	0.28970	No
523	H303	0.37410	0.93990	0.48970	No
524	H304	0.37410	0.93990	0.68970	No
525	H305	0.37410	0.93990	0.88970	No
526	H306	0.62590	0.06010	0.98970	No
527	H307	0.62590	0.06010	0.18970	No
528	H308	0.62590	0.06010	0.38970	No
529	H309	0.62590	0.06010	0.58970	No
530	H310	0.62590	0.06010	0.78970	No
531	H311	0.87410	0.56010	0.08970	No
532	H312	0.87410	0.56010	0.28970	No
533	H313	0.87410	0.56010	0.48970	No
534	H314	0.87410	0.56010	0.68970	No
535	H315	0.87410	0.56010	0.88970	No
536	H316	0.12590	0.43990	0.98970	No
537	H317	0.12590	0.43990	0.18970	No
538	H318	0.12590	0.43990	0.38970	No
539	H319	0.12590	0.43990	0.58970	No
540	H320	0.12590	0.43990	0.78970	No
541	H321	0.26160	0.89450	0.12342	No
542	H322	0.26160	0.89450	0.32342	No
543	H323	0.26160	0.89450	0.52342	No
544	H324	0.26160	0.89450	0.72342	No

545	H325	0.26160	0.89450	0.92342	No
546	H326	0.73840	0.10550	0.02342	No
547	H327	0.73840	0.10550	0.22342	No
548	H328	0.73840	0.10550	0.42342	No
549	H329	0.73840	0.10550	0.62342	No
550	H330	0.73840	0.10550	0.82342	No
551	H331	0.76160	0.60550	0.12342	No
552	H332	0.76160	0.60550	0.32342	No
553	H333	0.76160	0.60550	0.52342	No
554	H334	0.76160	0.60550	0.72342	No
555	H335	0.76160	0.60550	0.92342	No
556	H336	0.23840	0.39450	0.02342	No
557	H337	0.23840	0.39450	0.22342	No
558	H338	0.23840	0.39450	0.42342	No
559	H339	0.23840	0.39450	0.62342	No
560	H340	0.23840	0.39450	0.82342	No
561	H341	0.22810	0.00160	0.12678	No
562	H342	0.22810	0.00160	0.32678	No
563	H343	0.22810	0.00160	0.52678	No
564	H344	0.22810	0.00160	0.72678	No
565	H345	0.22810	0.00160	0.92678	No
566	H346	0.77190	0.99840	0.02678	No
567	H347	0.77190	0.99840	0.22678	No
568	H348	0.77190	0.99840	0.42678	No
569	H349	0.77190	0.99840	0.62678	No
570	H350	0.77190	0.99840	0.82678	No
571	H351	0.72810	0.49840	0.12678	No
572	H352	0.72810	0.49840	0.32678	No
573	H353	0.72810	0.49840	0.52678	No
574	H354	0.72810	0.49840	0.72678	No
575	H355	0.72810	0.49840	0.92678	No
576	H356	0.27190	0.50160	0.02678	No
577	H357	0.27190	0.50160	0.22678	No
578	H358	0.27190	0.50160	0.42678	No
579	H359	0.27190	0.50160	0.62678	No
580	H360	0.27190	0.50160	0.82678	No
581	Bi1	0.38917	0.62103	0.30063	No
582	Bi2	0.38917	0.62103	0.50063	No

583	Bi3	0.38917	0.62103	0.70063	No
584	Bi4	0.61083	0.37897	0.20063	No
585	Bi5	0.61083	0.37897	0.40063	No
586	Bi6	0.61083	0.37897	0.60063	No
587	Bi7	0.88917	0.87897	0.10063	No
588	Bi8	0.88917	0.87897	0.30063	No
589	Bi9	0.88917	0.87897	0.50063	No
590	Bi10	0.88917	0.87897	0.90063	No
591	Bi11	0.11083	0.12103	0.20063	No
592	Bi12	0.11083	0.12103	0.80063	No
593	N1	0.45000	0.29950	0.08598	No
594	N2	0.45000	0.29950	0.28598	No
595	N3	0.45000	0.29950	0.48598	No
596	N4	0.45000	0.29950	0.68598	No
597	N5	0.45000	0.29950	0.88598	No
598	N6	0.55000	0.70050	0.98598	No
599	N7	0.55000	0.70050	0.18598	No
600	N8	0.55000	0.70050	0.38598	No
601	N9	0.55000	0.70050	0.58598	No
602	N10	0.55000	0.70050	0.78598	No
603	N11	0.95000	0.20050	0.08598	No
604	N12	0.95000	0.20050	0.28598	No
605	N13	0.95000	0.20050	0.48598	No
606	N14	0.95000	0.20050	0.68598	No
607	N15	0.95000	0.20050	0.88598	No
608	N16	0.05000	0.79950	0.98598	No
609	N17	0.05000	0.79950	0.18598	No
610	N18	0.05000	0.79950	0.38598	No
611	N19	0.05000	0.79950	0.58598	No
612	N20	0.05000	0.79950	0.78598	No
613	N21	0.19340	0.94140	0.08536	No
614	N22	0.19340	0.94140	0.28536	No
615	N23	0.19340	0.94140	0.48536	No
616	N24	0.19340	0.94140	0.68536	No
617	N25	0.19340	0.94140	0.88536	No
618	N26	0.80660	0.05860	0.98536	No
619	N27	0.80660	0.05860	0.18536	No
620	N28	0.80660	0.05860	0.38536	No

621	N29	0.80660	0.05860	0.58536	No
622	N30	0.80660	0.05860	0.78536	No
623	N31	0.69340	0.55860	0.08536	No
624	N32	0.69340	0.55860	0.28536	No
625	N33	0.69340	0.55860	0.48536	No
626	N34	0.69340	0.55860	0.68536	No
627	N35	0.69340	0.55860	0.88536	No
628	N36	0.30660	0.44140	0.98536	No
629	N37	0.30660	0.44140	0.18536	No
630	N38	0.30660	0.44140	0.38536	No
631	N39	0.30660	0.44140	0.58536	No
632	N40	0.30660	0.44140	0.78536	No
633	Sb1	0.38917	0.62103	0.10063	No
634	Sb2	0.38917	0.62103	0.90063	No
635	Sb3	0.61083	0.37897	0.00063	No
636	Sb4	0.61083	0.37897	0.80063	No
637	Sb5	0.88917	0.87897	0.70063	No
638	Sb6	0.11083	0.12103	0.00063	No
639	Sb7	0.11083	0.12103	0.40063	No
640	Sb8	0.11083	0.12103	0.60063	No

Reflex Summary Report for Rietveld Refinement of 0.5[C₆N₂H₁₈][BiI₅+0.5[C₆N₂H₁₈][SbI₅ :

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.18922 ± 0.09999	Yes
b	14.07900 ± 0.09154	Yes
c	43.10229 ± 0.28796	Yes
α	86.18424 ± 0.04141	Yes
β	92.30210 ± 0.03933	Yes
γ	90.14920 ± 0.07023	Yes

Structure Parameters

Refined Motion Groups: 0
Refined Torsions: 0

Refined Angles: 0
Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
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1	C1	0.44190	0.21900	0.10840	No
2	C2	0.44190	0.21900	0.30840	No
3	C3	0.44190	0.21900	0.50840	No
4	C4	0.44190	0.21900	0.70840	No
5	C5	0.44190	0.21900	0.90840	No
6	C6	0.55810	0.78100	0.00840	No
7	C7	0.55810	0.78100	0.20840	No
8	C8	0.55810	0.78100	0.40840	No
9	C9	0.55810	0.78100	0.60840	No
10	C10	0.55810	0.78100	0.80840	No
11	C11	0.94190	0.28100	0.10840	No
12	C12	0.94190	0.28100	0.30840	No
13	C13	0.94190	0.28100	0.50840	No
14	C14	0.94190	0.28100	0.70840	No
15	C15	0.94190	0.28100	0.90840	No
16	C16	0.05810	0.71900	0.00840	No
17	C17	0.05810	0.71900	0.20840	No
18	C18	0.05810	0.71900	0.40840	No
19	C19	0.05810	0.71900	0.60840	No
20	C20	0.05810	0.71900	0.80840	No
21	C21	0.49640	0.13340	0.09722	No
22	C22	0.49640	0.13340	0.29722	No
23	C23	0.49640	0.13340	0.49722	No
24	C24	0.49640	0.13340	0.69722	No
25	C25	0.49640	0.13340	0.89722	No
26	C26	0.50360	0.86660	0.99722	No
27	C27	0.50360	0.86660	0.19722	No
28	C28	0.50360	0.86660	0.39722	No
29	C29	0.50360	0.86660	0.59722	No
30	C30	0.50360	0.86660	0.79722	No
31	C31	0.99640	0.36660	0.09722	No
32	C32	0.99640	0.36660	0.29722	No
33	C33	0.99640	0.36660	0.49722	No
34	C34	0.99640	0.36660	0.69722	No
35	C35	0.99640	0.36660	0.89722	No
36	C36	0.00360	0.63340	0.99722	No
37	C37	0.00360	0.63340	0.19722	No
38	C38	0.00360	0.63340	0.39722	No

39	C39	0.00360	0.63340	0.59722	No
40	C40	0.00360	0.63340	0.79722	No
41	C41	0.49500	0.05130	0.12030	No
42	C42	0.49500	0.05130	0.32030	No
43	C43	0.49500	0.05130	0.52030	No
44	C44	0.49500	0.05130	0.72030	No
45	C45	0.49500	0.05130	0.92030	No
46	C46	0.50500	0.94870	0.02030	No
47	C47	0.50500	0.94870	0.22030	No
48	C48	0.50500	0.94870	0.42030	No
49	C49	0.50500	0.94870	0.62030	No
50	C50	0.50500	0.94870	0.82030	No
51	C51	0.99500	0.44870	0.12030	No
52	C52	0.99500	0.44870	0.32030	No
53	C53	0.99500	0.44870	0.52030	No
54	C54	0.99500	0.44870	0.72030	No
55	C55	0.99500	0.44870	0.92030	No
56	C56	0.00500	0.55130	0.02030	No
57	C57	0.00500	0.55130	0.22030	No
58	C58	0.00500	0.55130	0.42030	No
59	C59	0.00500	0.55130	0.62030	No
60	C60	0.00500	0.55130	0.82030	No
61	C61	0.40380	0.01810	0.12902	No
62	C62	0.40380	0.01810	0.32902	No
63	C63	0.40380	0.01810	0.52902	No
64	C64	0.40380	0.01810	0.72902	No
65	C65	0.40380	0.01810	0.92902	No
66	C66	0.59620	0.98190	0.02902	No
67	C67	0.59620	0.98190	0.22902	No
68	C68	0.59620	0.98190	0.42902	No
69	C69	0.59620	0.98190	0.62902	No
70	C70	0.59620	0.98190	0.82902	No
71	C71	0.90380	0.48190	0.12902	No
72	C72	0.90380	0.48190	0.32902	No
73	C73	0.90380	0.48190	0.52902	No
74	C74	0.90380	0.48190	0.72902	No
75	C75	0.90380	0.48190	0.92902	No
76	C76	0.09620	0.51810	0.02902	No

77	C77	0.09620	0.51810	0.22902	No
78	C78	0.09620	0.51810	0.42902	No
79	C79	0.09620	0.51810	0.62902	No
80	C80	0.09620	0.51810	0.82902	No
81	C81	0.34450	0.99030	0.10188	No
82	C82	0.34450	0.99030	0.30188	No
83	C83	0.34450	0.99030	0.50188	No
84	C84	0.34450	0.99030	0.70188	No
85	C85	0.34450	0.99030	0.90188	No
86	C86	0.65550	0.00970	0.00188	No
87	C87	0.65550	0.00970	0.20188	No
88	C88	0.65550	0.00970	0.40188	No
89	C89	0.65550	0.00970	0.60188	No
90	C90	0.65550	0.00970	0.80188	No
91	C91	0.84450	0.50970	0.10188	No
92	C92	0.84450	0.50970	0.30188	No
93	C93	0.84450	0.50970	0.50188	No
94	C94	0.84450	0.50970	0.70188	No
95	C95	0.84450	0.50970	0.90188	No
96	C96	0.15550	0.49030	0.00188	No
97	C97	0.15550	0.49030	0.20188	No
98	C98	0.15550	0.49030	0.40188	No
99	C99	0.15550	0.49030	0.60188	No
100	C100	0.15550	0.49030	0.80188	No
101	C101	0.25450	0.95520	0.11224	No
102	C102	0.25450	0.95520	0.31224	No
103	C103	0.25450	0.95520	0.51224	No
104	C104	0.25450	0.95520	0.71224	No
105	C105	0.25450	0.95520	0.91224	No
106	C106	0.74550	0.04480	0.01224	No
107	C107	0.74550	0.04480	0.21224	No
108	C108	0.74550	0.04480	0.41224	No
109	C109	0.74550	0.04480	0.61224	No
110	C110	0.74550	0.04480	0.81224	No
111	C111	0.75450	0.54480	0.11224	No
112	C112	0.75450	0.54480	0.31224	No
113	C113	0.75450	0.54480	0.51224	No
114	C114	0.75450	0.54480	0.71224	No

115	C115	0.75450	0.54480	0.91224	No
116	C116	0.24550	0.45520	0.01224	No
117	C117	0.24550	0.45520	0.21224	No
118	C118	0.24550	0.45520	0.41224	No
119	C119	0.24550	0.45520	0.61224	No
120	C120	0.24550	0.45520	0.81224	No
121	I1	0.48458	0.51909	0.04212	No
122	I2	0.48458	0.51909	0.24212	No
123	I3	0.48458	0.51909	0.44212	No
124	I4	0.48458	0.51909	0.64212	No
125	I5	0.48458	0.51909	0.84212	No
126	I6	0.51542	0.48091	0.94212	No
127	I7	0.51542	0.48091	0.14212	No
128	I8	0.51542	0.48091	0.34212	No
129	I9	0.51542	0.48091	0.54212	No
130	I10	0.51542	0.48091	0.74212	No
131	I11	0.98458	0.98091	0.04212	No
132	I12	0.98458	0.98091	0.24212	No
133	I13	0.98458	0.98091	0.44212	No
134	I14	0.98458	0.98091	0.64212	No
135	I15	0.98458	0.98091	0.84212	No
136	I16	0.01542	0.01909	0.94212	No
137	I17	0.01542	0.01909	0.14212	No
138	I18	0.01542	0.01909	0.34212	No
139	I19	0.01542	0.01909	0.54212	No
140	I20	0.01542	0.01909	0.74212	No
141	I21	0.25948	0.45560	0.10194	No
142	I22	0.25948	0.45560	0.30194	No
143	I23	0.25948	0.45560	0.50194	No
144	I24	0.25948	0.45560	0.70194	No
145	I25	0.25948	0.45560	0.90194	No
146	I26	0.74052	0.54440	0.00194	No
147	I27	0.74052	0.54440	0.20194	No
148	I28	0.74052	0.54440	0.40194	No
149	I29	0.74052	0.54440	0.60194	No
150	I30	0.74052	0.54440	0.80194	No
151	I31	0.75948	0.04440	0.10194	No
152	I32	0.75948	0.04440	0.30194	No

