**Rubidium Bromide (RbBr)**

*Space group*: Fm-3m, 225, rocksalt

*Lattice vectors*: *R*1 = (-*a*/2, 0, *a*/2); *R*2 = (0, *a*/2, *a*/2); *R*3 = (-*a*/2, *a*/2, 0)

*Atom positions Cartesian*: Rb= (0, 0, 0); Br= (*a*/2, *a*/2, *a*/2)

*Atom positions crystallographic*: Rb= (0, 0, 0); Br= (1/2, 1/2, 1/2)

*Isotopes*: 72.17% 85Rb (84.912 amu); 27.83% 87Rb (86.909 amu);

50.69% 79Br (78.918 amu); 49.31% 81Br (80.916 amu)

*DFT*: Use VASP or QE. PBE PAW (**USE PLAIN PBE!!)** The QE website does not have pbesol for Rb)  
(QE: Rb.pbe-spn-kjpaw\_psl.1.0.0.UPF and Br.pbe-n-kjpaw\_psl.1.0.0.UPF;

VASP: standard version; Rb\_sv) –

**Checklist** (*all data should be reported for the 2-atom primitive cell*)

* Please provide all computational costs in cores\*hours

***Structure/electrons***

* Converged relaxed ‘temperature (T)=0’ lattice constant *a* (target accuracy < 0.005 Å)

- Single value with 4 significant figures: **7.018**

* Methods / convergence criteria→**Convergence\_Check\_Hamakawa.xlsx**

- Energy/force thresholds: **Energy 1e-10 Ry**

- Integration mesh / grid shifting: **k=(6, 6, 6), no shifting**

- Smearing used?: No

* Other notes / cpu hours (*e.g., multiple relaxations, compilers, hardware*)
* Intel 18.0.2.199
* Intel Xeon Gold 6150
* **36 core × 391 minutes**
* All input files to run fully converged calculations (*e.g., qe.scf.in, POSCAR*)
* **QE.scf.in**
* Converged electron band dispersion (target accuracy < 0.1 eV for Γ/X/L frequencies)

- Numerical data: normalized wavevectors (q) and band energies (E): top 3 valence bands and 5 conduction bands (excel file, text file, or google sheet)

- q in units of 2π/*a* and f in eV

- 3 segments: Γ→X, Γ→K→X, and Γ→L evenly divided with ~100 q points per segment

- 3 files, one for each segment. For each scaled q from 0 to 1 list (~100 rows): q, E1, E2, E3, E4, E5, E6, E7, E8

- **Band\_GX.txt, Band\_GKX.txt, Band\_GL.txt**

* Methods / convergence criteria
* Check convergence for Γ/X/L, target accuracy < 0.1 eV
* Evidence of converged band structure→**Convergence\_Check\_Hamakawa.xlsx**

- Band structure with varying integration meshes

* Other notes / cpu hours
  + **36 core × 10 minutes**
* All input files to run fully converged calculations
  + **submit\_band.sh**

***Harmonic***

* Converged dispersion (target accuracy < 0.1 THz for Γ/X/L frequencies)

- Numerical data: normalized wavevectors (q) and frequencies (f) for 6 polarizations (*j*) (excel or text file)

- q in units of 2π/*a* and f in THz (f=ω/2π)

- 3 segments: Γ→X, Γ→K→X, and Γ→L evenly divided with ~100 q points per segment

- 3 files, one for each segment. For each scaled q from 0 to 1 list (~100 rows): q, f1, f2, f3, f4, f5, f6

- **Harmonic\_GX.txt, Harmonic\_GKX.txt, Harmonic\_GL.txt**

* Converged harmonic interatomic force constants (IFCs)
* Supercell perturbations or DFPT (provide relevant details): **Supercell method**

- Standard format for code used (*e.g.*, QE, Phonopy): **fcs\_harmonic.xml**

- Will be supplied as supplemental material upon publication

* Long range Coulomb corrections→**borninfo**
* Dielectric matrix (1-3x3 matrix)
* Born effective charge matrices (2-3x3 matrices)
  + : Br
  + : Rb
* Method of long-range Coulomb corrections: **Ewald method**
* Methods / convergence criteria

