

## Electronic Supplementary Information

### Reported and Predicted Structures of $\text{Ba}(\text{Co},\text{Nb})_{1-\delta}\text{O}_3$ Hexagonal Perovskite Phases

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Below are the atomic coordinates of the lowest energy structures for the compositions  $\text{Ba}_3\text{CoNb}_2\text{O}_9$ ,  $\text{Ba}_5\text{Nb}_4\text{O}_{15}$ ,  $\text{Ba}_8\text{CoNb}_6\text{O}_{24}$ ,  $\text{Ba}_{11}\text{Co}_2\text{Nb}_8\text{O}_{33}$  and  $\text{Ba}_{13}\text{CoNb}_{10}\text{O}_{39}$  in  $2 \times 2 \times 1$  unit cells. For the first three compositions, this also corresponds to the experimental structure. They are given in VASP POSCAR format (for which a description can be found at: [http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR\\_file.html](http://cms.mpi.univie.ac.at/vasp/vasp/POSCAR_file.html)).

The file header indicates the VASP total energy for the converged structure, with settings as given in the main text.

#### $\text{Ba}_3\text{CoNb}_2\text{O}_9$

```
# Ba3CoNb2O9: energy = -459.11791318 eV
1.0000000000000000
 11.7081709476927731  0.0000000000000000 -0.0000000000000000
 -5.8540854738463839 10.1395734725528754 -0.0000000000000000
  0.0000000000000004  0.0000000000000008  7.2034988646604683
Ba Co Nb O
12 4 8 36
Direct
0.1866157999999984 0.3313744000000014 0.4707548317635327
0.0199490999999981 0.4980411000000018 0.1406488682364710
0.3532822999999965 0.6647077000000010 0.8057023000000001
0.5199490999999981 0.9980410000000006 0.1406487682364698
0.6866157999999984 0.8313744000000014 0.4707548317635327
0.8532823999999977 0.1647077000000010 0.8057019000000025
0.3532822999999965 0.1647077000000010 0.8057000000000016
0.5199490999999981 0.4980412000000030 0.1406487682364698
0.6866156999999973 0.3313744000000014 0.4707548317635327
0.8532823000000036 0.6647077000000010 0.8057019000000025
0.1866157999999984 0.8313745000000026 0.4707548317635327
0.0199493000000004 0.9980411000000018 0.1406489682364651
0.8532823999999977 0.1647075999999998 0.3057019999999966
0.3532826000000000 0.6647078000000022 0.3057025000000024
0.3532828000000023 0.1647079000000033 0.3056989999999971
0.8532823999999977 0.6647079000000033 0.3057020999999978
0.1866156999999973 0.8313745000000026 0.9836436141530619
0.0199489999999969 0.4980411000000018 0.6277599858469408
0.6866156999999973 0.8313744000000014 0.9836438141530642
0.5199490999999981 0.4980412000000030 0.6277597858469385
0.5199490999999981 0.9980408999999995 0.6277598858469396
0.0199488000000017 0.9980408999999995 0.6277597858469385
0.6866155000000020 0.3313743000000002 0.9836436141530619
0.1866156999999973 0.3313743000000002 0.9836436141530619
0.7675902367226396 0.2503996632773570 0.1314101653679674
0.2675904367226417 0.7503998632773591 0.1314101653679674
0.2675906367226440 0.9933240734452855 0.1314096653679616
```

0.5246661265547214 0.2503995632773558 0.1314100653679662  
0.0246665265547187 0.2503996632773570 0.1314102653679615  
0.7675904367226419 0.9933237734452820 0.1314101653679674  
0.1818982734452837 0.0790156367226440 0.4799932346320330  
0.5246664265547178 0.7503997632773579 0.1314103653679626  
0.4389743632773607 0.5790159367226405 0.4799934346320354  
0.1032822999999965 0.6647077000000010 0.8057019000000025  
0.4389743632773607 0.8360915265547189 0.4799934346320352  
0.4389745632773560 0.0790156367226441 0.4799930346320379  
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0.9389743632773605 0.3360917265547209 0.4799934346320354  
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0.6818984734452787 0.0790156367226440 0.4799935346320365  
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0.4389745632773560 0.3360920265547173 0.4799930346320376  
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0.6032823000000036 0.6647077000000010 0.8057019000000025  
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0.8532823000000036 0.4147077000000010 0.8057018000000014  
0.1032822000000024 0.1647075999999998 0.8057015999999990  
0.1032822999999965 0.4147077000000010 0.8057019000000025  
0.8532822000000024 0.9147077000000010 0.8057015999999990  
0.3532822999999965 0.4147078000000022 0.8057014999999978  
0.1818983734452849 0.5790157367226382 0.4799936346320377  
0.1032821000000013 0.9147075999999998 0.8057018000000014  
0.2675904367226417 0.4933236734452812 0.1314101653679674  
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0.3532822999999965 0.9147075999999998 0.8057015999999990  
0.0246665265547187 0.7503998632773591 0.1314103653679626

