

Crystal Structure and Physical Properties of BaHoLi2Pb2

Rank #3 · Score 72.8% Good Generated 8/4/2026, 10:14:56 PM

ABSTRACT

We report the computational discovery of BaHoLi2Pb2, a trigonal inorganic compound generated via generative diffusion modelling (MatterGen). The unit cell comprises 6 atoms with an estimated density of 5.422 g cm⁻³ and a packing fraction of 66.99%. Symmetry analysis identifies the space group as P-3m1 (No. 164), belonging to the trigonal crystal system with point group -3m. The shortest interatomic contact measures 2.848 Å. Bond length analysis reveals 12 bonds spanning 2.847–3.9143 Å (mean 3.3536 ± 0.368 Å). CHGNet DFT surrogate predicts a formation energy of -1.2985 eV/atom (stable). The structure achieved an absolute structural quality score of 72.8% (Good), ranking #3 in the current set.

1. COMPOUND IDENTIFICATION

Empirical formula	BaHoLi2Pb2
Atom count	6
Quality classification	Good (score 72.8%, rank #3)
Density (est.)	5.422 g cm ⁻³
Packing fraction	66.99 %
Min. interatomic dist.	2.848 Å

2. CRYSTAL STRUCTURE

Space group	P-3m1 (No. 164)
Crystal system	trigonal
Point group	-3m
Hall symbol	-P 3 2"
Symmetry operations	12
Laue class	Yes

2a. Lattice Parameters

a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	V (Å ³)
4.9147	4.9153	8.2798	90	89.99	120	173.2132

2b. Wyckoff Positions

Element	Site	Mult.	Fractional coordinates
Ba	b	1	0.7411, 0.5846, 0.8513
Li	d	2	0.4081, 0.9178, 0.1766

Element	Site	Mult.	Fractional coordinates
Li	d	2	0.0747, 0.2514, 0.5256
Ho	a	1	0.7414, 0.5845, 0.3512
Pb	d	2	0.0748, 0.2511, 0.1481
Pb	d	2	0.4081, 0.9180, 0.5543

3. BONDING ENVIRONMENT

Total bonds	12
Bond length range	2.847 – 3.9143 Å
Mean bond length	3.3536 Å
Std. deviation	0.368 Å

3a. Per-Pair Bond Statistics

Pair	Count	Min (Å)	Max (Å)	Mean (Å)
Ba-Li	2	3.9114	3.9143	3.9128
Ba-Pb	2	3.7522	3.7546	3.7534
Ho-Li	2	3.1831	3.1844	3.1837
Ho-Pb	2	3.2976	3.2985	3.298
Li-Pb	4	2.847	3.127	2.9868

4. COORDINATION ENVIRONMENT

Average coordination number: 8.67

#	Element	CN	Neighbor environment
0	Ba	12	Pb×6, Li×6
1	Li	7	Ho×3, Pb×4
2	Li	7	Pb×4, Ho×3
3	Ho	12	Li×6, Pb×6
4	Pb	7	Ba×3, Li×4
5	Pb	7	Li×4, Ba×3

5. DFT SURROGATE (CHGNET)

Stability **stable**

Formation energy	-1.2985 eV/atom
Total energy	-3.4911587238311768 eV/atom
Max force	0.1264 eV/Å
Max stress	63.564 GPa
Magnetic character	non-magnetic
Avg magmom	0.008 μB

CHGNet universal neural-network potential. Formation energy relative to DFT elemental references (Materials Project, PBE).

6. COMPUTATIONAL DETAILS

Generation method	MatterGen generative diffusion model
Scoring metric	Absolute structural quality composite
Score weights	Min. interatomic distance 40%, packing fraction 35%, density 25%
Ranking method	Gaussian proximity to ideal structural values → weighted sum
Property estimation	Derived from lattice geometry and atomic radii (geometric estimates)

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