153	I33	0.75948	0.04440	0.50194	No
154	I34	0.75948	0.04440	0.70194	No
155	I35	0.75948	0.04440	0.90194	No
156	I36	0.24052	0.95560	0.00194	No
157	I37	0.24052	0.95560	0.20194	No
158	I38	0.24052	0.95560	0.40194	No
159	I39	0.24052	0.95560	0.60194	No
160	I40	0.24052	0.95560	0.80194	No
161	I41	0.29912	0.73228	0.05329	No
162	I42	0.29912	0.73228	0.25329	No
163	I43	0.29912	0.73228	0.45329	No
164	I44	0.29912	0.73228	0.65329	No
165	I45	0.29912	0.73228	0.85329	No
166	I46	0.70088	0.26772	0.95329	No
167	I47	0.70088	0.26772	0.15329	No
168	I48	0.70088	0.26772	0.35329	No
169	I49	0.70088	0.26772	0.55329	No
170	I50	0.70088	0.26772	0.75329	No
171	I51	0.79912	0.76772	0.05329	No
172	I52	0.79912	0.76772	0.25329	No
173	I53	0.79912	0.76772	0.45329	No
174	I54	0.79912	0.76772	0.65329	No
175	I55	0.79912	0.76772	0.85329	No
176	I56	0.20088	0.23228	0.95329	No
177	I57	0.20088	0.23228	0.15329	No
178	I58	0.20088	0.23228	0.35329	No
179	I59	0.20088	0.23228	0.55329	No
180	I60	0.20088	0.23228	0.75329	No
181	I61	0.30809	0.69835	0.15768	No
182	I62	0.30809	0.69835	0.35768	No
183	I63	0.30809	0.69835	0.55768	No
184	I64	0.30809	0.69835	0.75768	No
185	I65	0.30809	0.69835	0.95768	No
186	I66	0.69191	0.30165	0.05768	No
187	I67	0.69191	0.30165	0.25768	No
188	I68	0.69191	0.30165	0.45768	No
189	I69	0.69191	0.30165	0.65768	No
190	I70	0.69191	0.30165	0.85768	No

191	I71	0.80809	0.80165	0.15768	No
192	I72	0.80809	0.80165	0.35768	No
193	I73	0.80809	0.80165	0.55768	No
194	I74	0.80809	0.80165	0.75768	No
195	I75	0.80809	0.80165	0.95768	No
196	I76	0.19191	0.19835	0.05768	No
197	I77	0.19191	0.19835	0.25768	No
198	I78	0.19191	0.19835	0.45768	No
199	I79	0.19191	0.19835	0.65768	No
200	I80	0.19191	0.19835	0.85768	No
201	I81	0.54645	0.76181	0.10427	No
202	I82	0.54645	0.76181	0.30427	No
203	I83	0.54645	0.76181	0.50427	No
204	I84	0.54645	0.76181	0.70427	No
205	I85	0.54645	0.76181	0.90427	No
206	I86	0.45355	0.23819	0.00427	No
207	I87	0.45355	0.23819	0.20427	No
208	I88	0.45355	0.23819	0.40427	No
209	I89	0.45355	0.23819	0.60427	No
210	I90	0.45355	0.23819	0.80427	No
211	I91	0.04645	0.73819	0.10427	No
212	I92	0.04645	0.73819	0.30427	No
213	I93	0.04645	0.73819	0.50427	No
214	I94	0.04645	0.73819	0.70427	No
215	I95	0.04645	0.73819	0.90427	No
216	I96	0.95355	0.26181	0.00427	No
217	I97	0.95355	0.26181	0.20427	No
218	I98	0.95355	0.26181	0.40427	No
219	I99	0.95355	0.26181	0.60427	No
220	I100	0.95355	0.26181	0.80427	No
221	H1	0.43960	0.27810	0.06640	No
222	H2	0.43960	0.27810	0.26640	No
223	H3	0.43960	0.27810	0.46640	No
224	H4	0.43960	0.27810	0.66640	No
225	H5	0.43960	0.27810	0.86640	No
226	H6	0.56040	0.72190	0.96640	No
227	H7	0.56040	0.72190	0.16640	No
228	H8	0.56040	0.72190	0.36640	No

229	H9	0.56040	0.72190	0.56640	No
230	H10	0.56040	0.72190	0.76640	No
231	H11	0.93960	0.22190	0.06640	No
232	H12	0.93960	0.22190	0.26640	No
233	H13	0.93960	0.22190	0.46640	No
234	H14	0.93960	0.22190	0.66640	No
235	H15	0.93960	0.22190	0.86640	No
236	H16	0.06040	0.77810	0.96640	No
237	H17	0.06040	0.77810	0.16640	No
238	H18	0.06040	0.77810	0.36640	No
239	H19	0.06040	0.77810	0.56640	No
240	H20	0.06040	0.77810	0.76640	No
241	H21	0.50570	0.32420	0.08704	No
242	H22	0.50570	0.32420	0.28704	No
243	H23	0.50570	0.32420	0.48704	No
244	H24	0.50570	0.32420	0.68704	No
245	H25	0.50570	0.32420	0.88704	No
246	H26	0.49430	0.67580	0.98704	No
247	H27	0.49430	0.67580	0.18704	No
248	H28	0.49430	0.67580	0.38704	No
249	H29	0.49430	0.67580	0.58704	No
250	H30	0.49430	0.67580	0.78704	No
251	H31	0.00570	0.17580	0.08704	No
252	H32	0.00570	0.17580	0.28704	No
253	H33	0.00570	0.17580	0.48704	No
254	H34	0.00570	0.17580	0.68704	No
255	H35	0.00570	0.17580	0.88704	No
256	H36	0.99430	0.82420	0.98704	No
257	H37	0.99430	0.82420	0.18704	No
258	H38	0.99430	0.82420	0.38704	No
259	H39	0.99430	0.82420	0.58704	No
260	H40	0.99430	0.82420	0.78704	No
261	H41	0.40970	0.34510	0.09086	No
262	H42	0.40970	0.34510	0.29086	No
263	H43	0.40970	0.34510	0.49086	No
264	H44	0.40970	0.34510	0.69086	No
265	H45	0.40970	0.34510	0.89086	No
266	H46	0.59030	0.65490	0.99086	No

267	H47	0.59030	0.65490	0.19086	No
268	H48	0.59030	0.65490	0.39086	No
269	H49	0.59030	0.65490	0.59086	No
270	H50	0.59030	0.65490	0.79086	No
271	H51	0.90970	0.15490	0.09086	No
272	H52	0.90970	0.15490	0.29086	No
273	H53	0.90970	0.15490	0.49086	No
274	H54	0.90970	0.15490	0.69086	No
275	H55	0.90970	0.15490	0.89086	No
276	H56	0.09030	0.84510	0.99086	No
277	H57	0.09030	0.84510	0.19086	No
278	H58	0.09030	0.84510	0.39086	No
279	H59	0.09030	0.84510	0.59086	No
280	H60	0.09030	0.84510	0.79086	No
281	H61	0.22060	0.90500	0.07076	No
282	H62	0.22060	0.90500	0.27076	No
283	H63	0.22060	0.90500	0.47076	No
284	H64	0.22060	0.90500	0.67076	No
285	H65	0.22060	0.90500	0.87076	No
286	H66	0.77940	0.09500	0.97076	No
287	H67	0.77940	0.09500	0.17076	No
288	H68	0.77940	0.09500	0.37076	No
289	H69	0.77940	0.09500	0.57076	No
290	H70	0.77940	0.09500	0.77076	No
291	H71	0.72060	0.59500	0.07076	No
292	H72	0.72060	0.59500	0.27076	No
293	H73	0.72060	0.59500	0.47076	No
294	H74	0.72060	0.59500	0.67076	No
295	H75	0.72060	0.59500	0.87076	No
296	H76	0.27940	0.40500	0.97076	No
297	H77	0.27940	0.40500	0.17076	No
298	H78	0.27940	0.40500	0.37076	No
299	H79	0.27940	0.40500	0.57076	No
300	H80	0.27940	0.40500	0.77076	No
301	H81	0.17940	0.99870	0.07702	No
302	H82	0.17940	0.99870	0.27702	No
303	H83	0.17940	0.99870	0.47702	No
304	H84	0.17940	0.99870	0.67702	No

305	H85	0.17940	0.99870	0.87702	No
306	H86	0.82060	0.00130	0.97702	No
307	H87	0.82060	0.00130	0.17702	No
308	H88	0.82060	0.00130	0.37702	No
309	H89	0.82060	0.00130	0.57702	No
310	H90	0.82060	0.00130	0.77702	No
311	H91	0.67940	0.50130	0.07702	No
312	H92	0.67940	0.50130	0.27702	No
313	H93	0.67940	0.50130	0.47702	No
314	H94	0.67940	0.50130	0.67702	No
315	H95	0.67940	0.50130	0.87702	No
316	H96	0.32060	0.49870	0.97702	No
317	H97	0.32060	0.49870	0.17702	No
318	H98	0.32060	0.49870	0.37702	No
319	H99	0.32060	0.49870	0.57702	No
320	H100	0.32060	0.49870	0.77702	No
321	H101	0.14300	0.91200	0.09190	No
322	H102	0.14300	0.91200	0.29190	No
323	H103	0.14300	0.91200	0.49190	No
324	H104	0.14300	0.91200	0.69190	No
325	H105	0.14300	0.91200	0.89190	No
326	H106	0.85700	0.08800	0.99190	No
327	H107	0.85700	0.08800	0.19190	No
328	H108	0.85700	0.08800	0.39190	No
329	H109	0.85700	0.08800	0.59190	No
330	H110	0.85700	0.08800	0.79190	No
331	H111	0.64300	0.58800	0.09190	No
332	H112	0.64300	0.58800	0.29190	No
333	H113	0.64300	0.58800	0.49190	No
334	H114	0.64300	0.58800	0.69190	No
335	H115	0.64300	0.58800	0.89190	No
336	H116	0.35700	0.41200	0.99190	No
337	H117	0.35700	0.41200	0.19190	No
338	H118	0.35700	0.41200	0.39190	No
339	H119	0.35700	0.41200	0.59190	No
340	H120	0.35700	0.41200	0.79190	No
341	H121	0.37870	0.20070	0.11042	No
342	H122	0.37870	0.20070	0.31042	No

343	H123	0.37870	0.20070	0.51042	No
344	H124	0.37870	0.20070	0.71042	No
345	H125	0.37870	0.20070	0.91042	No
346	H126	0.62130	0.79930	0.01042	No
347	H127	0.62130	0.79930	0.21042	No
348	H128	0.62130	0.79930	0.41042	No
349	H129	0.62130	0.79930	0.61042	No
350	H130	0.62130	0.79930	0.81042	No
351	H131	0.87870	0.29930	0.11042	No
352	H132	0.87870	0.29930	0.31042	No
353	H133	0.87870	0.29930	0.51042	No
354	H134	0.87870	0.29930	0.71042	No
355	H135	0.87870	0.29930	0.91042	No
356	H136	0.12130	0.70070	0.01042	No
357	H137	0.12130	0.70070	0.21042	No
358	H138	0.12130	0.70070	0.41042	No
359	H139	0.12130	0.70070	0.61042	No
360	H140	0.12130	0.70070	0.81042	No
361	H141	0.46340	0.23930	0.12906	No
362	H142	0.46340	0.23930	0.32906	No
363	H143	0.46340	0.23930	0.52906	No
364	H144	0.46340	0.23930	0.72906	No
365	H145	0.46340	0.23930	0.92906	No
366	H146	0.53660	0.76070	0.02906	No
367	H147	0.53660	0.76070	0.22906	No
368	H148	0.53660	0.76070	0.42906	No
369	H149	0.53660	0.76070	0.62906	No
370	H150	0.53660	0.76070	0.82906	No
371	H151	0.96340	0.26070	0.12906	No
372	H152	0.96340	0.26070	0.32906	No
373	H153	0.96340	0.26070	0.52906	No
374	H154	0.96340	0.26070	0.72906	No
375	H155	0.96340	0.26070	0.92906	No
376	H156	0.03660	0.73930	0.02906	No
377	H157	0.03660	0.73930	0.22906	No
378	H158	0.03660	0.73930	0.42906	No
379	H159	0.03660	0.73930	0.62906	No
380	H160	0.03660	0.73930	0.82906	No

381	H161	0.47240	0.11130	0.07710	No
382	H162	0.47240	0.11130	0.27710	No
383	H163	0.47240	0.11130	0.47710	No
384	H164	0.47240	0.11130	0.67710	No
385	H165	0.47240	0.11130	0.87710	No
386	H166	0.52760	0.88870	0.97710	No
387	H167	0.52760	0.88870	0.17710	No
388	H168	0.52760	0.88870	0.37710	No
389	H169	0.52760	0.88870	0.57710	No
390	H170	0.52760	0.88870	0.77710	No
391	H171	0.97240	0.38870	0.07710	No
392	H172	0.97240	0.38870	0.27710	No
393	H173	0.97240	0.38870	0.47710	No
394	H174	0.97240	0.38870	0.67710	No
395	H175	0.97240	0.38870	0.87710	No
396	H176	0.02760	0.61130	0.97710	No
397	H177	0.02760	0.61130	0.17710	No
398	H178	0.02760	0.61130	0.37710	No
399	H179	0.02760	0.61130	0.57710	No
400	H180	0.02760	0.61130	0.77710	No
401	H181	0.55860	0.15340	0.09382	No
402	H182	0.55860	0.15340	0.29382	No
403	H183	0.55860	0.15340	0.49382	No
404	H184	0.55860	0.15340	0.69382	No
405	H185	0.55860	0.15340	0.89382	No
406	H186	0.44140	0.84660	0.99382	No
407	H187	0.44140	0.84660	0.19382	No
408	H188	0.44140	0.84660	0.39382	No
409	H189	0.44140	0.84660	0.59382	No
410	H190	0.44140	0.84660	0.79382	No
411	H191	0.05860	0.34660	0.09382	No
412	H192	0.05860	0.34660	0.29382	No
413	H193	0.05860	0.34660	0.49382	No
414	H194	0.05860	0.34660	0.69382	No
415	H195	0.05860	0.34660	0.89382	No
416	H196	0.94140	0.65340	0.99382	No
417	H197	0.94140	0.65340	0.19382	No
418	H198	0.94140	0.65340	0.39382	No

