

Table S1. Atomic coordinates and coefficients of the equivalent isotropic displacement parameters for Cs₃[NO₃][B₁₂H₁₂] (**I**).

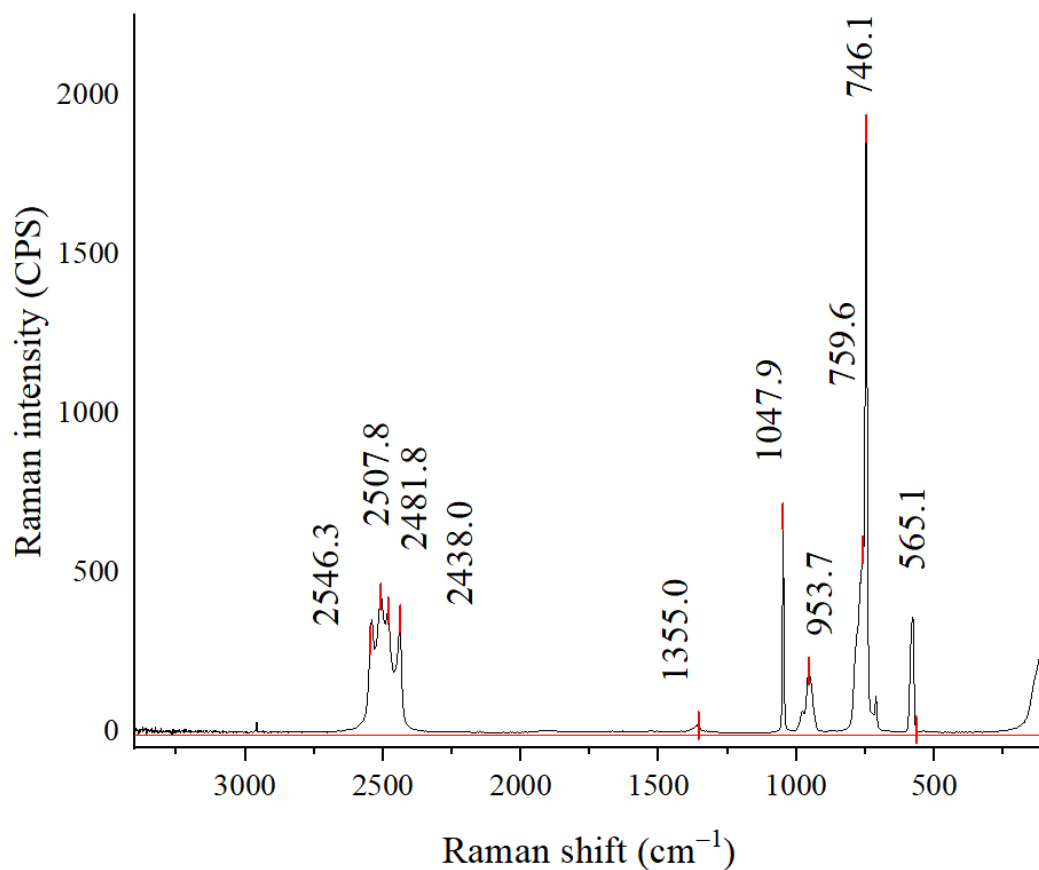
Atom	Wyckoff site	x/a	y/b	z/c	U_{eq}/pm^2
Cs1	4c	0.26627(5)	$1/4$	0.57549(2)	434.2(14)
Cs2	8d	0.22713(4)	0.00310(2)	0.341697(17)	423.2(13)
N	4c	0.0534(7)	$1/4$	0.7513(3)	448(11)
O1	4c	0.0646(9)	$1/4$	0.8230(3)	786(17)
O2	8d	0.0661(8)	0.1473(5)	0.7156(3)	1008(17)
B1	4c	0.1646(7)	$1/4$	0.1788(3)	346(11)
H1	4c	0.116	$1/4$	0.237	416
B2	4c	0.0418(7)	$1/4$	0.0962(3)	329(11)
H2	4c	-0.088	$1/4$	0.100	395
B3	4c	0.4384(7)	$1/4$	0.0823(3)	304(11)
H3	4c	0.568	$1/4$	0.078	365
B4	4c	0.3180(7)	$1/4$	0.0006(3)	349(11)
H4	4c	0.368	$1/4$	-0.057	418
B5	8d	0.3395(5)	0.1649(4)	0.1556(2)	328(8)
H5	8d	0.404	0.110	0.199	393
B6	8d	0.3266(5)	0.1116(4)	0.0598(2)	345(8)
H6	8d	0.382	0.022	0.041	413
B7	8d	0.1549(5)	0.1116(4)	0.1195(2)	325 (8)
H7	8d	0.099	0.022	0.139	390
B8	8d	0.1411(5)	0.1648(4)	0.0231(2)	371(8)
H8	8d	0.077	0.110	-0.020	445

