# Direct $Bi^{3+}$-$Bi^{3+}$ contacts mediated by lonepairs in the HP-$BiNiO(PO_4)$ polymorph

Marie Colmont,[1*] Anastasiia Zadoya,[1] Céline Darie,[2] Cyril Domingos, [2] Bastien Leclercq,[1] and Olivier Mentré[1]

[1] Université Lille, CNRS, Centrale Lille, ENSCL, Université Artois, UMR 8181, Unité de Catalyse et Chimie du Solide, Lille, F-59000, France.

[2] Université Grenoble Alpes et CNRS, Institut NEEL, F-38042 Grenoble, France

---

## SUPPLEMENTARY INFORMATION

---

**Table S1. Data collection and structure refinement form powder for HP-$BiNiO(PO_4)$**

| **Crystal data** | |
|---|---|
| Formula | HP-$BiNiO(PO_4)$ |
| Formula weight (g) | 378.6 |
| Temperature (K) | 293 |
| Cell setting | triclinic |
| Space group | *P* -1 |
| a (Å) | 7.421(1) |
| b (Å) | 6.561(1) |
| c (Å) | 5.163(8) |
| α ° | 83.817(2) |
| β ° | 110.727(2) |
| γ ° | 123.412(2) |
| V ($Å^3$) | 195.03(2) |
| Z | 1 |
| **Data collection** | |
| Diffractometer | Bruker D8 Advance A25 |
| Radiation; λ | Cu$K\alpha$; 1.5418 |
| 2θ step (deg) | 0.02 |
| Data range 2θ (°); | 5 – 119.68 ( 5 – 12.49 excluded region) |
| No. of measured points | 5615 |
| **Refinement** | |
| Profile function | Pseudo-Voigt |
| Weight scheme | sigma |
| $R_P$ (%) | 2.81 |
| $R_{wP}$ (%) | 3.76 |
| Goodness of fit | 3.53 |

## HT *X-ray Diffraction* of AP-BNPO

The evolution of powder diffraction patterns with increasing of temperature is shown on Figure S2 for AP- $BiNiO(PO_4)$ phase. No obvious phase transformation is detected.

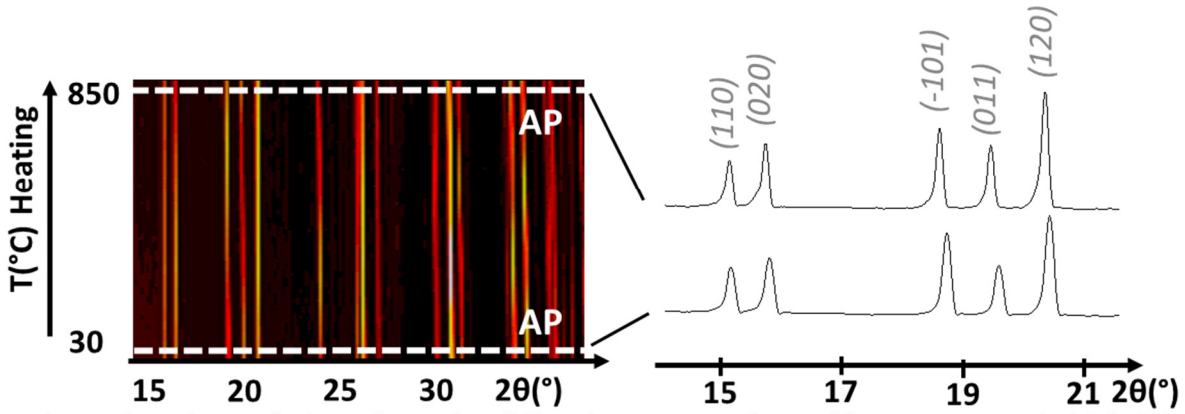


Figure S1. The evolution of powder diffraction patterns for ambient pressure $BiNiO(PO_4)$ phase.

