Supporting Information

Observation of Exceptional Stability in a Nonlinear Optical Crystal under Extreme Conditions

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Table SI. Crystallographic data of BZBP.

Space group	*Pmn2₁* space group (#31)
Pressure and temperature	ambient
a (Å) b (Å) c (Å) α, β, γ V (Å^3)	10.384147±0.001164 7.076825±0.001012 8.212868±0.000943 90^o 603.537±0.101
Atomic coordinates	Ba1: [0.23529, 0.44148, 0.94308] Ba2: [0.00000, 0.01743, 0.73221] Zn1: [0.50000, 0.72453, 0.85844] P1: [0.00000, 0.55703, 0.62695] B1: [0.51278, 1.28021, 0.52857] B2: [0.39896, 0.19574, 0.71177] B3: [0.50000, 0.53349, 0.53104] O1: [0.10057, 0.76399, 0.70912] O2: [0.50000, -0.10451, 0.73846] O3: [0.17692, 0.62447, 0.09474] O4: [0.00000, 0.68368, 0.64986] O5: [0.50000, 0.63225, 0.73460] O6: [0.00000, 0.67098, 0.50850] O7: [0.32867, 0.86095, 0.93891] O8: [0.27085, 0.05516, 0.79646] O9: [0.19451, 0.93943, -0.00499]

Table SII. The list of the Raman modes and their frequencies.

mode index	frequency (cm^{-1})	Raman mode
1	-1.47444833	A_1
2	-1.043802336	B_2
3	-0.769830597	B_1
4	46.94477408460345	A_1
5	59.36154312493942	A_2
6	69.55086507251464	A_1
7	70.55967438686262	B_1
8	71.83937476879194	B_2
9	77.60957909798016	A_1
10	79.22258626376644	A_2
11	84.44967327410303	B_2
12	88.17692529858924	A_1
13	90.15297287815602	B_1
14	93.06380986	B_1
15	95.24631239441717	B_2
16	98.90653148173685	A_2
17	101.17364220739681	A_2
18	109.7140696921142	A_1
19	110.52409264139516	B_2
20	118.63743726066998	A_1
21	119.06235698964029	B_1
22	120.59160174136296	B_2
23	128.54887154370476	A_2
24	134.20746172414684	B_1
25	139.50558642549873	B_2
26	140.50710840508657	A_2
27	146.8797215146885	A_2
28	147.1655595393411	B_1
29	149.09168219050935	A_1
30	151.02615579225423	A_1
31	154.2388543051879	B_2
32	157.14187978758622	A_2
33	165.12257518257593	A_1
34	169.15189169729192	B_1
35	169.22918770451878	B_2
36	171.3575270372032	A_2

37	182.09965870556502	A_2
38	185.5571354643891	B_1
39	185.86831733208143	B_2
40	186.13906123118397	A_1
41	188.7509912284501	B_2
42	192.12075054042583	B_1
43	201.96095766136796	A_1
44	210.73345027695794	B_2
45	211.16626982774434	B_1
46	212.54981433640006	A_1
47	213.29968752033867	A_2
48	215.51956589701115	A_1
49	217.3551152856587	B_2
50	217.97683196340458	B_1
51	229.13191915048296	A_2
52	252.74882159116817	A_2
53	270.8128560240491	A_1
54	281.84508088081424	B_2
55	287.84323866305556	B_1
56	294.4388658	B_1
57	297.1130982671134	B_2
58	314.32968251163294	B_2
59	324.88922888627036	A_2
60	327.54134923082023	A_1
61	337.1712962791078	A_2
62	344.6332181697926	B_1
63	359.9166083	B_2
64	375.8654451794923	A_1
65	384.6638218	A_1
66	396.35597696609926	A_2
67	397.4346155387941	B_1
68	403.26845414059676	B_2
69	413.2943921714216	B_2
70	413.91952838816064	A_2
71	416.93348599080656	A_1
72	430.2526404440588	B_2
73	436.7924743414507	B_1
74	446.70337055891486	A_1
75	448.6853940126312	A_2