419	H199	0.94140	0.65340	0.59382	No
420	H200	0.94140	0.65340	0.79382	No
421	H201	0.52810	0.99740	0.11126	No
422	H202	0.52810	0.99740	0.31126	No
423	H203	0.52810	0.99740	0.51126	No
424	H204	0.52810	0.99740	0.71126	No
425	H205	0.52810	0.99740	0.91126	No
426	H206	0.47190	0.00260	0.01126	No
427	H207	0.47190	0.00260	0.21126	No
428	H208	0.47190	0.00260	0.41126	No
429	H209	0.47190	0.00260	0.61126	No
430	H210	0.47190	0.00260	0.81126	No
431	H211	0.02810	0.50260	0.11126	No
432	H212	0.02810	0.50260	0.31126	No
433	H213	0.02810	0.50260	0.51126	No
434	H214	0.02810	0.50260	0.71126	No
435	H215	0.02810	0.50260	0.91126	No
436	H216	0.97190	0.49740	0.01126	No
437	H217	0.97190	0.49740	0.21126	No
438	H218	0.97190	0.49740	0.41126	No
439	H219	0.97190	0.49740	0.61126	No
440	H220	0.97190	0.49740	0.81126	No
441	H221	0.52650	0.07110	0.13938	No
442	H222	0.52650	0.07110	0.33938	No
443	H223	0.52650	0.07110	0.53938	No
444	H224	0.52650	0.07110	0.73938	No
445	H225	0.52650	0.07110	0.93938	No
446	H226	0.47350	0.92890	0.03938	No
447	H227	0.47350	0.92890	0.23938	No
448	H228	0.47350	0.92890	0.43938	No
449	H229	0.47350	0.92890	0.63938	No
450	H230	0.47350	0.92890	0.83938	No
451	H231	0.02650	0.42890	0.13938	No
452	H232	0.02650	0.42890	0.33938	No
453	H233	0.02650	0.42890	0.53938	No
454	H234	0.02650	0.42890	0.73938	No
455	H235	0.02650	0.42890	0.93938	No
456	H236	0.97350	0.57110	0.03938	No

457	H237	0.97350	0.57110	0.23938	No
458	H238	0.97350	0.57110	0.43938	No
459	H239	0.97350	0.57110	0.63938	No
460	H240	0.97350	0.57110	0.83938	No
461	H241	0.37400	0.06910	0.14084	No
462	H242	0.37400	0.06910	0.34084	No
463	H243	0.37400	0.06910	0.54084	No
464	H244	0.37400	0.06910	0.74084	No
465	H245	0.37400	0.06910	0.94084	No
466	H246	0.62600	0.93090	0.04084	No
467	H247	0.62600	0.93090	0.24084	No
468	H248	0.62600	0.93090	0.44084	No
469	H249	0.62600	0.93090	0.64084	No
470	H250	0.62600	0.93090	0.84084	No
471	H251	0.87400	0.43090	0.14084	No
472	H252	0.87400	0.43090	0.34084	No
473	H253	0.87400	0.43090	0.54084	No
474	H254	0.87400	0.43090	0.74084	No
475	H255	0.87400	0.43090	0.94084	No
476	H256	0.12600	0.56910	0.04084	No
477	H257	0.12600	0.56910	0.24084	No
478	H258	0.12600	0.56910	0.44084	No
479	H259	0.12600	0.56910	0.64084	No
480	H260	0.12600	0.56910	0.84084	No
481	H261	0.40970	0.96290	0.14300	No
482	H262	0.40970	0.96290	0.34300	No
483	H263	0.40970	0.96290	0.54300	No
484	H264	0.40970	0.96290	0.74300	No
485	H265	0.40970	0.96290	0.94300	No
486	H266	0.59030	0.03710	0.04300	No
487	H267	0.59030	0.03710	0.24300	No
488	H268	0.59030	0.03710	0.44300	No
489	H269	0.59030	0.03710	0.64300	No
490	H270	0.59030	0.03710	0.84300	No
491	H271	0.90970	0.53710	0.14300	No
492	H272	0.90970	0.53710	0.34300	No
493	H273	0.90970	0.53710	0.54300	No
494	H274	0.90970	0.53710	0.74300	No

495	H275	0.90970	0.53710	0.94300	No
496	H276	0.09030	0.46290	0.04300	No
497	H277	0.09030	0.46290	0.24300	No
498	H278	0.09030	0.46290	0.44300	No
499	H279	0.09030	0.46290	0.64300	No
500	H280	0.09030	0.46290	0.84300	No
501	H281	0.33640	0.04580	0.08812	No
502	H282	0.33640	0.04580	0.28812	No
503	H283	0.33640	0.04580	0.48812	No
504	H284	0.33640	0.04580	0.68812	No
505	H285	0.33640	0.04580	0.88812	No
506	H286	0.66360	0.95420	0.98812	No
507	H287	0.66360	0.95420	0.18812	No
508	H288	0.66360	0.95420	0.38812	No
509	H289	0.66360	0.95420	0.58812	No
510	H290	0.66360	0.95420	0.78812	No
511	H291	0.83640	0.45420	0.08812	No
512	H292	0.83640	0.45420	0.28812	No
513	H293	0.83640	0.45420	0.48812	No
514	H294	0.83640	0.45420	0.68812	No
515	H295	0.83640	0.45420	0.88812	No
516	H296	0.16360	0.54580	0.98812	No
517	H297	0.16360	0.54580	0.18812	No
518	H298	0.16360	0.54580	0.38812	No
519	H299	0.16360	0.54580	0.58812	No
520	H300	0.16360	0.54580	0.78812	No
521	H301	0.37410	0.93990	0.08970	No
522	H302	0.37410	0.93990	0.28970	No
523	H303	0.37410	0.93990	0.48970	No
524	H304	0.37410	0.93990	0.68970	No
525	H305	0.37410	0.93990	0.88970	No
526	H306	0.62590	0.06010	0.98970	No
527	H307	0.62590	0.06010	0.18970	No
528	H308	0.62590	0.06010	0.38970	No
529	H309	0.62590	0.06010	0.58970	No
530	H310	0.62590	0.06010	0.78970	No
531	H311	0.87410	0.56010	0.08970	No
532	H312	0.87410	0.56010	0.28970	No

533	H313	0.87410	0.56010	0.48970	No
534	H314	0.87410	0.56010	0.68970	No
535	H315	0.87410	0.56010	0.88970	No
536	H316	0.12590	0.43990	0.98970	No
537	H317	0.12590	0.43990	0.18970	No
538	H318	0.12590	0.43990	0.38970	No
539	H319	0.12590	0.43990	0.58970	No
540	H320	0.12590	0.43990	0.78970	No
541	H321	0.26160	0.89450	0.12342	No
542	H322	0.26160	0.89450	0.32342	No
543	H323	0.26160	0.89450	0.52342	No
544	H324	0.26160	0.89450	0.72342	No
545	H325	0.26160	0.89450	0.92342	No
546	H326	0.73840	0.10550	0.02342	No
547	H327	0.73840	0.10550	0.22342	No
548	H328	0.73840	0.10550	0.42342	No
549	H329	0.73840	0.10550	0.62342	No
550	H330	0.73840	0.10550	0.82342	No
551	H331	0.76160	0.60550	0.12342	No
552	H332	0.76160	0.60550	0.32342	No
553	H333	0.76160	0.60550	0.52342	No
554	H334	0.76160	0.60550	0.72342	No
555	H335	0.76160	0.60550	0.92342	No
556	H336	0.23840	0.39450	0.02342	No
557	H337	0.23840	0.39450	0.22342	No
558	H338	0.23840	0.39450	0.42342	No
559	H339	0.23840	0.39450	0.62342	No
560	H340	0.23840	0.39450	0.82342	No
561	H341	0.22810	0.00160	0.12678	No
562	H342	0.22810	0.00160	0.32678	No
563	H343	0.22810	0.00160	0.52678	No
564	H344	0.22810	0.00160	0.72678	No
565	H345	0.22810	0.00160	0.92678	No
566	H346	0.77190	0.99840	0.02678	No
567	H347	0.77190	0.99840	0.22678	No
568	H348	0.77190	0.99840	0.42678	No
569	H349	0.77190	0.99840	0.62678	No
570	H350	0.77190	0.99840	0.82678	No

571	H351	0.72810	0.49840	0.12678	No
572	H352	0.72810	0.49840	0.32678	No
573	H353	0.72810	0.49840	0.52678	No
574	H354	0.72810	0.49840	0.72678	No
575	H355	0.72810	0.49840	0.92678	No
576	H356	0.27190	0.50160	0.02678	No
577	H357	0.27190	0.50160	0.22678	No
578	H358	0.27190	0.50160	0.42678	No
579	H359	0.27190	0.50160	0.62678	No
580	H360	0.27190	0.50160	0.82678	No
581	Bi1	0.38917	0.62103	0.30063	No
582	Bi2	0.38917	0.62103	0.50063	No
583	Bi3	0.38917	0.62103	0.70063	No
584	Bi4	0.61083	0.37897	0.40063	No
585	Bi5	0.61083	0.37897	0.80063	No
586	Bi6	0.88917	0.87897	0.10063	No
587	Bi7	0.88917	0.87897	0.30063	No
588	Bi8	0.88917	0.87897	0.70063	No
589	Bi9	0.11083	0.12103	0.60063	No
590	Bi10	0.11083	0.12103	0.80063	No
591	N1	0.45000	0.29950	0.08598	No
592	N2	0.45000	0.29950	0.28598	No
593	N3	0.45000	0.29950	0.48598	No
594	N4	0.45000	0.29950	0.68598	No
595	N5	0.45000	0.29950	0.88598	No
596	N6	0.55000	0.70050	0.98598	No
597	N7	0.55000	0.70050	0.18598	No
598	N8	0.55000	0.70050	0.38598	No
599	N9	0.55000	0.70050	0.58598	No
600	N10	0.55000	0.70050	0.78598	No
601	N11	0.95000	0.20050	0.08598	No
602	N12	0.95000	0.20050	0.28598	No
603	N13	0.95000	0.20050	0.48598	No
604	N14	0.95000	0.20050	0.68598	No
605	N15	0.95000	0.20050	0.88598	No
606	N16	0.05000	0.79950	0.98598	No
607	N17	0.05000	0.79950	0.18598	No
608	N18	0.05000	0.79950	0.38598	No

609	N19	0.05000	0.79950	0.58598	No
610	N20	0.05000	0.79950	0.78598	No
611	N21	0.19340	0.94140	0.08536	No
612	N22	0.19340	0.94140	0.28536	No
613	N23	0.19340	0.94140	0.48536	No
614	N24	0.19340	0.94140	0.68536	No
615	N25	0.19340	0.94140	0.88536	No
616	N26	0.80660	0.05860	0.98536	No
617	N27	0.80660	0.05860	0.18536	No
618	N28	0.80660	0.05860	0.38536	No
619	N29	0.80660	0.05860	0.58536	No
620	N30	0.80660	0.05860	0.78536	No
621	N31	0.69340	0.55860	0.08536	No
622	N32	0.69340	0.55860	0.28536	No
623	N33	0.69340	0.55860	0.48536	No
624	N34	0.69340	0.55860	0.68536	No
625	N35	0.69340	0.55860	0.88536	No
626	N36	0.30660	0.44140	0.98536	No
627	N37	0.30660	0.44140	0.18536	No
628	N38	0.30660	0.44140	0.38536	No
629	N39	0.30660	0.44140	0.58536	No
630	N40	0.30660	0.44140	0.78536	No
631	Sb1	0.38917	0.62103	0.10063	No
632	Sb2	0.38917	0.62103	0.90063	No
633	Sb3	0.61083	0.37897	0.00063	No
634	Sb4	0.61083	0.37897	0.20063	No
635	Sb5	0.61083	0.37897	0.60063	No
636	Sb6	0.88917	0.87897	0.50063	No
637	Sb7	0.88917	0.87897	0.90063	No
638	Sb8	0.11083	0.12103	0.00063	No
639	Sb9	0.11083	0.12103	0.20063	No
640	Sb10	0.11083	0.12103	0.40063	No

Reflex Summary Report for Rietveld Refinement of 0.4[C₆N₂H₁₈]BiI₅+0.6[C₆N₂H₁₈]SbI₅:

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.32406 ± 0.09336	Yes

b	14.12210 ± 0.08511	Yes
c	43.83108 ± 0.26982	Yes
α	95.15920 ± 0.03655	Yes
β	87.56013 ± 0.03976	Yes
γ	90.13525 ± 0.05396	Yes

Structure Parameters

Refined Motion Groups: 0 Refined Torsions: 0

Refined Angles: 0 Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C1	0.44190	0.21900	0.10840	No
2	C2	0.44190	0.21900	0.30840	No
3	C3	0.44190	0.21900	0.50840	No
4	C4	0.44190	0.21900	0.70840	No
5	C5	0.44190	0.21900	0.90840	No
6	C6	0.55810	0.78100	0.00840	No
7	C7	0.55810	0.78100	0.20840	No
8	C8	0.55810	0.78100	0.40840	No
9	C9	0.55810	0.78100	0.60840	No
10	C10	0.55810	0.78100	0.80840	No
11	C11	0.94190	0.28100	0.10840	No
12	C12	0.94190	0.28100	0.30840	No
13	C13	0.94190	0.28100	0.50840	No
14	C14	0.94190	0.28100	0.70840	No
15	C15	0.94190	0.28100	0.90840	No
16	C16	0.05810	0.71900	0.00840	No
17	C17	0.05810	0.71900	0.20840	No
18	C18	0.05810	0.71900	0.40840	No
19	C19	0.05810	0.71900	0.60840	No
20	C20	0.05810	0.71900	0.80840	No
21	C21	0.49640	0.13340	0.09722	No
22	C22	0.49640	0.13340	0.29722	No
23	C23	0.49640	0.13340	0.49722	No
24	C24	0.49640	0.13340	0.69722	No
25	C25	0.49640	0.13340	0.89722	No
26	C26	0.50360	0.86660	0.99722	No

27	C27	0.50360	0.86660	0.19722	No
28	C28	0.50360	0.86660	0.39722	No
29	C29	0.50360	0.86660	0.59722	No
30	C30	0.50360	0.86660	0.79722	No
31	C31	0.99640	0.36660	0.09722	No
32	C32	0.99640	0.36660	0.29722	No
33	C33	0.99640	0.36660	0.49722	No
34	C34	0.99640	0.36660	0.69722	No
35	C35	0.99640	0.36660	0.89722	No
36	C36	0.00360	0.63340	0.99722	No
37	C37	0.00360	0.63340	0.19722	No
38	C38	0.00360	0.63340	0.39722	No
39	C39	0.00360	0.63340	0.59722	No
40	C40	0.00360	0.63340	0.79722	No
41	C41	0.49500	0.05130	0.12030	No
42	C42	0.49500	0.05130	0.32030	No
43	C43	0.49500	0.05130	0.52030	No
44	C44	0.49500	0.05130	0.72030	No
45	C45	0.49500	0.05130	0.92030	No
46	C46	0.50500	0.94870	0.02030	No
47	C47	0.50500	0.94870	0.22030	No
48	C48	0.50500	0.94870	0.42030	No
49	C49	0.50500	0.94870	0.62030	No
50	C50	0.50500	0.94870	0.82030	No
51	C51	0.99500	0.44870	0.12030	No
52	C52	0.99500	0.44870	0.32030	No
53	C53	0.99500	0.44870	0.52030	No
54	C54	0.99500	0.44870	0.72030	No
55	C55	0.99500	0.44870	0.92030	No
56	C56	0.00500	0.55130	0.02030	No
57	C57	0.00500	0.55130	0.22030	No
58	C58	0.00500	0.55130	0.42030	No
59	C59	0.00500	0.55130	0.62030	No
60	C60	0.00500	0.55130	0.82030	No
61	C61	0.40380	0.01810	0.12902	No
62	C62	0.40380	0.01810	0.32902	No
63	C63	0.40380	0.01810	0.52902	No
64	C64	0.40380	0.01810	0.72902	No

