

```

data_global
_chemical_name_mineral 'Uvarovite'
loop_
  _publ_author_name
  'Righter K'
  'sutton S'
  'Danielson L'
  'Pando K'
  'Schmidt G'
  'Yang H'
  'Berthet S'
  'Newville M'
  'Choi Y'
  'Downs R T'
  'Malavergne V'
  _publ_section_title
  ;
  The effect of fO2 on the partitioning and valence of V and Cr in garnet/melt
  pairs and the relation to terrestrial mantle V and Cr content
  Note: R060477
  ;
  _chemical_compound_source 'Saranovskiy mine, Sarany, Ural Mountains, Russia'
  _chemical_formula_sum 'Ca3 (Cr1.15 Al.82 Ti.03) Si3 O12'
  _cell_length_a 11.9204
  _cell_length_b 11.9204
  _cell_length_c 11.9204
  _cell_angle_alpha 90
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  _cell_volume 1693.840
  _exptl_crystal_density_diffn    3.763
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  'y,1/2-z,1/2+x'
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_atom_site_fract_z
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Cr 0.00000 0.00000 0.00000 0.57500 0.00670
Al 0.00000 0.00000 0.00000 0.41000 0.00670
Ti 0.00000 0.00000 0.00000 0.01500 0.00670
Si 0.37500 0.00000 0.25000 1.00000 0.00320
O 0.03880 0.04660 0.65260 1.00000 0.00940
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_atom_site_aniso_U_22
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_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
Ca 0.00140 0.00320 0.00320 0.00000 0.00000 0.00070
Cr 0.00670 0.00670 0.00670 0.00010 0.00010 0.00010
Al 0.00670 0.00670 0.00670 0.00010 0.00010 0.00010
Ti 0.00670 0.00670 0.00670 0.00010 0.00010 0.00010
Si 0.00360 0.00310 0.00310 0.00000 0.00000 0.00000
O 0.01060 0.00970 0.00790 0.00040 -0.00050 0.00030
END

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