76	495.28472816625225	B_1
77	511.0067842328732	B_2
78	512.2873923194253	A_2
79	519.8051419	A_1
80	529.4347643991741	B_2
81	529.6264639482013	A_1
82	534.7803348738286	A_1
83	542.5473450132662	B_1
84	556.2650869753497	A_1
85	556.7230425787584	B_1
86	558.5802776230206	A_2
87	562.9070212	B_2
88	574.4272227	B_2
89	601.9403826463164	A_1
90	608.4708809252652	B_1
91	616.9302067933431	B_2
92	621.3516003829288	A_2
93	637.4259361489964	B_2
94	665.0914734256078	B_1
95	666.5417962185927	A_1
96	673.7762683947141	A_1
97	674.5449882969381	B_2
98	675.1404371791145	A_2
99	683.8776005136722	B_1
100	693.4796136	B_2
101	694.4974797369767	A_2
102	724.3213587	A_1
103	729.6220655431291	B_2
104	734.3330986	A_1
105	765.3953506904808	A_2
106	781.8848534	B_1
107	840.5399584114821	A_1
108	849.8707012116079	B_1
109	875.1767117819006	B_2
110	889.6338414673446	B_2
111	895.8364827626447	B_2
112	896.0825416711726	A_1
113	902.6405108713546	A_2
114	909.9819394939926	B_1

115	915.4627501520416	A_2
116	933.6401077159541	A_1
117	985.2511733988863	B_2
118	985.6730578213447	A_1
119	989.0866375452405	A_1
120	990.1271623305629	B_1
121	999.8431114289759	B_1
122	1000.3541845761225	A_2
123	1014.0998813775504	A_2
124	1020.3200125357877	A_1
125	1022.4754327398663	B_2
126	1037.2088008455592	B_2
127	1049.186032757844	A_1
128	1071.4193914670777	B_2
129	1084.0321050631649	A_2
130	1096.5485920390338	B_1
131	1118.4361271818839	B_2
132	1124.6730908583029	A_1
133	1215.1112556107669	A_2
134	1226.322563	A_1
135	1243.4662496114736	B_1
136	1298.0654575344784	B_2
137	1312.1103762763078	A_2
138	1332.0213300669902	B_1
139	1347.3548807930242	A_1
140	1358.670424915281	B_2
141	1376.2013700867874	B_1
142	1389.9437837535875	A_2
143	1406.6211485124693	A_1
144	1419.6287139563656	B_2

Table SIII. The list of the indices of Raman bands, the corresponding vibrational modes, ω_o, and $\frac{\partial \omega_t}{\partial T}$. The latter two values were obtained from the linear fitting using equation (3).

Index of Raman band	Vibrational mode	ω_o	$\frac{\partial \omega_t}{\partial T}$
123	A_2	1010.1(1.58)	-0.015964(0.00274)
116	A_1	933.49(0.695)	-0.0077105(0.00121)
104	A_1	747.24 ± 0.391	-0.00050218 ± 0.00222
102	A_1	714.58 ± 1.28	-0.0040845 ± 0.00222
92	A_2	628.65 ± 1.24	-0.0049833 ± 0.00215
88	B_2	587.56 ± 0.694	-0.0068422 ± 0.0012
86	A_2	559.6 ± 0.629	-0.0045294 ± 0.00109
73	B_1	437.46 ± 0.411	0.00062033 ± 0.000713
60	A_1	337.37 ± 0.795	-0.01287 ± 0.00138
53	A_1	280.47 ± 1.28	-0.023446 ± 0.00223
51	A_2	232.29 ± 1.27	-0.012511 ± 0.0022
29	A_1	155.57 ± 0.834	-0.013018 ± 0.00145
12	A_1	90.863 ± 0.685	-0.0058114 ± 0.00119
7	B_1	72.986 ± 0.507	-0.0060612 ± 0.000879