65	C65	0.40380	0.01810	0.92902	No
66	C66	0.59620	0.98190	0.02902	No
67	C67	0.59620	0.98190	0.22902	No
68	C68	0.59620	0.98190	0.42902	No
69	C69	0.59620	0.98190	0.62902	No
70	C70	0.59620	0.98190	0.82902	No
71	C71	0.90380	0.48190	0.12902	No
72	C72	0.90380	0.48190	0.32902	No
73	C73	0.90380	0.48190	0.52902	No
74	C74	0.90380	0.48190	0.72902	No
75	C75	0.90380	0.48190	0.92902	No
76	C76	0.09620	0.51810	0.02902	No
77	C77	0.09620	0.51810	0.22902	No
78	C78	0.09620	0.51810	0.42902	No
79	C79	0.09620	0.51810	0.62902	No
80	C80	0.09620	0.51810	0.82902	No
81	C81	0.34450	0.99030	0.10188	No
82	C82	0.34450	0.99030	0.30188	No
83	C83	0.34450	0.99030	0.50188	No
84	C84	0.34450	0.99030	0.70188	No
85	C85	0.34450	0.99030	0.90188	No
86	C86	0.65550	0.00970	0.00188	No
87	C87	0.65550	0.00970	0.20188	No
88	C88	0.65550	0.00970	0.40188	No
89	C89	0.65550	0.00970	0.60188	No
90	C90	0.65550	0.00970	0.80188	No
91	C91	0.84450	0.50970	0.10188	No
92	C92	0.84450	0.50970	0.30188	No
93	C93	0.84450	0.50970	0.50188	No
94	C94	0.84450	0.50970	0.70188	No
95	C95	0.84450	0.50970	0.90188	No
96	C96	0.15550	0.49030	0.00188	No
97	C97	0.15550	0.49030	0.20188	No
98	C98	0.15550	0.49030	0.40188	No
99	C99	0.15550	0.49030	0.60188	No
100	C100	0.15550	0.49030	0.80188	No
101	C101	0.25450	0.95520	0.11224	No
102	C102	0.25450	0.95520	0.31224	No

103	C103	0.25450	0.95520	0.51224	No
104	C104	0.25450	0.95520	0.71224	No
105	C105	0.25450	0.95520	0.91224	No
106	C106	0.74550	0.04480	0.01224	No
107	C107	0.74550	0.04480	0.21224	No
108	C108	0.74550	0.04480	0.41224	No
109	C109	0.74550	0.04480	0.61224	No
110	C110	0.74550	0.04480	0.81224	No
111	C111	0.75450	0.54480	0.11224	No
112	C112	0.75450	0.54480	0.31224	No
113	C113	0.75450	0.54480	0.51224	No
114	C114	0.75450	0.54480	0.71224	No
115	C115	0.75450	0.54480	0.91224	No
116	C116	0.24550	0.45520	0.01224	No
117	C117	0.24550	0.45520	0.21224	No
118	C118	0.24550	0.45520	0.41224	No
119	C119	0.24550	0.45520	0.61224	No
120	C120	0.24550	0.45520	0.81224	No
121	I1	0.48458	0.51909	0.04212	No
122	I2	0.48458	0.51909	0.24212	No
123	I3	0.48458	0.51909	0.44212	No
124	I4	0.48458	0.51909	0.64212	No
125	I5	0.48458	0.51909	0.84212	No
126	I6	0.51542	0.48091	0.94212	No
127	I7	0.51542	0.48091	0.14212	No
128	I8	0.51542	0.48091	0.34212	No
129	I9	0.51542	0.48091	0.54212	No
130	I10	0.51542	0.48091	0.74212	No
131	I11	0.98458	0.98091	0.04212	No
132	I12	0.98458	0.98091	0.24212	No
133	I13	0.98458	0.98091	0.44212	No
134	I14	0.98458	0.98091	0.64212	No
135	I15	0.98458	0.98091	0.84212	No
136	I16	0.01542	0.01909	0.94212	No
137	I17	0.01542	0.01909	0.14212	No
138	I18	0.01542	0.01909	0.34212	No
139	I19	0.01542	0.01909	0.54212	No
140	I20	0.01542	0.01909	0.74212	No

141	I21	0.25948	0.45560	0.10194	No
142	I22	0.25948	0.45560	0.30194	No
143	I23	0.25948	0.45560	0.50194	No
144	I24	0.25948	0.45560	0.70194	No
145	I25	0.25948	0.45560	0.90194	No
146	I26	0.74052	0.54440	0.00194	No
147	I27	0.74052	0.54440	0.20194	No
148	I28	0.74052	0.54440	0.40194	No
149	I29	0.74052	0.54440	0.60194	No
150	I30	0.74052	0.54440	0.80194	No
151	I31	0.75948	0.04440	0.10194	No
152	I32	0.75948	0.04440	0.30194	No
153	I33	0.75948	0.04440	0.50194	No
154	I34	0.75948	0.04440	0.70194	No
155	I35	0.75948	0.04440	0.90194	No
156	I36	0.24052	0.95560	0.00194	No
157	I37	0.24052	0.95560	0.20194	No
158	I38	0.24052	0.95560	0.40194	No
159	I39	0.24052	0.95560	0.60194	No
160	I40	0.24052	0.95560	0.80194	No
161	I41	0.29912	0.73228	0.05329	No
162	I42	0.29912	0.73228	0.25329	No
163	I43	0.29912	0.73228	0.45329	No
164	I44	0.29912	0.73228	0.65329	No
165	I45	0.29912	0.73228	0.85329	No
166	I46	0.70088	0.26772	0.95329	No
167	I47	0.70088	0.26772	0.15329	No
168	I48	0.70088	0.26772	0.35329	No
169	I49	0.70088	0.26772	0.55329	No
170	I50	0.70088	0.26772	0.75329	No
171	I51	0.79912	0.76772	0.05329	No
172	I52	0.79912	0.76772	0.25329	No
173	I53	0.79912	0.76772	0.45329	No
174	I54	0.79912	0.76772	0.65329	No
175	I55	0.79912	0.76772	0.85329	No
176	I56	0.20088	0.23228	0.95329	No
177	I57	0.20088	0.23228	0.15329	No
178	I58	0.20088	0.23228	0.35329	No

179	I59	0.20088	0.23228	0.55329	No
180	I60	0.20088	0.23228	0.75329	No
181	I61	0.30809	0.69835	0.15768	No
182	I62	0.30809	0.69835	0.35768	No
183	I63	0.30809	0.69835	0.55768	No
184	I64	0.30809	0.69835	0.75768	No
185	I65	0.30809	0.69835	0.95768	No
186	I66	0.69191	0.30165	0.05768	No
187	I67	0.69191	0.30165	0.25768	No
188	I68	0.69191	0.30165	0.45768	No
189	I69	0.69191	0.30165	0.65768	No
190	I70	0.69191	0.30165	0.85768	No
191	I71	0.80809	0.80165	0.15768	No
192	I72	0.80809	0.80165	0.35768	No
193	I73	0.80809	0.80165	0.55768	No
194	I74	0.80809	0.80165	0.75768	No
195	I75	0.80809	0.80165	0.95768	No
196	I76	0.19191	0.19835	0.05768	No
197	I77	0.19191	0.19835	0.25768	No
198	I78	0.19191	0.19835	0.45768	No
199	I79	0.19191	0.19835	0.65768	No
200	I80	0.19191	0.19835	0.85768	No
201	I81	0.54645	0.76181	0.10427	No
202	I82	0.54645	0.76181	0.30427	No
203	I83	0.54645	0.76181	0.50427	No
204	I84	0.54645	0.76181	0.70427	No
205	I85	0.54645	0.76181	0.90427	No
206	I86	0.45355	0.23819	0.00427	No
207	I87	0.45355	0.23819	0.20427	No
208	I88	0.45355	0.23819	0.40427	No
209	I89	0.45355	0.23819	0.60427	No
210	I90	0.45355	0.23819	0.80427	No
211	I91	0.04645	0.73819	0.10427	No
212	I92	0.04645	0.73819	0.30427	No
213	I93	0.04645	0.73819	0.50427	No
214	I94	0.04645	0.73819	0.70427	No
215	I95	0.04645	0.73819	0.90427	No
216	I96	0.95355	0.26181	0.00427	No

217	I97	0.95355	0.26181	0.20427	No
218	I98	0.95355	0.26181	0.40427	No
219	I99	0.95355	0.26181	0.60427	No
220	I100	0.95355	0.26181	0.80427	No
221	H1	0.43960	0.27810	0.06640	No
222	H2	0.43960	0.27810	0.26640	No
223	H3	0.43960	0.27810	0.46640	No
224	H4	0.43960	0.27810	0.66640	No
225	H5	0.43960	0.27810	0.86640	No
226	H6	0.56040	0.72190	0.96640	No
227	H7	0.56040	0.72190	0.16640	No
228	H8	0.56040	0.72190	0.36640	No
229	H9	0.56040	0.72190	0.56640	No
230	H10	0.56040	0.72190	0.76640	No
231	H11	0.93960	0.22190	0.06640	No
232	H12	0.93960	0.22190	0.26640	No
233	H13	0.93960	0.22190	0.46640	No
234	H14	0.93960	0.22190	0.66640	No
235	H15	0.93960	0.22190	0.86640	No
236	H16	0.06040	0.77810	0.96640	No
237	H17	0.06040	0.77810	0.16640	No
238	H18	0.06040	0.77810	0.36640	No
239	H19	0.06040	0.77810	0.56640	No
240	H20	0.06040	0.77810	0.76640	No
241	H21	0.50570	0.32420	0.08704	No
242	H22	0.50570	0.32420	0.28704	No
243	H23	0.50570	0.32420	0.48704	No
244	H24	0.50570	0.32420	0.68704	No
245	H25	0.50570	0.32420	0.88704	No
246	H26	0.49430	0.67580	0.98704	No
247	H27	0.49430	0.67580	0.18704	No
248	H28	0.49430	0.67580	0.38704	No
249	H29	0.49430	0.67580	0.58704	No
250	H30	0.49430	0.67580	0.78704	No
251	H31	0.00570	0.17580	0.08704	No
252	H32	0.00570	0.17580	0.28704	No
253	H33	0.00570	0.17580	0.48704	No
254	H34	0.00570	0.17580	0.68704	No

255	H35	0.00570	0.17580	0.88704	No
256	H36	0.99430	0.82420	0.98704	No
257	H37	0.99430	0.82420	0.18704	No
258	H38	0.99430	0.82420	0.38704	No
259	H39	0.99430	0.82420	0.58704	No
260	H40	0.99430	0.82420	0.78704	No
261	H41	0.40970	0.34510	0.09086	No
262	H42	0.40970	0.34510	0.29086	No
263	H43	0.40970	0.34510	0.49086	No
264	H44	0.40970	0.34510	0.69086	No
265	H45	0.40970	0.34510	0.89086	No
266	H46	0.59030	0.65490	0.99086	No
267	H47	0.59030	0.65490	0.19086	No
268	H48	0.59030	0.65490	0.39086	No
269	H49	0.59030	0.65490	0.59086	No
270	H50	0.59030	0.65490	0.79086	No
271	H51	0.90970	0.15490	0.09086	No
272	H52	0.90970	0.15490	0.29086	No
273	H53	0.90970	0.15490	0.49086	No
274	H54	0.90970	0.15490	0.69086	No
275	H55	0.90970	0.15490	0.89086	No
276	H56	0.09030	0.84510	0.99086	No
277	H57	0.09030	0.84510	0.19086	No
278	H58	0.09030	0.84510	0.39086	No
279	H59	0.09030	0.84510	0.59086	No
280	H60	0.09030	0.84510	0.79086	No
281	H61	0.22060	0.90500	0.07076	No
282	H62	0.22060	0.90500	0.27076	No
283	H63	0.22060	0.90500	0.47076	No
284	H64	0.22060	0.90500	0.67076	No
285	H65	0.22060	0.90500	0.87076	No
286	H66	0.77940	0.09500	0.97076	No
287	H67	0.77940	0.09500	0.17076	No
288	H68	0.77940	0.09500	0.37076	No
289	H69	0.77940	0.09500	0.57076	No
290	H70	0.77940	0.09500	0.77076	No
291	H71	0.72060	0.59500	0.07076	No
292	H72	0.72060	0.59500	0.27076	No

293	H73	0.72060	0.59500	0.47076	No
294	H74	0.72060	0.59500	0.67076	No
295	H75	0.72060	0.59500	0.87076	No
296	H76	0.27940	0.40500	0.97076	No
297	H77	0.27940	0.40500	0.17076	No
298	H78	0.27940	0.40500	0.37076	No
299	H79	0.27940	0.40500	0.57076	No
300	H80	0.27940	0.40500	0.77076	No
301	H81	0.17940	0.99870	0.07702	No
302	H82	0.17940	0.99870	0.27702	No
303	H83	0.17940	0.99870	0.47702	No
304	H84	0.17940	0.99870	0.67702	No
305	H85	0.17940	0.99870	0.87702	No
306	H86	0.82060	0.00130	0.97702	No
307	H87	0.82060	0.00130	0.17702	No
308	H88	0.82060	0.00130	0.37702	No
309	H89	0.82060	0.00130	0.57702	No
310	H90	0.82060	0.00130	0.77702	No
311	H91	0.67940	0.50130	0.07702	No
312	H92	0.67940	0.50130	0.27702	No
313	H93	0.67940	0.50130	0.47702	No
314	H94	0.67940	0.50130	0.67702	No
315	H95	0.67940	0.50130	0.87702	No
316	H96	0.32060	0.49870	0.97702	No
317	H97	0.32060	0.49870	0.17702	No
318	H98	0.32060	0.49870	0.37702	No
319	H99	0.32060	0.49870	0.57702	No
320	H100	0.32060	0.49870	0.77702	No
321	H101	0.14300	0.91200	0.09190	No
322	H102	0.14300	0.91200	0.29190	No
323	H103	0.14300	0.91200	0.49190	No
324	H104	0.14300	0.91200	0.69190	No
325	H105	0.14300	0.91200	0.89190	No
326	H106	0.85700	0.08800	0.99190	No
327	H107	0.85700	0.08800	0.19190	No
328	H108	0.85700	0.08800	0.39190	No
329	H109	0.85700	0.08800	0.59190	No
330	H110	0.85700	0.08800	0.79190	No

