



## *Supplement of*

# **Theoretical infrared spectra of OH defects in corundum ( $\alpha$ -Al<sub>2</sub>O<sub>3</sub>)**

**Etienne Balan**

*Correspondence to:* Etienne Balan ([etienne.balan@sorbonne-universite.fr](mailto:etienne.balan@sorbonne-universite.fr))

- [ejm-32-457-2020-supplement-title-page.pdf](#)
- [\\_\\_MACOSX](#)
  - [structures\\_corundum\\_Table\\_1\\_EA](#)
    - \* [\\_.DS\\_Store](#)
    - \* [1V\\_defects](#)
    - \* [2V\\_defects](#)
    - \* [intrinsic defects](#)
- [structures\\_corundum\\_Table\\_1\\_EA](#)
  - [.DS\\_Store](#)
  - [1Ti\\_defects](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al1.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al1.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al10.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al10.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al2.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al2.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al3.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al3.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al4.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al4.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al5.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al5.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al6.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al6.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al7.cif](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al7.vesta](#)
    - \* [corundum\\_221\\_VAl\\_Ti\\_1H\\_Al8.cif](#)

- \* corundum\_221\_VAl\_Ti\_1H\_Al8.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al9.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al9.vesta
- 1V\_defects
  - \* .DS\_Store
  - \* corundum\_221\_VAl\_V\_1H\_Al1.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al1.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al10.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al10.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al2.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al2.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al4.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al4.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al8.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al8.vesta
- 2Ti\_defects
  - \* corundum\_221\_VAl\_Ti\_1H\_Al10\_Al2.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al10\_Al2.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al10.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al10.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al2.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al2.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al4.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al4.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al5.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al5.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al8.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al8.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al9.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al1\_Al9.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al4.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al4.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al5.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al5.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al8.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al8.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al9.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al2\_Al9.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al10.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al10.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al5.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al5.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al8.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al8.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al9.cif
  - \* corundum\_221\_VAl\_Ti\_1H\_Al4\_Al9.vesta
  - \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al10.cif

- \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al10.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al8.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al8.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al9.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al5\_Al9.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al8\_Al10.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al8\_Al10.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al8\_Al9.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al8\_Al9.vesta
- \* corundum\_221\_VAl\_Ti\_1H\_Al9\_Al10.cif
- \* corundum\_221\_VAl\_Ti\_1H\_Al9\_Al10.vesta
- 2V\_defects
  - \* .DS\_Store
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al10.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al10.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al2.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al2.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al4.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al1\_Al4.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al2\_Al10.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al2\_Al10.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al4\_Al10.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al4\_Al10.vesta
  - \* corundum\_221\_VAl\_V\_1H\_Al8\_Al10.cif
  - \* corundum\_221\_VAl\_V\_1H\_Al8\_Al10.vesta
- Mg\_defects
  - \* corundum\_221\_Mg\_1H\_Al1.cif
  - \* corundum\_221\_Mg\_1H\_Al1.vesta
  - \* corundum\_221\_Mg\_1H\_Al2.cif
  - \* corundum\_221\_Mg\_1H\_Al2.vesta
  - \* corundum\_221\_Mg\_1H\_Al3.cif
  - \* corundum\_221\_Mg\_1H\_Al3.vesta
  - \* corundum\_221\_Mg\_1H\_Al4.cif
  - \* corundum\_221\_Mg\_1H\_Al4.vesta
- intrinsic defects
  - \* .DS\_Store
  - \* corundum\_221\_1H\_Hi.cif
  - \* corundum\_221\_1H\_Hi.vesta
  - \* corundum\_221\_VAl\_1H\_Oc.cif
  - \* corundum\_221\_VAl\_1H\_Oc.vesta
  - \* corundum\_221\_VAl\_1H\_Oe.cif
  - \* corundum\_221\_VAl\_1H\_Oe.vesta
  - \* corundum\_221\_VAl\_1H\_VOa.cif
  - \* corundum\_221\_VAl\_1H\_VOa.vesta
  - \* corundum\_221\_VAl\_1H\_VOb.cif
  - \* corundum\_221\_VAl\_1H\_VOb.vesta
  - \* corundum\_221\_VAl\_1H\_VOd.cif

- \* corundum\_221\_VAl\_1H\_VOd.vesta
- \* corundum\_221\_VAl\_1H\_VOe.cif
- \* corundum\_221\_VAl\_1H\_VOe.vesta
- \* corundum\_221\_VAl\_1H\_VOf.cif
- \* corundum\_221\_VAl\_1H\_VOf.vesta
- \* corundum\_221\_VAl\_2H.cif
- \* corundum\_221\_VAl\_2H.vesta

The copyright of individual parts of the supplement might differ from the CC BY 4.0 License.