# Ba<sub>5</sub>Nb<sub>4</sub>O<sub>15</sub>

# Ba<sub>5</sub>Nb<sub>4</sub>O<sub>15</sub>: energy = -769.38441134 eV

1.0000000000000000

11.7762624066164232 -0.0015364228893497 0.0000193176250818

-5.8880239019268572 10.1982084234882944 -0.0001144905597196

0.0000425935640684 -0.0001163106556492 11.9980115303445203

Ba Nb O

20 16 60

Direct

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0.6111966070662953 0.2924798473622336 0.2806188593264700  
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0.1112706656424035 0.7924636717161191 0.2805930779900692  
0.9445458392032261 0.9591182887711359 0.4222861817424949  
0.9444606392636420 0.9592407120382497 0.0597190874189117  
0.7778719160477997 0.1260066127616178 0.8515651957055893  
0.4445467392032225 0.9591177887711372 0.4222858817424914  
0.7779105554161957 0.6260252828378723 0.8515190645307557  
0.4446254510448584 0.4590989403608618 0.4222311522138841  
0.2779104554161937 0.6260251828378711 0.8515189645307545  
0.9445167642204206 0.4592482707428800 0.0596678908669474  
0.1111974070662975 0.2924796473622313 0.2806179593264737  
0.1110819965774516 0.7922881480161365 0.6431327926924741  
0.2778720160478015 0.1260068127616201 0.8515651957055893  
0.1110232382089502 0.2922634646594216 0.6432083586884546  
0.4444607392636499 0.9592408120382508 0.0597189874189106  
0.6110831965774512 0.7922885480161340 0.6431322926924754  
0.4445166642204197 0.4592481707428788 0.0596675908669510  
0.6110224382089481 0.2922628646594217 0.6432090586884486  
0.6111267171573151 0.7925028390370993 0.9563515068670266  
0.4445482252169071 0.4592217874359527 0.7465211562586627  
0.4445121445228822 0.9592366207785611 0.7465088199369371  
0.9445481252169062 0.4592214874359491 0.7465211562586627  
0.9445122445228764 0.9592369207785646 0.7465087199369359  
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0.1111508087169185 0.2925463556497098 0.9563497641566537  
0.6111509087169126 0.2925463556497097 0.9563498641566549  
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0.2776725641274378 0.1257984809927655 0.1681311261906929  
0.2777816363326958 0.6257786148737804 0.1681017943070137  
0.7777155638498676 0.1257210076220724 0.5348731571090443  
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0.6966472704357574 0.4618759497446753 0.4641462911279076  
0.6953699663850237 0.7069367724947692 0.4640463008456261  
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0.3624367222120640 0.2956200663891413 0.6595253714432511  
0.3629313750876071 0.5419053600266943 0.6598092852520276  
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0.5281755194357924 0.8765753538438901 0.8514507297685896  
0.1939587336810725 0.4570137840376692 0.0431366331507173  
0.1928169107151440 0.7103212259303722 0.0433030847570698  
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0.6939052798877123 0.9569959849272132 0.0431437499616947  
0.6927176303914296 0.2102763364932765 0.0432518096115165  
0.4473197452777842 0.7113318591263648 0.0432204884930876  
0.6939591336810704 0.4570138840376703 0.0431367331507185  
0.0281755194357928 0.8765753538438901 0.8514508297685908  
0.8585445692441885 0.7896878270815552 0.2386857770240579  
0.7783569480489938 0.3763039207409102 0.8515008244695119  
0.3629547207140700 0.0418941034338962 0.6597293408371019  
0.8629301750876076 0.5419042600266957 0.6598094852520229  
0.6088647139633424 0.0414871459483052 0.6597692505045293  
0.8625042247039503 0.7956638354314588 0.6594493157512180  
0.8629554207140704 0.0418948034338972 0.6597289408370972  
0.2783568480489929 0.3763042207409137 0.8515005244695084  
0.5281315684808954 0.1267950461289086 0.8513771567231811  
0.5281886974417355 0.3766300568285760 0.8514576227623145  
0.2783612298370119 0.8762890351737114 0.8514886467282718  
0.5282343612168999 0.6267654268947127 0.8513446763636411  
0.8624367222120637 0.2956199663891401 0.6595252714432570  
0.6928174107151430 0.7103216259303697 0.0433028847570746