Table S2. Atomic coordinates and coefficients of the equivalent isotropic displacement parameters for Cs₃[ClO₃][B₁₂H₁₂] (**II**).

Atom	Wyckoff site	x/a	y/b	z/c	U_{eq}/pm^2
Cs1	4c	0.26127(7)	$1/4$	0.57179 (4)	497(3)
Cs2	8d	0.23179(5)	0.00982(5)	0.34315(3)	475(2)
Cl	4c	0.0097(2)	$1/4$	0.75085(13)	470(6)
O1	4c	0.0740(9)	$1/4$	0.8277(4)	678(22)
O2	8d	0.0738(7)	0.1394(5)	0.7119(3)	717(17)
B1	4c	0.1668(11)	$1/4$	0.1770(6)	35(2)
H1	4c	0.119	$1/4$	0.235	422
B2	4c	0.0411(11)	$1/4$	0.0975(6)	394(22)
H2	4c	-0.089	$1/4$	0.103	469
B3	4c	0.4394(11)	$1/4$	0.0829(6)	360(23)
H3	4c	0.570	$1/4$	0.079	432
B4	4c	0.3179(11)	$1/4$	0.0011(6)	411(26)
H4	4c	0.369	$1/4$	0.944	493
B5	8d	0.3379(8)	0.1663(7)	0.1551(4)	350(17)
H5	8d	0.402	0.112	0.198	422
B6	8d	0.3259(8)	0.1155(7)	0.0600(4)	399(18)
H6	8d	0.382	0.028	0.041	478
B7	8d	0.1556(8)	0.1144(7)	0.1187(4)	419(19)
H7	8d	0.100	0.027	0.137	503
B8	8d	0.1412(8)	0.1666(7)	0.0229(4)	391(18)
H8	8d	0.076	0.113	-0.0201	469

Table S3. Atomic coordinates and coefficients of the equivalent isotropic displacement parameters for Cs₃[ClO₄][B₁₂H₁₂] (**III**).

Atom	Wyckoff site	x/a	y/b	z/c	U_{eq}/pm^2
Cs1	4c	0.27314(3)	$1/4$	0.571528(17)	372.8(10)
Cs2	8d	0.22891(2)	0.007474(18)	0.342365(12)	342.1(9)
Cl	4c	0.01695(9)	$1/4$	0.74841(6)	258(2)
O1	4c	0.0690(3)	$1/4$	0.82737(17)	376(7)
O2	4c	0.3561(3)	$1/4$	0.7515(18)	416(8)
O3	8d	0.0696(2)	0.13879(19)	0.70885(12)	359(5)
B1	4c	0.1765(5)	$1/4$	0.1822(3)	272(10)
H1	4c	0.131(5)	$1/4$	0.246(3)	405(125)
B2	4c	0.0526(5)	$1/4$	0.1011(3)	292 (11)
H2	4c	0.424(4)	$1/4$	0.392(2)	161(94)
B3	4c	0.4292(5)	$1/4$	0.0800(3)	272(10)
H3	4c	0.056(5)	$1/4$	0.423(2)	335(121)
B4	4c	0.3093(5)	$1/4$	0.9982(3)	305 (11)
H4	4c	0.352(5)	$1/4$	0.938(3)	348(12)
B5	8d	0.3404(4)	0.1656(3)	0.15604(19)	262(7)
H5	8d	0.402(3)	0.114(3)	0.207(17)	225(73)
B6	8d	0.3204(4)	0.1127(3)	0.0585(2)	2867(7)
H6	8d	0.367(4)	0.022(3)	0.0397(18)	391(91)
B7	8d	0.1625(4)	0.1129(3)	0.1222(2)	2770(72)
H7	8d	0.111(4)	0.020(3)	0.1449(18)	430(100)
B8	8d	0.1430(4)	0.1657(3)	0.0240(2)	316(8)
H8	8d	0.075(3)	0.111(3)	0.9801(18)	402(88)