LeBail Pattern matching was used to determine unit cell parameters from room temperature to 850ºC with a 100ºC step. The evolution of unit cell parameters is shown on graphics on figure S3.

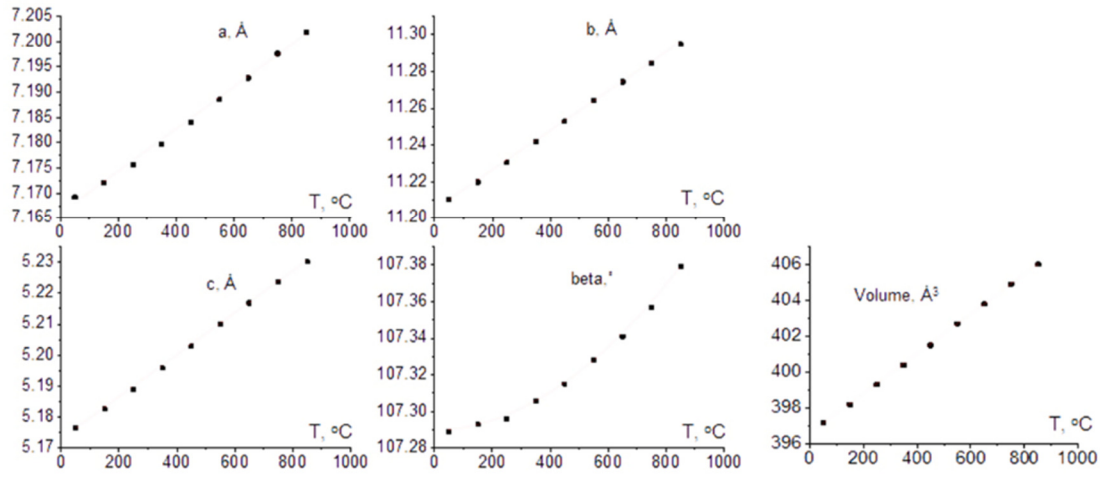


Figure S2. Evolution of unit cell parameters of the ambient pressure $BiNiO(PO_4)$. phase.

The evolution of powder diffraction patterns for HP-$BiNiO(PO_4)$ phase is presented in the main text. The determination and evolution of unit cell parameters of HP-$BiNiPO_5$ were provided with a 100ºC step from ambient temperature to 800ºC using LeBail Pattern matching in Jana2006 software. [3] The evolution of unit cell parameters is shown on Figure S4. The HP-BNPO sample heated at 950°C during 2h shows a relative amount in mass of the main AP-BNPO phase of about 85%, the rest corresponding to the HP modification.