331	H111	0.64300	0.58800	0.09190	No
332	H112	0.64300	0.58800	0.29190	No
333	H113	0.64300	0.58800	0.49190	No
334	H114	0.64300	0.58800	0.69190	No
335	H115	0.64300	0.58800	0.89190	No
336	H116	0.35700	0.41200	0.99190	No
337	H117	0.35700	0.41200	0.19190	No
338	H118	0.35700	0.41200	0.39190	No
339	H119	0.35700	0.41200	0.59190	No
340	H120	0.35700	0.41200	0.79190	No
341	H121	0.37870	0.20070	0.11042	No
342	H122	0.37870	0.20070	0.31042	No
343	H123	0.37870	0.20070	0.51042	No
344	H124	0.37870	0.20070	0.71042	No
345	H125	0.37870	0.20070	0.91042	No
346	H126	0.62130	0.79930	0.01042	No
347	H127	0.62130	0.79930	0.21042	No
348	H128	0.62130	0.79930	0.41042	No
349	H129	0.62130	0.79930	0.61042	No
350	H130	0.62130	0.79930	0.81042	No
351	H131	0.87870	0.29930	0.11042	No
352	H132	0.87870	0.29930	0.31042	No
353	H133	0.87870	0.29930	0.51042	No
354	H134	0.87870	0.29930	0.71042	No
355	H135	0.87870	0.29930	0.91042	No
356	H136	0.12130	0.70070	0.01042	No
357	H137	0.12130	0.70070	0.21042	No
358	H138	0.12130	0.70070	0.41042	No
359	H139	0.12130	0.70070	0.61042	No
360	H140	0.12130	0.70070	0.81042	No
361	H141	0.46340	0.23930	0.12906	No
362	H142	0.46340	0.23930	0.32906	No
363	H143	0.46340	0.23930	0.52906	No
364	H144	0.46340	0.23930	0.72906	No
365	H145	0.46340	0.23930	0.92906	No
366	H146	0.53660	0.76070	0.02906	No
367	H147	0.53660	0.76070	0.22906	No
368	H148	0.53660	0.76070	0.42906	No

369	H149	0.53660	0.76070	0.62906	No
370	H150	0.53660	0.76070	0.82906	No
371	H151	0.96340	0.26070	0.12906	No
372	H152	0.96340	0.26070	0.32906	No
373	H153	0.96340	0.26070	0.52906	No
374	H154	0.96340	0.26070	0.72906	No
375	H155	0.96340	0.26070	0.92906	No
376	H156	0.03660	0.73930	0.02906	No
377	H157	0.03660	0.73930	0.22906	No
378	H158	0.03660	0.73930	0.42906	No
379	H159	0.03660	0.73930	0.62906	No
380	H160	0.03660	0.73930	0.82906	No
381	H161	0.47240	0.11130	0.07710	No
382	H162	0.47240	0.11130	0.27710	No
383	H163	0.47240	0.11130	0.47710	No
384	H164	0.47240	0.11130	0.67710	No
385	H165	0.47240	0.11130	0.87710	No
386	H166	0.52760	0.88870	0.97710	No
387	H167	0.52760	0.88870	0.17710	No
388	H168	0.52760	0.88870	0.37710	No
389	H169	0.52760	0.88870	0.57710	No
390	H170	0.52760	0.88870	0.77710	No
391	H171	0.97240	0.38870	0.07710	No
392	H172	0.97240	0.38870	0.27710	No
393	H173	0.97240	0.38870	0.47710	No
394	H174	0.97240	0.38870	0.67710	No
395	H175	0.97240	0.38870	0.87710	No
396	H176	0.02760	0.61130	0.97710	No
397	H177	0.02760	0.61130	0.17710	No
398	H178	0.02760	0.61130	0.37710	No
399	H179	0.02760	0.61130	0.57710	No
400	H180	0.02760	0.61130	0.77710	No
401	H181	0.55860	0.15340	0.09382	No
402	H182	0.55860	0.15340	0.29382	No
403	H183	0.55860	0.15340	0.49382	No
404	H184	0.55860	0.15340	0.69382	No
405	H185	0.55860	0.15340	0.89382	No
406	H186	0.44140	0.84660	0.99382	No

407	H187	0.44140	0.84660	0.19382	No
408	H188	0.44140	0.84660	0.39382	No
409	H189	0.44140	0.84660	0.59382	No
410	H190	0.44140	0.84660	0.79382	No
411	H191	0.05860	0.34660	0.09382	No
412	H192	0.05860	0.34660	0.29382	No
413	H193	0.05860	0.34660	0.49382	No
414	H194	0.05860	0.34660	0.69382	No
415	H195	0.05860	0.34660	0.89382	No
416	H196	0.94140	0.65340	0.99382	No
417	H197	0.94140	0.65340	0.19382	No
418	H198	0.94140	0.65340	0.39382	No
419	H199	0.94140	0.65340	0.59382	No
420	H200	0.94140	0.65340	0.79382	No
421	H201	0.52810	0.99740	0.11126	No
422	H202	0.52810	0.99740	0.31126	No
423	H203	0.52810	0.99740	0.51126	No
424	H204	0.52810	0.99740	0.71126	No
425	H205	0.52810	0.99740	0.91126	No
426	H206	0.47190	0.00260	0.01126	No
427	H207	0.47190	0.00260	0.21126	No
428	H208	0.47190	0.00260	0.41126	No
429	H209	0.47190	0.00260	0.61126	No
430	H210	0.47190	0.00260	0.81126	No
431	H211	0.02810	0.50260	0.11126	No
432	H212	0.02810	0.50260	0.31126	No
433	H213	0.02810	0.50260	0.51126	No
434	H214	0.02810	0.50260	0.71126	No
435	H215	0.02810	0.50260	0.91126	No
436	H216	0.97190	0.49740	0.01126	No
437	H217	0.97190	0.49740	0.21126	No
438	H218	0.97190	0.49740	0.41126	No
439	H219	0.97190	0.49740	0.61126	No
440	H220	0.97190	0.49740	0.81126	No
441	H221	0.52650	0.07110	0.13938	No
442	H222	0.52650	0.07110	0.33938	No
443	H223	0.52650	0.07110	0.53938	No
444	H224	0.52650	0.07110	0.73938	No

445	H225	0.52650	0.07110	0.93938	No
446	H226	0.47350	0.92890	0.03938	No
447	H227	0.47350	0.92890	0.23938	No
448	H228	0.47350	0.92890	0.43938	No
449	H229	0.47350	0.92890	0.63938	No
450	H230	0.47350	0.92890	0.83938	No
451	H231	0.02650	0.42890	0.13938	No
452	H232	0.02650	0.42890	0.33938	No
453	H233	0.02650	0.42890	0.53938	No
454	H234	0.02650	0.42890	0.73938	No
455	H235	0.02650	0.42890	0.93938	No
456	H236	0.97350	0.57110	0.03938	No
457	H237	0.97350	0.57110	0.23938	No
458	H238	0.97350	0.57110	0.43938	No
459	H239	0.97350	0.57110	0.63938	No
460	H240	0.97350	0.57110	0.83938	No
461	H241	0.37400	0.06910	0.14084	No
462	H242	0.37400	0.06910	0.34084	No
463	H243	0.37400	0.06910	0.54084	No
464	H244	0.37400	0.06910	0.74084	No
465	H245	0.37400	0.06910	0.94084	No
466	H246	0.62600	0.93090	0.04084	No
467	H247	0.62600	0.93090	0.24084	No
468	H248	0.62600	0.93090	0.44084	No
469	H249	0.62600	0.93090	0.64084	No
470	H250	0.62600	0.93090	0.84084	No
471	H251	0.87400	0.43090	0.14084	No
472	H252	0.87400	0.43090	0.34084	No
473	H253	0.87400	0.43090	0.54084	No
474	H254	0.87400	0.43090	0.74084	No
475	H255	0.87400	0.43090	0.94084	No
476	H256	0.12600	0.56910	0.04084	No
477	H257	0.12600	0.56910	0.24084	No
478	H258	0.12600	0.56910	0.44084	No
479	H259	0.12600	0.56910	0.64084	No
480	H260	0.12600	0.56910	0.84084	No
481	H261	0.40970	0.96290	0.14300	No
482	H262	0.40970	0.96290	0.34300	No

483	H263	0.40970	0.96290	0.54300	No
484	H264	0.40970	0.96290	0.74300	No
485	H265	0.40970	0.96290	0.94300	No
486	H266	0.59030	0.03710	0.04300	No
487	H267	0.59030	0.03710	0.24300	No
488	H268	0.59030	0.03710	0.44300	No
489	H269	0.59030	0.03710	0.64300	No
490	H270	0.59030	0.03710	0.84300	No
491	H271	0.90970	0.53710	0.14300	No
492	H272	0.90970	0.53710	0.34300	No
493	H273	0.90970	0.53710	0.54300	No
494	H274	0.90970	0.53710	0.74300	No
495	H275	0.90970	0.53710	0.94300	No
496	H276	0.09030	0.46290	0.04300	No
497	H277	0.09030	0.46290	0.24300	No
498	H278	0.09030	0.46290	0.44300	No
499	H279	0.09030	0.46290	0.64300	No
500	H280	0.09030	0.46290	0.84300	No
501	H281	0.33640	0.04580	0.08812	No
502	H282	0.33640	0.04580	0.28812	No
503	H283	0.33640	0.04580	0.48812	No
504	H284	0.33640	0.04580	0.68812	No
505	H285	0.33640	0.04580	0.88812	No
506	H286	0.66360	0.95420	0.98812	No
507	H287	0.66360	0.95420	0.18812	No
508	H288	0.66360	0.95420	0.38812	No
509	H289	0.66360	0.95420	0.58812	No
510	H290	0.66360	0.95420	0.78812	No
511	H291	0.83640	0.45420	0.08812	No
512	H292	0.83640	0.45420	0.28812	No
513	H293	0.83640	0.45420	0.48812	No
514	H294	0.83640	0.45420	0.68812	No
515	H295	0.83640	0.45420	0.88812	No
516	H296	0.16360	0.54580	0.98812	No
517	H297	0.16360	0.54580	0.18812	No
518	H298	0.16360	0.54580	0.38812	No
519	H299	0.16360	0.54580	0.58812	No
520	H300	0.16360	0.54580	0.78812	No

521	H301	0.37410	0.93990	0.08970	No
522	H302	0.37410	0.93990	0.28970	No
523	H303	0.37410	0.93990	0.48970	No
524	H304	0.37410	0.93990	0.68970	No
525	H305	0.37410	0.93990	0.88970	No
526	H306	0.62590	0.06010	0.98970	No
527	H307	0.62590	0.06010	0.18970	No
528	H308	0.62590	0.06010	0.38970	No
529	H309	0.62590	0.06010	0.58970	No
530	H310	0.62590	0.06010	0.78970	No
531	H311	0.87410	0.56010	0.08970	No
532	H312	0.87410	0.56010	0.28970	No
533	H313	0.87410	0.56010	0.48970	No
534	H314	0.87410	0.56010	0.68970	No
535	H315	0.87410	0.56010	0.88970	No
536	H316	0.12590	0.43990	0.98970	No
537	H317	0.12590	0.43990	0.18970	No
538	H318	0.12590	0.43990	0.38970	No
539	H319	0.12590	0.43990	0.58970	No
540	H320	0.12590	0.43990	0.78970	No
541	H321	0.26160	0.89450	0.12342	No
542	H322	0.26160	0.89450	0.32342	No
543	H323	0.26160	0.89450	0.52342	No
544	H324	0.26160	0.89450	0.72342	No
545	H325	0.26160	0.89450	0.92342	No
546	H326	0.73840	0.10550	0.02342	No
547	H327	0.73840	0.10550	0.22342	No
548	H328	0.73840	0.10550	0.42342	No
549	H329	0.73840	0.10550	0.62342	No
550	H330	0.73840	0.10550	0.82342	No
551	H331	0.76160	0.60550	0.12342	No
552	H332	0.76160	0.60550	0.32342	No
553	H333	0.76160	0.60550	0.52342	No
554	H334	0.76160	0.60550	0.72342	No
555	H335	0.76160	0.60550	0.92342	No
556	H336	0.23840	0.39450	0.02342	No
557	H337	0.23840	0.39450	0.22342	No
558	H338	0.23840	0.39450	0.42342	No

559	H339	0.23840	0.39450	0.62342	No
560	H340	0.23840	0.39450	0.82342	No
561	H341	0.22810	0.00160	0.12678	No
562	H342	0.22810	0.00160	0.32678	No
563	H343	0.22810	0.00160	0.52678	No
564	H344	0.22810	0.00160	0.72678	No
565	H345	0.22810	0.00160	0.92678	No
566	H346	0.77190	0.99840	0.02678	No
567	H347	0.77190	0.99840	0.22678	No
568	H348	0.77190	0.99840	0.42678	No
569	H349	0.77190	0.99840	0.62678	No
570	H350	0.77190	0.99840	0.82678	No
571	H351	0.72810	0.49840	0.12678	No
572	H352	0.72810	0.49840	0.32678	No
573	H353	0.72810	0.49840	0.52678	No
574	H354	0.72810	0.49840	0.72678	No
575	H355	0.72810	0.49840	0.92678	No
576	H356	0.27190	0.50160	0.02678	No
577	H357	0.27190	0.50160	0.22678	No
578	H358	0.27190	0.50160	0.42678	No
579	H359	0.27190	0.50160	0.62678	No
580	H360	0.27190	0.50160	0.82678	No
581	Bi1	0.38917	0.62103	0.30063	No
582	Bi2	0.38917	0.62103	0.90063	No
583	Bi3	0.88917	0.87897	0.50063	No
584	Bi4	0.88917	0.87897	0.70063	No
585	Bi5	0.88917	0.87897	0.90063	No
586	Bi6	0.11083	0.12103	0.00063	No
587	Bi7	0.11083	0.12103	0.40063	No
588	Bi8	0.11083	0.12103	0.80063	No
589	N1	0.45000	0.29950	0.08598	No
590	N2	0.45000	0.29950	0.28598	No
591	N3	0.45000	0.29950	0.48598	No
592	N4	0.45000	0.29950	0.68598	No
593	N5	0.45000	0.29950	0.88598	No
594	N6	0.55000	0.70050	0.98598	No
595	N7	0.55000	0.70050	0.18598	No
596	N8	0.55000	0.70050	0.38598	No

