Supplementary Material (ESI) for *PCCP*

Databases of virtual inorganic crystal structures and their applications †

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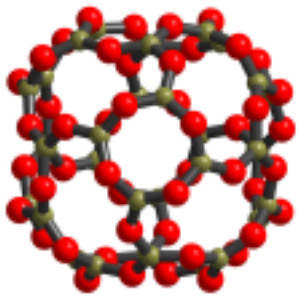

Graphical abstract : The PCOD (Predicted Crystallography Open Database) contains more than 1000000 entries including this nanosphere with $B_{32}O_{48}$ formulation as proposed by the *GRINSP* software.

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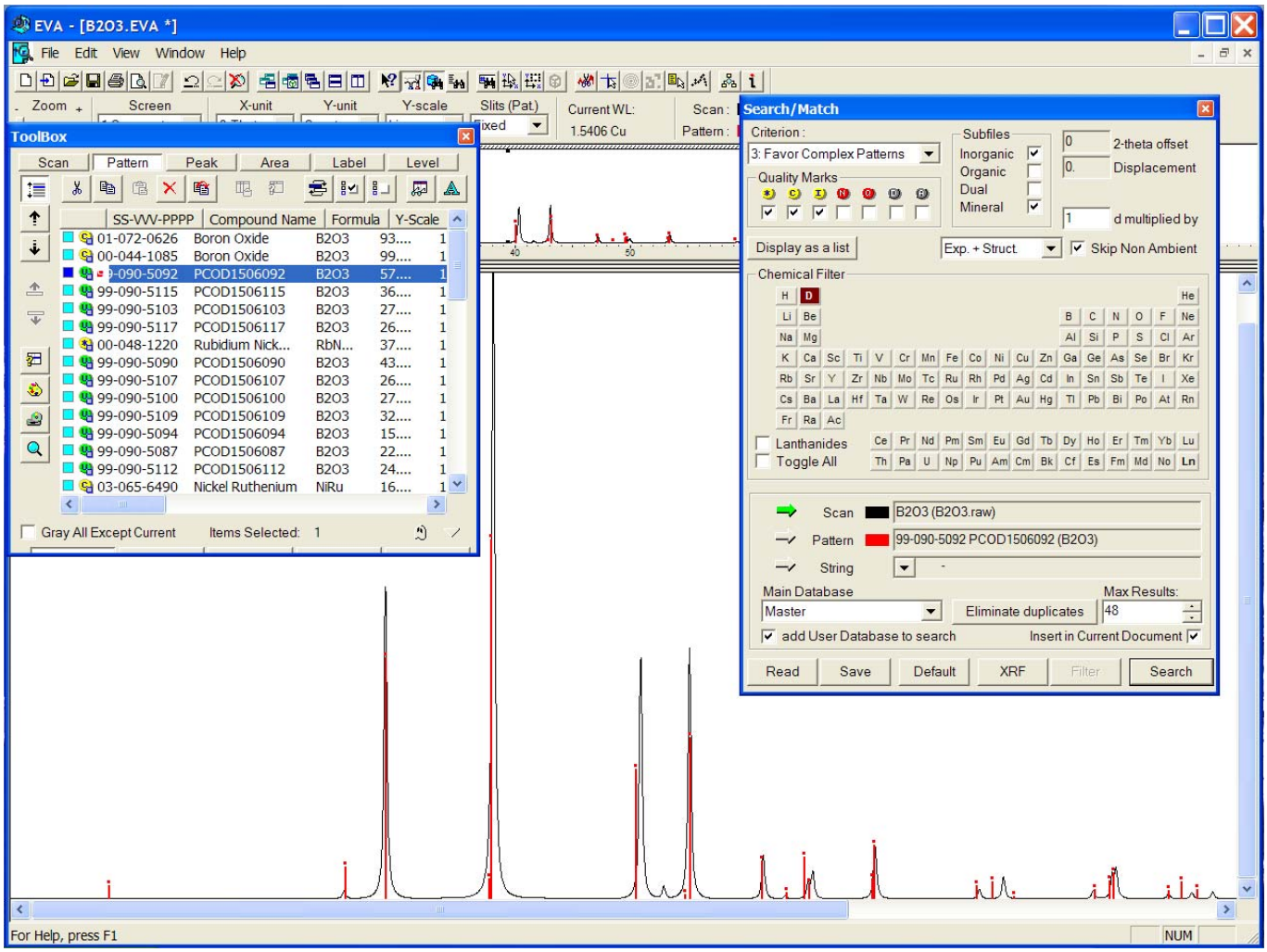

Figure S1. Positive search match by the *EVA*-Bruker program combined with the P2D2 database. Identification of B_2O_3 form I as being predicted by *GRINSP*.