# Ba<sub>8</sub>CoNb<sub>6</sub>O<sub>24</sub>

# Ba8CoNb6O24: energy = -1228.51536919 eV

1.0000000000000000

11.7506158653766342 0.0003008856931004 0.0000448459983034  
-5.8750457946848806 10.1789455151226313 0.0001664038946425  
0.0000737789709302 0.0003567811040585 19.2007682465907479

Ba Co Nb O  
32 4 24 96

Direct

0.5001535192038833 0.5029670475198359 0.2977780254701839  
0.1668412646486940 0.3363762875202662 0.2094798633194518  
0.3335218822801223 0.1695847075508284 0.9389407759312983  
0.0002614630852209 0.5030047509512787 0.0706071598359172  
0.5002261743253953 0.5029333440898638 0.0706574124133637  
0.5002091066668619 0.0029539179607819 0.0706364482095776  
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0.8335576111478337 0.6695075285945883 0.9389183577880266  
0.3335784792139000 0.6695812748696672 0.9389374278519385  
0.6668237139973193 0.3363739210712162 0.2094761952013651  
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0.0000902741822858 0.5030538617324802 0.8742732547027566  
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0.1669680593710104 0.8364291169644205 0.6329302579321884  
0.6669783182751132 0.8363142483196647 0.0065381664521096  
0.6668795687539664 0.3362779515107779 0.0065273754454041  
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0.6695958502182919 0.5839745040469722 0.1827940268378104  
0.2553057897877447 0.0056253334743860 0.3245137056049138  
0.9200712469947055 0.8414735998826929 0.8189222037404951  
0.4193859369402086 0.0915301473144558 0.1827427277925670  
0.1695750885139818 0.0839603260801358 0.1828138793119511  
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0.9975150998190593 0.7554685116808988 0.3244938516104752  
0.2552889153256592 0.5056151381434955 0.3245096042694723  
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0.9975251254938136 0.2554872982702852 0.3244915543345479  
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0.9199449036152511 0.3414180418697276 0.8189070532543726  
0.9163904998487996 0.8384669222774160 0.4468528846319841  
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0.9193340349333542 0.0867058889439165 0.4469132393393400  
0.7481101603111937 0.7560819992633945 0.6887168942093761  
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0.2485154760317481 0.7565118216386271 0.6885507164493156  
0.5053679792093213 0.2549331704153269 0.6886455565983901  
0.7471359069054566 0.9978469457017998 0.6883547482418644  
0.0820413013548456 0.9192996848517621 0.5671055352746724  
0.0839025016076533 0.6684928031130708 0.5671745413225512  
0.8346022727148970 0.9209624444134107 0.5671102999765609  
0.7480436788065565 0.2559763004707636 0.6886400778135222  
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# Ba<sub>11</sub>Co<sub>2</sub>Nb<sub>8</sub>O<sub>33</sub>

# Ba11Co2Nb8O33: energy = -1687.55833156 eV

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Ba Co Nb O

44 8 32 132

Direct

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# Ba<sub>13</sub>CoNb<sub>10</sub>O<sub>39</sub>

# Ba13CoNb10O39: energy = -1997.89023854 eV

1.0000000000000000

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-0.0003480056743607 0.0022580251952968 31.1976239719942186

Ba Co Nb O

52 4 40 156

Direct

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