597	N9	0.55000	0.70050	0.58598	No
598	N10	0.55000	0.70050	0.78598	No
599	N11	0.95000	0.20050	0.08598	No
600	N12	0.95000	0.20050	0.28598	No
601	N13	0.95000	0.20050	0.48598	No
602	N14	0.95000	0.20050	0.68598	No
603	N15	0.95000	0.20050	0.88598	No
604	N16	0.05000	0.79950	0.98598	No
605	N17	0.05000	0.79950	0.18598	No
606	N18	0.05000	0.79950	0.38598	No
607	N19	0.05000	0.79950	0.58598	No
608	N20	0.05000	0.79950	0.78598	No
609	N21	0.19340	0.94140	0.08536	No
610	N22	0.19340	0.94140	0.28536	No
611	N23	0.19340	0.94140	0.48536	No
612	N24	0.19340	0.94140	0.68536	No
613	N25	0.19340	0.94140	0.88536	No
614	N26	0.80660	0.05860	0.98536	No
615	N27	0.80660	0.05860	0.18536	No
616	N28	0.80660	0.05860	0.38536	No
617	N29	0.80660	0.05860	0.58536	No
618	N30	0.80660	0.05860	0.78536	No
619	N31	0.69340	0.55860	0.08536	No
620	N32	0.69340	0.55860	0.28536	No
621	N33	0.69340	0.55860	0.48536	No
622	N34	0.69340	0.55860	0.68536	No
623	N35	0.69340	0.55860	0.88536	No
624	N36	0.30660	0.44140	0.98536	No
625	N37	0.30660	0.44140	0.18536	No
626	N38	0.30660	0.44140	0.38536	No
627	N39	0.30660	0.44140	0.58536	No
628	N40	0.30660	0.44140	0.78536	No
629	Sb1	0.38917	0.62103	0.10063	No
630	Sb2	0.38917	0.62103	0.50063	No
631	Sb3	0.38917	0.62103	0.70063	No
632	Sb4	0.61083	0.37897	0.00063	No
633	Sb5	0.61083	0.37897	0.20063	No
634	Sb6	0.61083	0.37897	0.40063	No

635	Sb7	0.61083	0.37897	0.60063	No
636	Sb8	0.61083	0.37897	0.80063	No
637	Sb9	0.88917	0.87897	0.10063	No
638	Sb10	0.88917	0.87897	0.30063	No
639	Sb11	0.11083	0.12103	0.20063	No
640	Sb12	0.11083	0.12103	0.60063	No

Reflex Summary Report for Rietveld Refinement of 0.2[C₆N₂H₁₈]BiI₅+0.4[C₆N₂H₁₈]SbI₅:

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.48409 ± 0.15342	Yes
b	14.06560 ± 0.13733	Yes
c	43.17725 ± 0.42772	Yes
α	86.72315 ± 0.06700	Yes
β	86.08317 ± 0.08071	Yes
γ	88.86027 ± 0.04541	Yes

Structure Parameters

Refined Motion Groups: 0 Refined Torsions: 0

Refined Angles: 0 Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	C1	0.44165	0.21915	0.10807	No
2	C2	0.44165	0.21915	0.30807	No
3	C3	0.44165	0.21915	0.50807	No
4	C4	0.44165	0.21915	0.70807	No
5	C5	0.44165	0.21915	0.90807	No
6	C6	0.55779	0.78140	0.00781	No
7	C7	0.55779	0.78140	0.20781	No
8	C8	0.55779	0.78140	0.40781	No
9	C9	0.55779	0.78140	0.60781	No
10	C10	0.55779	0.78140	0.80781	No
11	C11	0.94137	0.28125	0.10776	No
12	C12	0.94137	0.28125	0.30776	No
13	C13	0.94137	0.28125	0.50776	No
14	C14	0.94137	0.28125	0.70776	No

15	C15	0.94137	0.28125	0.90776	No
16	C16	0.05807	0.71931	0.00812	No
17	C17	0.05807	0.71931	0.20812	No
18	C18	0.05807	0.71931	0.40812	No
19	C19	0.05807	0.71931	0.60812	No
20	C20	0.05807	0.71931	0.80812	No
21	C21	0.49612	0.13352	0.09689	No
22	C22	0.49612	0.13352	0.29689	No
23	C23	0.49612	0.13352	0.49689	No
24	C24	0.49612	0.13352	0.69689	No
25	C25	0.49612	0.13352	0.89689	No
26	C26	0.50332	0.86703	0.99663	No
27	C27	0.50332	0.86703	0.19663	No
28	C28	0.50332	0.86703	0.39663	No
29	C29	0.50332	0.86703	0.59663	No
30	C30	0.50332	0.86703	0.79663	No
31	C31	0.99584	0.36689	0.09652	No
32	C32	0.99584	0.36689	0.29652	No
33	C33	0.99584	0.36689	0.49652	No
34	C34	0.99584	0.36689	0.69652	No
35	C35	0.99584	0.36689	0.89652	No
36	C36	0.00360	0.63367	0.99700	No
37	C37	0.00360	0.63367	0.19700	No
38	C38	0.00360	0.63367	0.39700	No
39	C39	0.00360	0.63367	0.59700	No
40	C40	0.00360	0.63367	0.79700	No
41	C41	0.49472	0.05139	0.12000	No
42	C42	0.49472	0.05139	0.32000	No
43	C43	0.49472	0.05139	0.52000	No
44	C44	0.49472	0.05139	0.72000	No
45	C45	0.49472	0.05139	0.92000	No
46	C46	0.50472	0.94917	0.01969	No
47	C47	0.50472	0.94917	0.21969	No
48	C48	0.50472	0.94917	0.41969	No
49	C49	0.50472	0.94917	0.61969	No
50	C50	0.50472	0.94917	0.81969	No
51	C51	0.99444	0.44902	0.11957	No
52	C52	0.99444	0.44902	0.31957	No

53	C53	0.99444	0.44902	0.51957	No
54	C54	0.99444	0.44902	0.71957	No
55	C55	0.99444	0.44902	0.91957	No
56	C56	0.00500	0.55153	0.02011	No
57	C57	0.00500	0.55153	0.22011	No
58	C58	0.00500	0.55153	0.42011	No
59	C59	0.00500	0.55153	0.62011	No
60	C60	0.00500	0.55153	0.82011	No
61	C61	0.40357	0.01816	0.12878	No
62	C62	0.40357	0.01816	0.32878	No
63	C63	0.40357	0.01816	0.52878	No
64	C64	0.40357	0.01816	0.72878	No
65	C65	0.40357	0.01816	0.92878	No
66	C66	0.59587	0.98239	0.02834	No
67	C67	0.59587	0.98239	0.22834	No
68	C68	0.59587	0.98239	0.42834	No
69	C69	0.59587	0.98239	0.62834	No
70	C70	0.59587	0.98239	0.82834	No
71	C71	0.90329	0.48223	0.12833	No
72	C72	0.90329	0.48223	0.32833	No
73	C73	0.90329	0.48223	0.52833	No
74	C74	0.90329	0.48223	0.72833	No
75	C75	0.90329	0.48223	0.92833	No
76	C76	0.09615	0.51833	0.02879	No
77	C77	0.09615	0.51833	0.22879	No
78	C78	0.09615	0.51833	0.42879	No
79	C79	0.09615	0.51833	0.62879	No
80	C80	0.09615	0.51833	0.82879	No
81	C81	0.34431	0.99076	0.10134	No
82	C82	0.34431	0.99076	0.30134	No
83	C83	0.34431	0.99076	0.50134	No
84	C84	0.34431	0.99076	0.70134	No
85	C85	0.34431	0.99076	0.90134	No
86	C86	0.65513	0.00979	0.00150	No
87	C87	0.65513	0.00979	0.20150	No
88	C88	0.65513	0.00979	0.40150	No
89	C89	0.65513	0.00979	0.60150	No
90	C90	0.65513	0.00979	0.80150	No

91	C91	0.84403	0.51003	0.10122	No
92	C92	0.84403	0.51003	0.30122	No
93	C93	0.84403	0.51003	0.50122	No
94	C94	0.84403	0.51003	0.70122	No
95	C95	0.84403	0.51003	0.90122	No
96	C96	0.15541	0.49053	0.00162	No
97	C97	0.15541	0.49053	0.20162	No
98	C98	0.15541	0.49053	0.40162	No
99	C99	0.15541	0.49053	0.60162	No
100	C100	0.15541	0.49053	0.80162	No
101	C101	0.25436	0.95563	0.11177	No
102	C102	0.25436	0.95563	0.31177	No
103	C103	0.25436	0.95563	0.51177	No
104	C104	0.25436	0.95563	0.71177	No
105	C105	0.25436	0.95563	0.91177	No
106	C106	0.74508	0.04492	0.01179	No
107	C107	0.74508	0.04492	0.21179	No
108	C108	0.74508	0.04492	0.41179	No
109	C109	0.74508	0.04492	0.61179	No
110	C110	0.74508	0.04492	0.81179	No
111	C111	0.75408	0.54513	0.11162	No
112	C112	0.75408	0.54513	0.31162	No
113	C113	0.75408	0.54513	0.51162	No
114	C114	0.75408	0.54513	0.71162	No
115	C115	0.75408	0.54513	0.91162	No
116	C116	0.24536	0.45542	0.01194	No
117	C117	0.24536	0.45542	0.21194	No
118	C118	0.24536	0.45542	0.41194	No
119	C119	0.24536	0.45542	0.61194	No
120	C120	0.24536	0.45542	0.81194	No
121	I1	0.48431	0.51937	0.04166	No
122	I2	0.48431	0.51937	0.24166	No
123	I3	0.48431	0.51937	0.44166	No
124	I4	0.48431	0.51937	0.64166	No
125	I5	0.48431	0.51937	0.84166	No
126	I6	0.51513	0.48118	0.94166	No
127	I7	0.51513	0.48118	0.14166	No
128	I8	0.51513	0.48118	0.34166	No

129	I9	0.51513	0.48118	0.54166	No
130	I10	0.51513	0.48118	0.74166	No
131	I11	0.98403	0.98146	0.04122	No
132	I12	0.98403	0.98146	0.24122	No
133	I13	0.98403	0.98146	0.44122	No
134	I14	0.98403	0.98146	0.64122	No
135	I15	0.98403	0.98146	0.84122	No
136	I16	0.01541	0.01910	0.94210	No
137	I17	0.01541	0.01910	0.14210	No
138	I18	0.01541	0.01910	0.34210	No
139	I19	0.01541	0.01910	0.54210	No
140	I20	0.01541	0.01910	0.74210	No
141	I21	0.25933	0.45583	0.10163	No
142	I22	0.25933	0.45583	0.30163	No
143	I23	0.25933	0.45583	0.50163	No
144	I24	0.25933	0.45583	0.70163	No
145	I25	0.25933	0.45583	0.90163	No
146	I26	0.74011	0.54473	0.00132	No
147	I27	0.74011	0.54473	0.20132	No
148	I28	0.74011	0.54473	0.40132	No
149	I29	0.74011	0.54473	0.60132	No
150	I30	0.74011	0.54473	0.80132	No
151	I31	0.75905	0.04452	0.10148	No
152	I32	0.75905	0.04452	0.30148	No
153	I33	0.75905	0.04452	0.50148	No
154	I34	0.75905	0.04452	0.70148	No
155	I35	0.75905	0.04452	0.90148	No
156	I36	0.24039	0.95603	0.00147	No
157	I37	0.24039	0.95603	0.20147	No
158	I38	0.24039	0.95603	0.40147	No
159	I39	0.24039	0.95603	0.60147	No
160	I40	0.24039	0.95603	0.80147	No
161	I41	0.29895	0.73263	0.05287	No
162	I42	0.29895	0.73263	0.25287	No
163	I43	0.29895	0.73263	0.45287	No
164	I44	0.29895	0.73263	0.65287	No
165	I45	0.29895	0.73263	0.85287	No
166	I46	0.70049	0.26793	0.95279	No

167	I47	0.70049	0.26793	0.15279	No
168	I48	0.70049	0.26793	0.35279	No
169	I49	0.70049	0.26793	0.55279	No
170	I50	0.70049	0.26793	0.75279	No
171	I51	0.79867	0.76815	0.05257	No
172	I52	0.79867	0.76815	0.25257	No
173	I53	0.79867	0.76815	0.45257	No
174	I54	0.79867	0.76815	0.65257	No
175	I55	0.79867	0.76815	0.85257	No
176	I56	0.20077	0.23240	0.95309	No
177	I57	0.20077	0.23240	0.15309	No
178	I58	0.20077	0.23240	0.35309	No
179	I59	0.20077	0.23240	0.55309	No
180	I60	0.20077	0.23240	0.75309	No
181	I61	0.30792	0.69868	0.15727	No
182	I62	0.30792	0.69868	0.35727	No
183	I63	0.30792	0.69868	0.55727	No
184	I64	0.30792	0.69868	0.75727	No
185	I65	0.30792	0.69868	0.95727	No
186	I66	0.69152	0.30187	0.05718	No
187	I67	0.69152	0.30187	0.25718	No
188	I68	0.69152	0.30187	0.45718	No
189	I69	0.69152	0.30187	0.65718	No
190	I70	0.69152	0.30187	0.85718	No
191	I71	0.80764	0.80210	0.15694	No
192	I72	0.80764	0.80210	0.35694	No
193	I73	0.80764	0.80210	0.55694	No
194	I74	0.80764	0.80210	0.75694	No
195	I75	0.80764	0.80210	0.95694	No
196	I76	0.19180	0.19846	0.05751	No
197	I77	0.19180	0.19846	0.25751	No
198	I78	0.19180	0.19846	0.45751	No
199	I79	0.19180	0.19846	0.65751	No
200	I80	0.19180	0.19846	0.85751	No
201	I81	0.54614	0.76220	0.10369	No
202	I82	0.54614	0.76220	0.30369	No
203	I83	0.54614	0.76220	0.50369	No
204	I84	0.54614	0.76220	0.70369	No

205	I85	0.54614	0.76220	0.90369	No
206	I86	0.45330	0.23835	0.00392	No
207	I87	0.45330	0.23835	0.20392	No
208	I88	0.45330	0.23835	0.40392	No
209	I89	0.45330	0.23835	0.60392	No
210	I90	0.45330	0.23835	0.80392	No
211	I91	0.04642	0.73851	0.10399	No
212	I92	0.04642	0.73851	0.30399	No
213	I93	0.04642	0.73851	0.50399	No
214	I94	0.04642	0.73851	0.70399	No
215	I95	0.04642	0.73851	0.90399	No
216	I96	0.95302	0.26205	0.00363	No
217	I97	0.95302	0.26205	0.20363	No
218	I98	0.95302	0.26205	0.40362	No
219	I99	0.95302	0.26205	0.60362	No
220	I100	0.95302	0.26205	0.80362	No
221	H1	0.43935	0.27828	0.06605	No
222	H2	0.43935	0.27828	0.26605	No
223	H3	0.43935	0.27828	0.46605	No
224	H4	0.43935	0.27828	0.66605	No
225	H5	0.43935	0.27828	0.86605	No
226	H6	0.56009	0.72228	0.96583	No
227	H7	0.56009	0.72228	0.16583	No
228	H8	0.56009	0.72228	0.36583	No
229	H9	0.56009	0.72228	0.56583	No
230	H10	0.56009	0.72228	0.76583	No
231	H11	0.93907	0.22212	0.06578	No
232	H12	0.93907	0.22212	0.26578	No
233	H13	0.93907	0.22212	0.46578	No
234	H14	0.93907	0.22212	0.66578	No
235	H15	0.93907	0.22212	0.86578	No
236	H16	0.06037	0.77843	0.96610	No
237	H17	0.06037	0.77843	0.16610	No
238	H18	0.06037	0.77843	0.36610	No
239	H19	0.06037	0.77843	0.56610	No
240	H20	0.06037	0.77843	0.76610	No
241	H21	0.50542	0.32441	0.08664	No
242	H22	0.50542	0.32441	0.28664	No

