Local Structural Distortion and Interrelated Phonon Mode Studies in Yttrium Chromite

Venkateswara rao Mannepalli1), Rajamani Raghunathan2), R.Ranjith1)**\***, A. David 3) and W. Prellier3)

*1) Department of Materials science and Metallurgical Engineering*

*Indian Institute of Technology Hyderabad, Hyderabad, Telangana, India-502205*

*2) Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, India-560012*.

*3) Laboratoire CRISMAT, ENSICAEN/CNRS, 6 Boulevard du Maréchal Juin, 14050 Caen Cedex 4, France*

TABLE SI: Frequencies,$ \overbar{ϑ}$ (cm-1) of various Phonon modes as a function of displacement (Å). SM, BM, OHD, AS correspond to Scissor, Bending, Octahedral displacement, and Antistretch modes respectively.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 0.000 | 0.008 | 0.015 | 0.030 | 0.038 |
| Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 |
| SM | B1u | 473.2 | SM | B1u | 473.3 | SM | B1u | 473.4 | BM | B1u | 472.8 | SMBM | B1u | 472.7 |
| SMBM | B3g | 474 | SMBM | B3g | 474.2 | SMBM | B3g | 474.6 | SMBM | B3g | 476.1 | BM | B3g | 477.2 |
| OHD | B2u | 479.4 | OHD | B2u | 479.4 | OHD | B2u | 479.4 | OHD | B2u | 479.3 | OHD | B2u | 479.2 |
| AS | B3u | 507.6 | AS | B3u | 507.2 | AS | B3u | 507.0 | AS | B3u | 506.5 | AS | B3u | 506.2 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 0.045 | 0.053 | 0.060 | 0.075 | 0.113 |
| Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 |
| SMBM | B1u | 472.6 | SMBM | B1u | 472.6 | SMBM | B1u | 472.5 | SMBM | B1u | 472.3 | SMBM | B1u | 472.4 |
| SM | B3g | 478.5 | SM | B2u | 479.0 | BM | B2u | 478.8 | OHD | B2u | 478.4 | OHD | B2u | 477.3 |
| OHD | B2u | 479.0 | OHD | B3g | 479.8 | OHD | B3g | 481.3 | SM | B3g | 484.8 | SM | B3g | 494.1 |
| AS | B3u | 505.9 | AS | B3u | 505.7 | AS | B3u | 505.3 | AS | B3u | 504.5 | AS | B3u | 502.5 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| 0.128 | 0.143 | 0.151 | 0.189 | 0.226 |
| Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 | Mode | Sym. | $$\overbar{ϑ}$$cm-1 |
| SMBM | B1u | 472.3 | SMBM | B1u | 472.2 | SMBM | B1u | 472.2 | SMBM | B2u | 473.5 | OHD | B2u | 471.0 |
| OHD | B2u | 476.1 | OHD | B2u | 476.1 | OHD | B2u | 475.7 | OHD | B1u | 474.5 | SMBM | B1u | 480.8 |
| SM | B3g | 497.3 | SM | B3g | 499.4 | AS | B3u | 499.8 | AS | B3u | 493.4 | AS | B3u | 488.8 |
| AS | B3u | 500.2 | AS | B3u | 500.2 | BM | B3g | 499.9 | OPS | B3g | 500.2 | OPS | B3g | 497.8 |