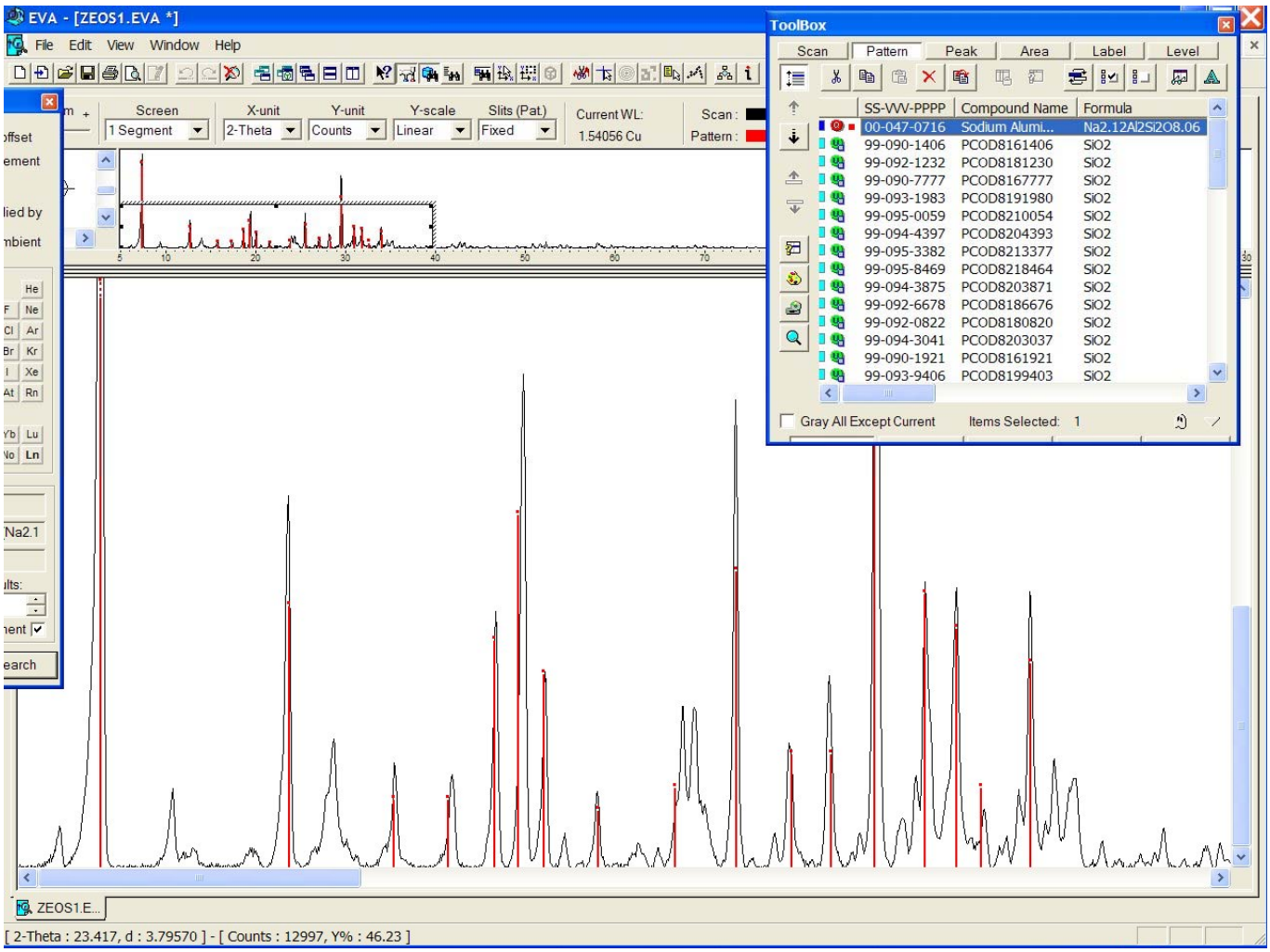

Figure S2. Positive search-matching for the "supposed to be" zeolite LZ-200 by using the *EVA*-Bruker software combined with the ICDD PDF (Powder Diffraction File). The matching PDF card 00-047-0716 (unindexed) does not explain all peaks suggesting that the sample contains impurities.