243	H23	0.50542	0.32441	0.48664	No
244	H24	0.50542	0.32441	0.68664	No
245	H25	0.50542	0.32441	0.88664	No
246	H26	0.49402	0.67615	0.98652	No
247	H27	0.49402	0.67615	0.18652	No
248	H28	0.49402	0.67615	0.38652	No
249	H29	0.49402	0.67615	0.58652	No
250	H30	0.49402	0.67615	0.78652	No
251	H31	0.00570	0.17587	0.08698	No
252	H32	0.00570	0.17587	0.28698	No
253	H33	0.00570	0.17587	0.48698	No
254	H34	0.00570	0.17587	0.68698	No
255	H35	0.00570	0.17587	0.88698	No
256	H36	0.99374	0.82468	0.98618	No
257	H37	0.99374	0.82468	0.18618	No
258	H38	0.99374	0.82468	0.38618	No
259	H39	0.99374	0.82468	0.58618	No
260	H40	0.99374	0.82468	0.78618	No
261	H41	0.40947	0.34530	0.09051	No
262	H42	0.40947	0.34530	0.29051	No
263	H43	0.40947	0.34530	0.49051	No
264	H44	0.40947	0.34530	0.69051	No
265	H45	0.40947	0.34530	0.89051	No
266	H46	0.58997	0.65526	0.99030	No
267	H47	0.58997	0.65526	0.19030	No
268	H48	0.58997	0.65526	0.39030	No
269	H49	0.58997	0.65526	0.59030	No
270	H50	0.58997	0.65526	0.79030	No
271	H51	0.90919	0.15509	0.09028	No
272	H52	0.90919	0.15509	0.29028	No
273	H53	0.90919	0.15509	0.49028	No
274	H54	0.90919	0.15509	0.69028	No
275	H55	0.90919	0.15509	0.89028	No
276	H56	0.09025	0.84547	0.99052	No
277	H57	0.09025	0.84547	0.19052	No
278	H58	0.09025	0.84547	0.39052	No
279	H59	0.09025	0.84547	0.59052	No
280	H60	0.09025	0.84547	0.79052	No

281	H61	0.22048	0.90541	0.07033	No
282	H62	0.22048	0.90541	0.27032	No
283	H63	0.22048	0.90541	0.47032	No
284	H64	0.22048	0.90541	0.67032	No
285	H65	0.22048	0.90541	0.87032	No
286	H66	0.77896	0.09515	0.97028	No
287	H67	0.77896	0.09515	0.17028	No
288	H68	0.77896	0.09515	0.37028	No
289	H69	0.77896	0.09515	0.57028	No
290	H70	0.77896	0.09515	0.77028	No
291	H71	0.72020	0.59535	0.07014	No
292	H72	0.72020	0.59535	0.27014	No
293	H73	0.72020	0.59535	0.47014	No
294	H74	0.72020	0.59535	0.67014	No
295	H75	0.72020	0.59535	0.87014	No
296	H76	0.27924	0.40521	0.97046	No
297	H77	0.27924	0.40521	0.17046	No
298	H78	0.27924	0.40521	0.37046	No
299	H79	0.27924	0.40521	0.57046	No
300	H80	0.27924	0.40521	0.77046	No
301	H81	0.17930	0.99914	0.07658	No
302	H82	0.17930	0.99914	0.27658	No
303	H83	0.17930	0.99914	0.47658	No
304	H84	0.17930	0.99914	0.67658	No
305	H85	0.17930	0.99914	0.87658	No
306	H86	0.82014	0.00141	0.97654	No
307	H87	0.82014	0.00141	0.17654	No
308	H88	0.82014	0.00141	0.37654	No
309	H89	0.82014	0.00141	0.57654	No
310	H90	0.82014	0.00141	0.77654	No
311	H91	0.67902	0.50160	0.07646	No
312	H92	0.67902	0.50160	0.27646	No
313	H93	0.67902	0.50160	0.47646	No
314	H94	0.67902	0.50160	0.67646	No
315	H95	0.67902	0.50160	0.87646	No
316	H96	0.32042	0.49895	0.97666	No
317	H97	0.32042	0.49895	0.17667	No
318	H98	0.32042	0.49895	0.37666	No

319	H99	0.32042	0.49895	0.57666	No
320	H100	0.32042	0.49895	0.77666	No
321	H101	0.14292	0.91240	0.09151	No
322	H102	0.14292	0.91240	0.29151	No
323	H103	0.14292	0.91240	0.49151	No
324	H104	0.14292	0.91240	0.69151	No
325	H105	0.14292	0.91240	0.89151	No
326	H106	0.85652	0.08815	0.99137	No
327	H107	0.85652	0.08815	0.19137	No
328	H108	0.85652	0.08815	0.39137	No
329	H109	0.85652	0.08815	0.59137	No
330	H110	0.85652	0.08815	0.79137	No
331	H111	0.64264	0.58833	0.09133	No
332	H112	0.64264	0.58833	0.29133	No
333	H113	0.64264	0.58833	0.49133	No
334	H114	0.64264	0.58833	0.69133	No
335	H115	0.64264	0.58833	0.89133	No
336	H116	0.35680	0.41222	0.99155	No
337	H117	0.35680	0.41222	0.19155	No
338	H118	0.35680	0.41222	0.39155	No
339	H119	0.35680	0.41222	0.59155	No
340	H120	0.35680	0.41222	0.79155	No
341	H121	0.37849	0.20084	0.11013	No
342	H122	0.37849	0.20084	0.31013	No
343	H123	0.37849	0.20084	0.51013	No
344	H124	0.37849	0.20084	0.71013	No
345	H125	0.37849	0.20084	0.91013	No
346	H126	0.62095	0.79972	0.00979	No
347	H127	0.62095	0.79972	0.20979	No
348	H128	0.62095	0.79972	0.40979	No
349	H129	0.62095	0.79972	0.60979	No
350	H130	0.62095	0.79972	0.80979	No
351	H131	0.87821	0.29955	0.10981	No
352	H132	0.87821	0.29955	0.30981	No
353	H133	0.87821	0.29955	0.50981	No
354	H134	0.87821	0.29955	0.70981	No
355	H135	0.87821	0.29955	0.90981	No
356	H136	0.12123	0.70101	0.01011	No

357	H137	0.12123	0.70101	0.21011	No
358	H138	0.12123	0.70101	0.41011	No
359	H139	0.12123	0.70101	0.61011	No
360	H140	0.12123	0.70101	0.81011	No
361	H141	0.46314	0.23946	0.12871	No
362	H142	0.46314	0.23946	0.32871	No
363	H143	0.46314	0.23946	0.52871	No
364	H144	0.46314	0.23946	0.72871	No
365	H145	0.46314	0.23946	0.92871	No
366	H146	0.53630	0.76109	0.02849	No
367	H147	0.53630	0.76109	0.22849	No
368	H148	0.53630	0.76109	0.42849	No
369	H149	0.53630	0.76109	0.62849	No
370	H150	0.53630	0.76109	0.82849	No
371	H151	0.96286	0.26094	0.12841	No
372	H152	0.96286	0.26094	0.32841	No
373	H153	0.96286	0.26094	0.52841	No
374	H154	0.96286	0.26094	0.72841	No
375	H155	0.96286	0.26094	0.92841	No
376	H156	0.03658	0.73961	0.02879	No
377	H157	0.03658	0.73961	0.22879	No
378	H158	0.03658	0.73961	0.42879	No
379	H159	0.03658	0.73961	0.62879	No
380	H160	0.03658	0.73961	0.82879	No
381	H161	0.47214	0.11141	0.07679	No
382	H162	0.47214	0.11141	0.27679	No
383	H163	0.47214	0.11141	0.47679	No
384	H164	0.47214	0.11141	0.67679	No
385	H165	0.47214	0.11141	0.87679	No
386	H166	0.52730	0.88914	0.97649	No
387	H167	0.52730	0.88914	0.17649	No
388	H168	0.52730	0.88914	0.37649	No
389	H169	0.52730	0.88914	0.57649	No
390	H170	0.52730	0.88914	0.77649	No
391	H171	0.97186	0.38900	0.07641	No
392	H172	0.97186	0.38900	0.27641	No
393	H173	0.97186	0.38900	0.47640	No
394	H174	0.97186	0.38900	0.67640	No

395	H175	0.97186	0.38900	0.87640	No
396	H176	0.02758	0.61156	0.97688	No
397	H177	0.02758	0.61156	0.17688	No
398	H178	0.02758	0.61156	0.37688	No
399	H179	0.02758	0.61156	0.57688	No
400	H180	0.02758	0.61156	0.77688	No
401	H181	0.55829	0.15354	0.09344	No
402	H182	0.55829	0.15354	0.29344	No
403	H183	0.55829	0.15354	0.49344	No
404	H184	0.55829	0.15354	0.69344	No
405	H185	0.55829	0.15354	0.89344	No
406	H186	0.44115	0.84702	0.99328	No
407	H187	0.44115	0.84702	0.19328	No
408	H188	0.44115	0.84702	0.39328	No
409	H189	0.44115	0.84702	0.59328	No
410	H190	0.44115	0.84702	0.79328	No
411	H191	0.05857	0.34675	0.09367	No
412	H192	0.05857	0.34675	0.29367	No
413	H193	0.05857	0.34675	0.49367	No
414	H194	0.05857	0.34675	0.69367	No
415	H195	0.05857	0.34675	0.89367	No
416	H196	0.94087	0.65380	0.99305	No
417	H197	0.94087	0.65380	0.19305	No
418	H198	0.94087	0.65380	0.39305	No
419	H199	0.94087	0.65380	0.59305	No
420	H200	0.94087	0.65380	0.79305	No
421	H201	0.52780	0.99789	0.11062	No
422	H202	0.52780	0.99789	0.31062	No
423	H203	0.52780	0.99789	0.51062	No
424	H204	0.52780	0.99789	0.71062	No
425	H205	0.52780	0.99789	0.91062	No
426	H206	0.47164	0.00267	0.01099	No
427	H207	0.47164	0.00267	0.21099	No
428	H208	0.47164	0.00267	0.41099	No
429	H209	0.47164	0.00267	0.61099	No
430	H210	0.47164	0.00267	0.81099	No
431	H211	0.02808	0.50281	0.11107	No
432	H212	0.02808	0.50281	0.31107	No

433	H213	0.02808	0.50281	0.51107	No
434	H214	0.02808	0.50281	0.71107	No
435	H215	0.02808	0.50281	0.91107	No
436	H216	0.97136	0.49774	0.01053	No
437	H217	0.97136	0.49774	0.21053	No
438	H218	0.97136	0.49774	0.41053	No
439	H219	0.97136	0.49774	0.61053	No
440	H220	0.97136	0.49774	0.81053	No
441	H221	0.52621	0.07120	0.13905	No
442	H222	0.52621	0.07120	0.33905	No
443	H223	0.52621	0.07120	0.53905	No
444	H224	0.52621	0.07120	0.73905	No
445	H225	0.52621	0.07120	0.93905	No
446	H226	0.47323	0.92935	0.03879	No
447	H227	0.47323	0.92935	0.23879	No
448	H228	0.47323	0.92935	0.43879	No
449	H229	0.47323	0.92935	0.63879	No
450	H230	0.47323	0.92935	0.83879	No
451	H231	0.02649	0.42908	0.13922	No
452	H232	0.02649	0.42908	0.33922	No
453	H233	0.02649	0.42908	0.53922	No
454	H234	0.02649	0.42908	0.73922	No
455	H235	0.02649	0.42908	0.93922	No
456	H236	0.97295	0.57147	0.03862	No
457	H237	0.97295	0.57147	0.23862	No
458	H238	0.97295	0.57147	0.43862	No
459	H239	0.97295	0.57147	0.63862	No
460	H240	0.97295	0.57147	0.83862	No
461	H241	0.37379	0.06918	0.14060	No
462	H242	0.37379	0.06918	0.34060	No
463	H243	0.37379	0.06918	0.54060	No
464	H244	0.37379	0.06918	0.74060	No
465	H245	0.37379	0.06918	0.94060	No
466	H246	0.62565	0.93138	0.04016	No
467	H247	0.62565	0.93138	0.24016	No
468	H248	0.62565	0.93138	0.44016	No
469	H249	0.62565	0.93138	0.64016	No
470	H250	0.62565	0.93138	0.84016	No

471	H251	0.87351	0.43120	0.14019	No
472	H252	0.87351	0.43120	0.34019	No
473	H253	0.87351	0.43120	0.54019	No
474	H254	0.87351	0.43120	0.74019	No
475	H255	0.87351	0.43120	0.94019	No
476	H256	0.12593	0.56936	0.04057	No
477	H257	0.12593	0.56936	0.24057	No
478	H258	0.12593	0.56936	0.44057	No
479	H259	0.12593	0.56936	0.64057	No
480	H260	0.12593	0.56936	0.84057	No
481	H261	0.40947	0.96336	0.14244	No
482	H262	0.40947	0.96336	0.34244	No
483	H263	0.40947	0.96336	0.54244	No
484	H264	0.40947	0.96336	0.74244	No
485	H265	0.40947	0.96336	0.94244	No
486	H266	0.58997	0.03720	0.04265	No
487	H267	0.58997	0.03720	0.24265	No
488	H268	0.58997	0.03720	0.44265	No
489	H269	0.58997	0.03720	0.64265	No
490	H270	0.58997	0.03720	0.84265	No
491	H271	0.90919	0.53745	0.14229	No
492	H272	0.90919	0.53745	0.34229	No
493	H273	0.90919	0.53745	0.54229	No
494	H274	0.90919	0.53745	0.74229	No
495	H275	0.90919	0.53745	0.94229	No
496	H276	0.09025	0.46311	0.04279	No
497	H277	0.09025	0.46311	0.24279	No
498	H278	0.09025	0.46311	0.44279	No
499	H279	0.09025	0.46311	0.64279	No
500	H280	0.09025	0.46311	0.84279	No
501	H281	0.33621	0.04587	0.08791	No
502	H282	0.33621	0.04587	0.28791	No
503	H283	0.33621	0.04587	0.48791	No
504	H284	0.33621	0.04587	0.68791	No
505	H285	0.33621	0.04587	0.88791	No
506	H286	0.66323	0.95469	0.98741	No
507	H287	0.66323	0.95469	0.18741	No
508	H288	0.66323	0.95469	0.38741	No

