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Cite this: DOI: 10.1039/c0xx00000x

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COMMUNICATION

Relativity and the mercury battery (supplementary material)

Patryk Zaleski-Ejgierd[a] and Pekka Pyykkö[a]

Received (in XXX, XXX) Xth XXXXXXXXX 20XX, Accepted Xth XXXXXXXXX 20XX
DOI: 10.1039/b00000

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1. **Crystal structure of Zn(s)**
2. **Crystal structure of ZnO(s)**
3. **Crystal structure of Hg(s)**
4. **Crystal structure of HgO(s)**

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1. Structure of Zn(s)

```
#======================================================================================================
# CRYSTAL DATA
#------------------------------------------------------------------------------------------------------

data_VESTA_phase_Zn

_pd_phase_name                         'Zn'
_cell_length_a                         2.66480
_cell_length_b                         2.66480
_cell_length_c                         4.94670
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_symmetry_space_group_name_H-M         'P 63/m m c'
_symmetry_Int_Tables_number            194

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'
   '-x, -y, -z'
   '-y, x-y, z'
   'y, -x+y, -z'
   '-x+y, -x, z'
   'x-y, x, -z'
   '-x, -y, z+1/2'
   'x, y, -z+1/2'
   'y, -x+y, z+1/2'
   '-y, x-y, -z+1/2'
   'x-y, x, z+1/2'
   '-x+y, -x, -z+1/2'
   'y, x, -z'
   '-y, -x, z'
   'x-y, -y, -z'
   '-x+y, y, z'
   '-x, -x+y, -z'
   'x, x-y, z'
   '-y, -x, -z+1/2'
   'y, x, z+1/2'
   '-x+y, y, -z+1/2'
   'x-y, -y, z+1/2'
   'x, x-y, -z+1/2'
   '-x, -x+y, z+1/2'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_thermal_displace_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Zn       1.0    0.33333      0.66667      0.25000     Biso  1.000  Zn

#------------------------------------------------------------------------------------------------------
```


2. Crystal structure of ZnO(s)

```
#======================================================================================================
# CRYSTAL DATA
#------------------------------------------------------------------------------------------------------

data_VESTA_phase_ZnO


_pd_phase_name                         'Zn O'
_cell_length_a                         3.24900
_cell_length_b                         3.24900
_cell_length_c                         5.20700
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      120
_symmetry_space_group_name_H-M         'P 63 m c'
_symmetry_Int_Tables_number            186

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'
   '-y, x-y, z'
   '-x+y, -x, z'
   '-x, -y, z+1/2'
   'y, -x+y, z+1/2'
   'x-y, x, z+1/2'
   '-y, -x, z'
   '-x+y, y, z'
   'x, x-y, z'
   'y, x, z+1/2'
   'x-y, -y, z+1/2'
   '-x, -x+y, z+1/2'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_thermal_displace_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Zn       1.0    0.66667      0.33333      0           Biso  1.000  Zn
   O        1.0    0.66667      0.33333      0.34500     Biso  1.000  O


#------------------------------------------------------------------------------------------------------
```

3. Crystal structure of Hg(s)

```
#======================================================================================================
# CRYSTAL DATA
#------------------------------------------------------------------------------------------------------

data_VESTA_phase_1


_pd_phase_name                          'Hg'
_cell_length_a                         3.00504
_cell_length_b                         3.00504
_cell_length_c                         3.00504
_cell_angle_alpha                      70.54171
_cell_angle_beta                       70.54171
_cell_angle_gamma                      70.54171
_symmetry_space_group_name_H-M         'P 1'
_symmetry_Int_Tables_number            1

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_thermal_displace_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   Hg1      1.0    0            0            0           Biso  1.000  Hg
```

4. Crystal structure of HgO(s)

```
#======================================================================================================
# CRYSTAL DATA
#------------------------------------------------------------------------------------------------------

data_VESTA_phase_HgO


_pd_phase_name                         'Hg O'
_cell_length_a                         6.61290
_cell_length_b                         5.52080
_cell_length_c                         3.52190
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_symmetry_space_group_name_H-M         'P n m a'
_symmetry_Int_Tables_number            62

loop_
_symmetry_equiv_pos_as_xyz
   'x, y, z'
   '-x, -y, -z'
   '-x+1/2, -y, z+1/2'
   'x+1/2, y, -z+1/2'
   '-x, y+1/2, -z'
   'x, -y+1/2, z'
   'x+1/2, -y+1/2, -z+1/2'
   '-x+1/2, y+1/2, z+1/2'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_thermal_displace_type
   _atom_site_U_iso_or_equiv
   _atom_site_type_symbol
   Hg        1.0    0.11360      0.25000      0.24560     Uiso  0.015  Hg
   O         1.0    0.35920      0.25000      0.59550     Uiso  0.019  O
```

```
#------------------------------------------------------------------------------------------------------
```