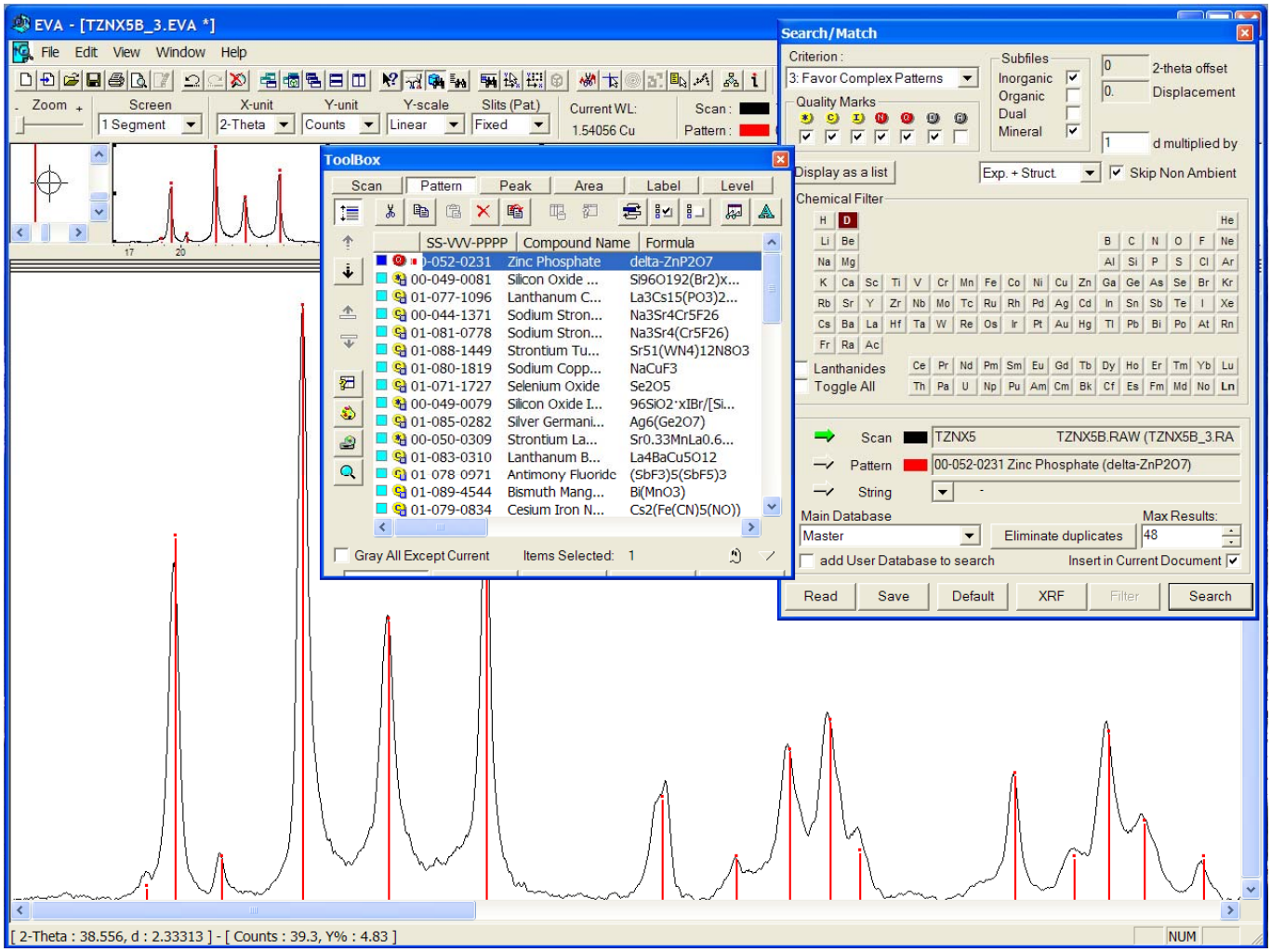

Figure S3. The poor quality and uncertainly indexed powder pattern of δ-$Zn_2P_2O_7$ of which the crystal structure can be proposed as a challenge to the ICSP community for its prediction.