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Structural and Electronic Properties of Monoclinic TiO_2 (B) Polymorph MICHEL POSTERNAK, ALFONSO BALDERESCHI, EPF-Lausanne, Switzerland, BERNARD DELLEY, Paul Scherrer Institut, Switzerland — Three major polymorphs of TiO_2 are known: rutile, anatase, and brookite. A further phase, TiO_2 (B), which coexists with, and derives from natural anatase has recently been identified[1]. It is monoclinic with C_{2h}^3 space group, and its conventional cell contains 8 TiO_2 formula units. Using the DMol[3] approach[2], we study the structural and electronic properties of this polymorph in terms of the OTi_3 complex, that we have recently shown[3] to be the relevant building block for describing the electronic properties of the three major polymorphs. At variance with these latter cases, the 16 O atoms in TiO_2 (B) are *not* all threefold coordinated: indeed, 12 O atoms belong to anataselike OTi_3 structural units, and the remaining 4 O atoms are twofold coordinated. The outcome of structural differences on the electronic properties of the TiO_2 phases is analyzed.

[1]J.F.Banfield *et al.*, Am. Mineral. **76**, 343 (1991).
[2]B. Delley, J. Chem. Phys. **113**, 7756 (2000).
[3]M. Posternak *et al.*, Phys. Rev. B **74**, 125113 (2006).

Michel A. Posternak
EPFL SB ITP CPNMC, PH D2 345, Station 3, CH-1015 Lausanne

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