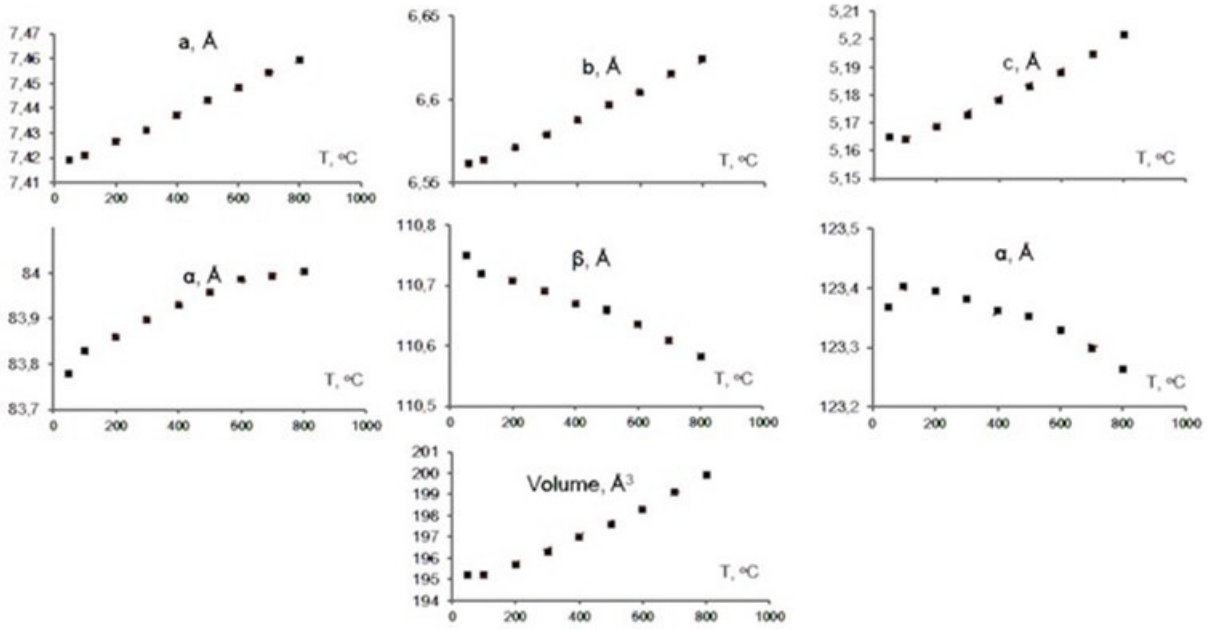


Figure S3. The evolution of unit cell lattice parameters for triclinic high pressure $BiNiO(PO_4)$ phase.

## Magnetic properties

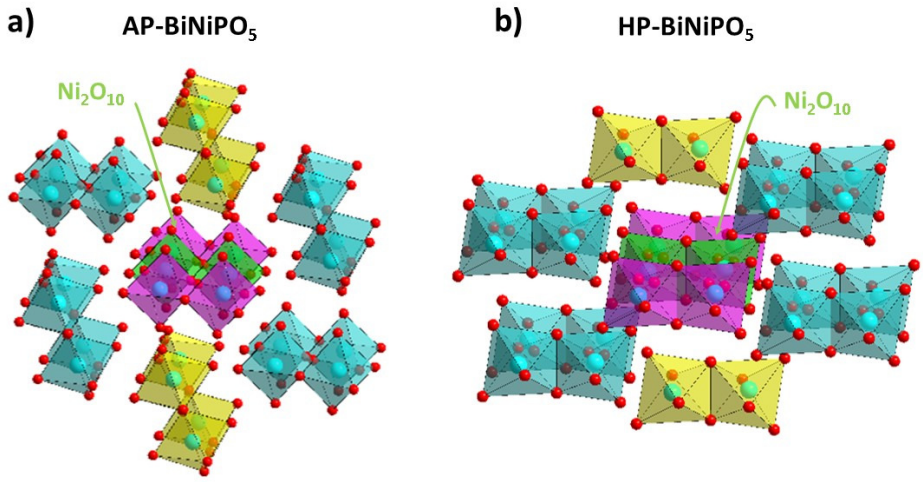


Figure S4: respective number of dimers neighbor of $Ni_2O_{10}$ dimer at the center of the figure (in green) for a) AP (14) and b) HP (12) $BiNiO(PO_4)$.

## References

O Mentre et al 2008 J. Phys.: Condens. Matter 20 41521, doi:10.1088/0953-8984/20/41/415211

The Belt-type apparatus was used to provide HP-HT experiment at 5GPa and 600˚C. The experiment was provided under supervision of Celine Darie in Neel Institute (Grenoble). Polycrystalline sample of initial compound was well grinded in agate mortar, loaded in 5x2 mm2 platinum capsule surrounded by a carbon furnace and pyrophyllite gasket.

Petricek, V., Dusek, M., Palatinus, L. (2014). Z. Kristallogr. 229(5), 345-352. DOI 10.1515/zkri-2014-1737

Brese, N. E., O'keeffe, M. Acta Cryst. (1991). B47, 192-197

T. Langreiter & V. Kahlenberg (2015) TEV – a program for the determination and visualization of the thermal expansion tensor from diffraction data. Crystals, 5, 143-153.