- Thresholds: **Check target accuracy < 0.1 THz for Γ/X/L frequencies**

- Supercell size / integration mesh: **2×2×2 / 2×2×2**

- Symmetries / irreducibility / number of calculations (*linked to cpu hours below*): **Space group: Fm-3m (225) / / 2**

- Post-processing (*e.g., enforce invariance constraints*): **Translational Invariance**

* Evidence of converged dispersion→**Convergence\_Check\_Hamakawa.xlsx**

- Dispersions with varying supercell sizes and integration meshes

* Other notes / cpu hours (*e.g., accuracy vs cpu cost, shifted meshes*)
  + **36 core × 7634 minutes**
* All input files to run fully converged calculations
  + **submit\_DFT.sh, submit\_born.sh, submit\_dispersion.sh**

***Anharmonic thermal transport***

* Four converged T-dependent thermal conductivities (*k*) (target accuracy <2% difference between successive grids - please contact us if a problem): natural isotopes with full BTE solution (*knat,full*), natural isotopes with the relaxation time approximation (RTA) (*knat,RTA*), isotopically pure (*e.g.*, 100% 85Rb and 100% 79Br) with full BTE solution (*kpure,full*), and isotopically pure with RTA (*kpure,RTA*). If only RTA available, then only *knat,RTA* and *kpure,RTA*

- Do not include boundary scattering, even at low T. We want to see how the codes behave at low T without this extrinsic scattering.

- Numerical data: T (K) and *k* (W/m/K) in range 10K < T < 1000K (excel or text file)

- For 10K ≤ T ≤ 50K increments of 10K (5 data points); for 50K < T ≤ 300K increments of 25K (10 data points); for 300K < T ≤ 1000K increments of 100K (7 data points).

- 1 file with T from 10K to 1000K list (22 rows): T, *knat,full*, *knat,RTA*, *kpure,full*, *kpure,RTA*

- Masses used for pure and natural calculations: **pure Rb:84.912 Br:78.918, nat Rb:85.4677651 Br:79.9032138**

- **kappa\_temp.txt**

* Accumulated T=300K *kacc* vs frequency and *kacc* vs mean free path (mfp) for converged *knat,RTA* value: **accum\_freq.txt, accum\_mfp.txt**

- Numerical data for each mode (q, *j*) sampled in the Brillouin zone integration: f (THz), mfp=|sqrt(*vx*2+*vy*2+*vz*2)×lifetime| (nm), mode contribution to *k* (W/m/K) for *knat,RTA*

- 1 file (excel or text) with row for each mode (q, *j*): f, mfp, mode contribution to *k*

- **mode\_kappa.txt**

* RTA T=300K three-phonon scattering rates (1/*τ3ph*) and phonon-isotope scattering rates for natural abundance (1/*τiso*)

- Numerical data: f (THz), 1/*τ3ph* (THz=1/ps), and 1/*τiso* (THz)

- 1 file (excel or text) with row for each mode (q, j): f, 1/*τ3ph*, 1/*τiso*

- **tau\_all.txt**

* Converged third-order anharmonic IFCs

- Standard format for code used

- Will be supplied as supplemental material upon publication

- **fcs\_anharmonic.xml**

* Methods / convergence criteria: thermal conductivity

- Delta function representation (*with details; e.g., adaptive smearing, cutoff*): **Tetrahedron**

- Integration grid: **30×30×30**

- Symmetries used

* Methods / convergence criteria: anharmonic IFCs→**Convergence\_Check\_Hamakawa.xlsx**

- Cutoff radius, supercell size, integration mesh, thresholds, displacement parameter for supercell derivatives

- Post-processing

* Evidence of converged *k* at T=300K →**Convergence\_Check\_Hamakawa.xlsx**

- Varying integration meshes

- Target accuracy <2% difference between successive grids

* Other notes / cpu hours
  + IFC calculation: **36 core × 90226 minutes**
  + Calculation thermal conductivity: **36 core × 3468 minutes**
* All input files to run fully converged calculations
  + **submit\_suggest.sh, submit\_fp.sh, submit\_thermal.sh**