**Figure S1.** Raman spectrum of Cs₃[NO₃][B₁₂H₁₂] (**I**).

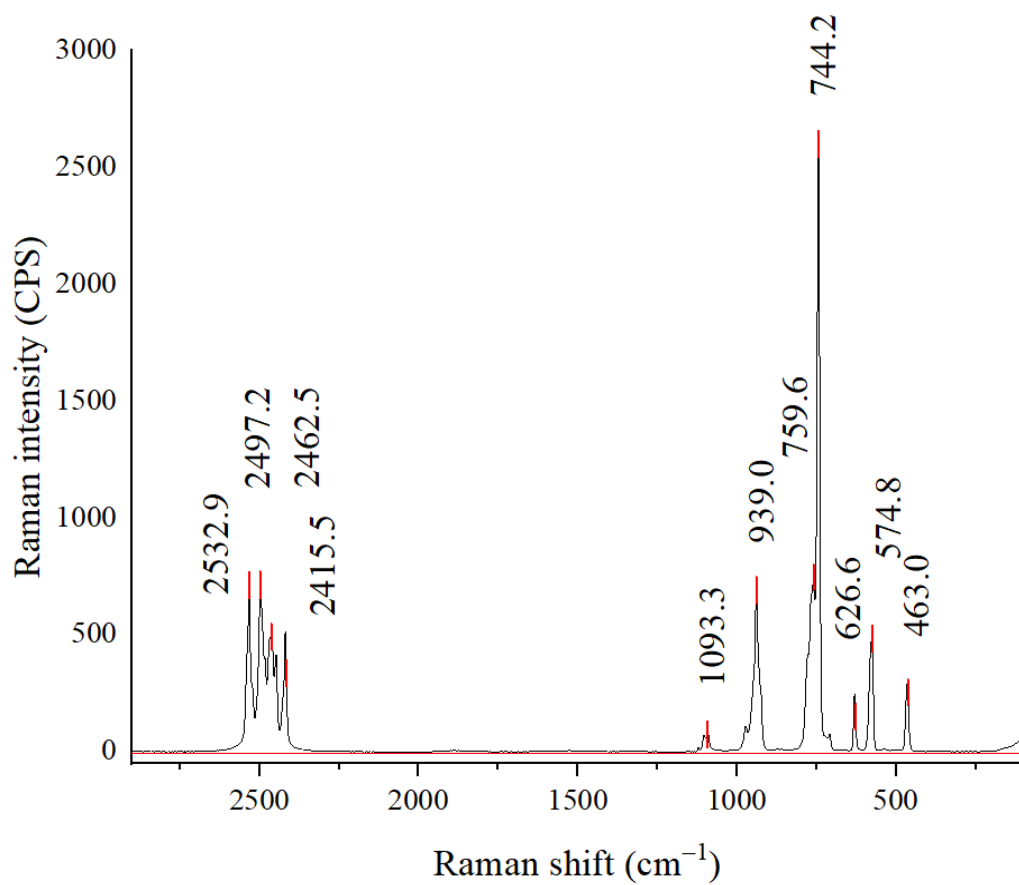


Figure S2. Raman spectrum of $\text{Cs}_3[\text{ClO}_4][\text{B}_{12}\text{H}_{12}]$ (**III**).