509	H289	0.66323	0.95469	0.58741	No
510	H290	0.66323	0.95469	0.78741	No
511	H291	0.83593	0.45451	0.08748	No
512	H292	0.83593	0.45451	0.28748	No
513	H293	0.83593	0.45451	0.48748	No
514	H294	0.83593	0.45451	0.68748	No
515	H295	0.83593	0.45451	0.88748	No
516	H296	0.16351	0.54605	0.98784	No
517	H297	0.16351	0.54605	0.18784	No
518	H298	0.16351	0.54605	0.38784	No
519	H299	0.16351	0.54605	0.58784	No
520	H300	0.16351	0.54605	0.78784	No
521	H301	0.37389	0.94034	0.08916	No
522	H302	0.37389	0.94034	0.28916	No
523	H303	0.37389	0.94034	0.48916	No
524	H304	0.37389	0.94034	0.68916	No
525	H305	0.37389	0.94034	0.88916	No
526	H306	0.62555	0.06021	0.98932	No
527	H307	0.62555	0.06021	0.18932	No
528	H308	0.62555	0.06021	0.38932	No
529	H309	0.62555	0.06021	0.58932	No
530	H310	0.62555	0.06021	0.78932	No
531	H311	0.87361	0.56045	0.08900	No
532	H312	0.87361	0.56045	0.28900	No
533	H313	0.87361	0.56045	0.48900	No
534	H314	0.87361	0.56045	0.68900	No
535	H315	0.87361	0.56045	0.88900	No
536	H316	0.12583	0.44010	0.98948	No
537	H317	0.12583	0.44010	0.18948	No
538	H318	0.12583	0.44010	0.38948	No
539	H319	0.12583	0.44010	0.58948	No
540	H320	0.12583	0.44010	0.78948	No
541	H321	0.26145	0.89491	0.12296	No
542	H322	0.26145	0.89491	0.32296	No
543	H323	0.26145	0.89491	0.52296	No
544	H324	0.26145	0.89491	0.72296	No
545	H325	0.26145	0.89491	0.92296	No
546	H326	0.73799	0.10565	0.02296	No

547	H327	0.73799	0.10565	0.22296	No
548	H328	0.73799	0.10565	0.42296	No
549	H329	0.73799	0.10565	0.62296	No
550	H330	0.73799	0.10565	0.82296	No
551	H331	0.76117	0.60586	0.12277	No
552	H332	0.76117	0.60586	0.32277	No
553	H333	0.76117	0.60586	0.52277	No
554	H334	0.76117	0.60586	0.72277	No
555	H335	0.76117	0.60586	0.92277	No
556	H336	0.23827	0.39470	0.02315	No
557	H337	0.23827	0.39470	0.22315	No
558	H338	0.23827	0.39470	0.42315	No
559	H339	0.23827	0.39470	0.62315	No
560	H340	0.23827	0.39470	0.82315	No
561	H341	0.22797	0.00163	0.12665	No
562	H342	0.22797	0.00163	0.32665	No
563	H343	0.22797	0.00163	0.52665	No
564	H344	0.22797	0.00163	0.72665	No
565	H345	0.22797	0.00163	0.92665	No
566	H346	0.77147	0.99892	0.02599	No
567	H347	0.77147	0.99892	0.22599	No
568	H348	0.77147	0.99892	0.42599	No
569	H349	0.77147	0.99892	0.62599	No
570	H350	0.77147	0.99892	0.82599	No
571	H351	0.72769	0.49871	0.12619	No
572	H352	0.72769	0.49871	0.32619	No
573	H353	0.72769	0.49871	0.52619	No
574	H354	0.72769	0.49871	0.72619	No
575	H355	0.72769	0.49871	0.92619	No
576	H356	0.27175	0.50185	0.02645	No
577	H357	0.27175	0.50185	0.22645	No
578	H358	0.27175	0.50185	0.42645	No
579	H359	0.27175	0.50185	0.62645	No
580	H360	0.27175	0.50185	0.82645	No
581	Bi1	0.38895	0.62134	0.10019	No
582	Bi2	0.38895	0.62134	0.70019	No
583	Bi3	0.61049	0.37921	0.80015	No
584	Bi4	0.11077	0.12110	0.20052	No

585	N1	0.44975	0.29969	0.08562	No
586	N2	0.44975	0.29969	0.28562	No
587	N3	0.44975	0.29969	0.48562	No
588	N4	0.44975	0.29969	0.68562	No
589	N5	0.44975	0.29969	0.88562	No
590	N6	0.54969	0.70087	0.98542	No
591	N7	0.54969	0.70087	0.18542	No
592	N8	0.54969	0.70087	0.38542	No
593	N9	0.54969	0.70087	0.58542	No
594	N10	0.54969	0.70087	0.78542	No
595	N11	0.94947	0.20071	0.08536	No
596	N12	0.94947	0.20071	0.28536	No
597	N13	0.94947	0.20071	0.48536	No
598	N14	0.94947	0.20071	0.68536	No
599	N15	0.94947	0.20071	0.88536	No
600	N16	0.04997	0.79984	0.98568	No
601	N17	0.04997	0.79984	0.18568	No
602	N18	0.04997	0.79984	0.38568	No
603	N19	0.04997	0.79984	0.58568	No
604	N20	0.04997	0.79984	0.78568	No
605	N21	0.19329	0.94182	0.08493	No
606	N22	0.19329	0.94182	0.28493	No
607	N23	0.19329	0.94182	0.48493	No
608	N24	0.19329	0.94182	0.68493	No
609	N25	0.19329	0.94182	0.88493	No
610	N26	0.80615	0.05874	0.98487	No
611	N27	0.80615	0.05874	0.18487	No
612	N28	0.80615	0.05874	0.38487	No
613	N29	0.80615	0.05874	0.58487	No
614	N30	0.80615	0.05874	0.78487	No
615	N31	0.69301	0.55893	0.08477	No
616	N32	0.69301	0.55893	0.28477	No
617	N33	0.69301	0.55893	0.48477	No
618	N34	0.69301	0.55893	0.68477	No
619	N35	0.69301	0.55893	0.88477	No
620	N36	0.30643	0.44163	0.98503	No
621	N37	0.30643	0.44163	0.18503	No
622	N38	0.30643	0.44163	0.38503	No

623	N39	0.30643	0.44163	0.58503	No
624	N40	0.30643	0.44163	0.78503	No
625	Sb1	0.38895	0.62134	0.30019	No
626	Sb2	0.38895	0.62134	0.50019	No
627	Sb3	0.38895	0.62134	0.90019	No
628	Sb4	0.61049	0.37921	0.00015	No
629	Sb5	0.61049	0.37921	0.20015	No
630	Sb6	0.61049	0.37921	0.40015	No
631	Sb7	0.61049	0.37921	0.60015	No
632	Sb8	0.88867	0.87946	0.09982	No
633	Sb9	0.88867	0.87946	0.29982	No
634	Sb10	0.88867	0.87946	0.49982	No
635	Sb11	0.88867	0.87946	0.69982	No
636	Sb12	0.88867	0.87946	0.89982	No
637	Sb13	0.11077	0.12110	0.00052	No
638	Sb14	0.11077	0.12110	0.40052	No
639	Sb15	0.11077	0.12110	0.60052	No
640	Sb16	0.11077	0.12110	0.80052	No

Reflex Summary Report for Rietveld Refinement of [C₆N₂H₁₈]*Sb*I₅ :

Lattice Parameters

Lattice Type: Triclinic Space Group: P 1

Parameter	Value	Refined?
a	15.05779 ± <i>0.15659</i>	Yes
b	14.21729 ± <i>0.14699</i>	Yes
c	8.48135 ± <i>0.08922</i>	Yes
α	90.00000 ± <i>15995162.17605</i>	Yes
β	90.00000 ± <i>0.00000</i>	Yes
γ	89.99999 ± <i>5007.80545</i>	Yes

Errors are unusually large: This may be due to correlations between refined parameters.

Structure Parameters

Refined Motion Groups: 0 Refined Torsions: 0

Refined Angles: 0 Refined Distances: 0

Number of Refined DOF: 0

Fractional Coordinates

No.	Name	u	v	w	Refined?
1	Sb1	0.38917	0.62103	0.50315	No

2	Sb2	0.61083	0.37897	0.00315	No
3	Sb3	0.88917	0.87897	0.50315	No
4	Sb4	0.11083	0.12103	0.00315	No
5	I1	0.48458	0.51909	0.21060	No
6	I2	0.51542	0.48091	0.71060	No
7	I3	0.98458	0.98091	0.21060	No
8	I4	0.01542	0.01909	0.71060	No
9	I5	0.25948	0.45560	0.50969	No
10	I6	0.74052	0.54440	0.00969	No
11	I7	0.75948	0.04440	0.50969	No
12	I8	0.24052	0.95560	0.00969	No
13	I9	0.29912	0.73228	0.26645	No
14	I10	0.70088	0.26772	0.76645	No
15	I11	0.79912	0.76772	0.26645	No
16	I12	0.20088	0.23228	0.76645	No
17	I13	0.30809	0.69835	0.78842	No
18	I14	0.69191	0.30165	0.28842	No
19	I15	0.80809	0.80165	0.78842	No
20	I16	0.19191	0.19835	0.28842	No
21	I17	0.54645	0.76181	0.52133	No
22	I18	0.45355	0.23819	0.02133	No
23	I19	0.04645	0.73819	0.52133	No
24	I20	0.95355	0.26181	0.02133	No
25	N1	0.45000	0.29950	0.42990	No
26	N2	0.55000	0.70050	0.92990	No
27	N3	0.95000	0.20050	0.42990	No
28	N4	0.05000	0.79950	0.92990	No
29	N5	0.19340	0.94140	0.42680	No
30	N6	0.80660	0.05860	0.92680	No
31	N7	0.69340	0.55860	0.42680	No
32	N8	0.30660	0.44140	0.92680	No
33	H1	0.43960	0.27810	0.33200	No
34	H2	0.56040	0.72190	0.83200	No
35	H3	0.93960	0.22190	0.33200	No
36	H4	0.06040	0.77810	0.83200	No
37	H5	0.50570	0.32420	0.43520	No
38	H6	0.49430	0.67580	0.93520	No
39	H7	0.00570	0.17580	0.43520	No

40	H8	0.99430	0.82420	0.93520	No
41	H9	0.40970	0.34510	0.45430	No
42	H10	0.59030	0.65490	0.95430	No
43	H11	0.90970	0.15490	0.45430	No
44	H12	0.09030	0.84510	0.95430	No
45	H13	0.22060	0.90500	0.35380	No
46	H14	0.77940	0.09500	0.85380	No
47	H15	0.72060	0.59500	0.35380	No
48	H16	0.27940	0.40500	0.85380	No
49	H17	0.17940	0.99870	0.38510	No
50	H18	0.82060	0.00130	0.88510	No
51	H19	0.67940	0.50130	0.38510	No
52	H20	0.32060	0.49870	0.88510	No
53	H21	0.14300	0.91200	0.45950	No
54	H22	0.85700	0.08800	0.95950	No
55	H23	0.64300	0.58800	0.45950	No
56	H24	0.35700	0.41200	0.95950	No
57	H25	0.37870	0.20070	0.55210	No
58	H26	0.62130	0.79930	0.05210	No
59	H27	0.87870	0.29930	0.55210	No
60	H28	0.12130	0.70070	0.05210	No
61	H29	0.46340	0.23930	0.64530	No
62	H30	0.53660	0.76070	0.14530	No
63	H31	0.96340	0.26070	0.64530	No
64	H32	0.03660	0.73930	0.14530	No
65	H33	0.47240	0.11130	0.38550	No
66	H34	0.52760	0.88870	0.88550	No
67	H35	0.97240	0.38870	0.38550	No
68	H36	0.02760	0.61130	0.88550	No
69	H37	0.55860	0.15340	0.46910	No
70	H38	0.44140	0.84660	0.96910	No
71	H39	0.05860	0.34660	0.46910	No
72	H40	0.94140	0.65340	0.96910	No
73	H41	0.52810	0.99740	0.55630	No
74	H42	0.47190	0.00260	0.05630	No
75	H43	0.02810	0.50260	0.55630	No
76	H44	0.97190	0.49740	0.05630	No
77	H45	0.52650	0.07110	0.69690	No

78	H46	0.47350	0.92890	0.19690	No
79	H47	0.02650	0.42890	0.69690	No
80	H48	0.97350	0.57110	0.19690	No
81	H49	0.37400	0.06910	0.70420	No
82	H50	0.62600	0.93090	0.20420	No
83	H51	0.87400	0.43090	0.70420	No
84	H52	0.12600	0.56910	0.20420	No
85	H53	0.40970	0.96290	0.71500	No
86	H54	0.59030	0.03710	0.21500	No
87	H55	0.90970	0.53710	0.71500	No
88	H56	0.09030	0.46290	0.21500	No
89	H57	0.33640	0.04580	0.44060	No
90	H58	0.66360	0.95420	0.94060	No
91	H59	0.83640	0.45420	0.44060	No
92	H60	0.16360	0.54580	0.94060	No
93	H61	0.37410	0.93990	0.44850	No
94	H62	0.62590	0.06010	0.94850	No
95	H63	0.87410	0.56010	0.44850	No
96	H64	0.12590	0.43990	0.94850	No
97	H65	0.26160	0.89450	0.61710	No
98	H66	0.73840	0.10550	0.11710	No
99	H67	0.76160	0.60550	0.61710	No
100	H68	0.23840	0.39450	0.11710	No
101	H69	0.22810	0.00160	0.63390	No
102	H70	0.77190	0.99840	0.13390	No
103	H71	0.72810	0.49840	0.63390	No
104	H72	0.27190	0.50160	0.13390	No
105	C1	0.44190	0.21900	0.54200	No
106	C2	0.55810	0.78100	0.04200	No
107	C3	0.94190	0.28100	0.54200	No
108	C4	0.05810	0.71900	0.04200	No
109	C5	0.49640	0.13340	0.48610	No
110	C6	0.50360	0.86660	0.98610	No
111	C7	0.99640	0.36660	0.48610	No
112	C8	0.00360	0.63340	0.98610	No
113	C9	0.49500	0.05130	0.60150	No
114	C10	0.50500	0.94870	0.10150	No
115	C11	0.99500	0.44870	0.60150	No

116	C12	0.00500	0.55130	0.10150	No
117	C13	0.40380	0.01810	0.64510	No
118	C14	0.59620	0.98190	0.14510	No
119	C15	0.90380	0.48190	0.64510	No
120	C16	0.09620	0.51810	0.14510	No
121	C17	0.34450	0.99030	0.50940	No
122	C18	0.65550	0.00970	0.00940	No
123	C19	0.84450	0.50970	0.50940	No
124	C20	0.15550	0.49030	0.00940	No
125	C21	0.25450	0.95520	0.56120	No
126	C22	0.74550	0.04480	0.06120	No
127	C23	0.75450	0.54480	0.56120	No
128	C24	0.24550	0.45520	0.06120	No