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Supporting information for article:

Ab initio crystal structure prediction of magnesium (poly)sulfides and calculation of their NMR parameters

Gregor Mali

S1. CIF for the CSP-predicted rocksalt form of MgS

```
data_MgS_rocksalt
_audit_creation_date              2016-12-16
_audit_creation_method            'Crystal structure prediction (USPEX interfaced with Quantum Espresso)'
_symmetry_space_group_name_H-M    'FM-3M'
_symmetry_Int_Tables_number       225
_symmetry_cell_setting            cubic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x,-y,z
  -x,y,-z
  x,-y,-z
  z,x,y
  z,-x,-y
  -z,-x,y
  -z,x,-y
  y,z,x
  -y,z,-x
  y,-z,-x
  -y,-z,x
  y,x,-z
  -y,-x,-z
  y,-x,z
  -y,x,z
  x,z,-y
  -x,z,y
  -x,-z,-y
  x,-z,y
  z,y,-x
  z,-y,x
  -z,y,x
  -z,-y,-x
  -x,-y,-z
  x,y,-z
  x,-y,z
  -x,y,z
  -z,-x,-y
  -z,x,y
  z,x,-y
  z,-x,y
  -y,-z,-x
  y,-z,x
  -y,z,x
  y,z,-x
  -y,-x,z
  y,x,z
  -y,x,-z
  y,-x,-z
  -x,-z,y
  x,-z,-y
  x,z,y
  -x,z,-y
  -z,-y,x
  -z,y,-x
  z,-y,-x
  z,y,x
  x,y+1/2,z+1/2
  -x,-y+1/2,z+1/2
```

-x,y+1/2,-z+1/2
x,-y+1/2,-z+1/2
z,x+1/2,y+1/2
z,-x+1/2,-y+1/2
-z,-x+1/2,y+1/2
-z,x+1/2,-y+1/2
y,z+1/2,x+1/2
-y,z+1/2,-x+1/2
y,-z+1/2,-x+1/2
-y,-z+1/2,x+1/2
y,x+1/2,-z+1/2
-y,-x+1/2,-z+1/2
y,-x+1/2,z+1/2
-y,x+1/2,z+1/2
x,z+1/2,-y+1/2
-x,z+1/2,y+1/2
-x,-z+1/2,-y+1/2
x,-z+1/2,y+1/2
z,y+1/2,-x+1/2
z,-y+1/2,x+1/2
-z,y+1/2,x+1/2
-z,-y+1/2,-x+1/2
-x,-y+1/2,-z+1/2
x,y+1/2,-z+1/2
x,-y+1/2,z+1/2
-x,y+1/2,z+1/2
-z,-x+1/2,-y+1/2
-z,x+1/2,y+1/2
z,x+1/2,-y+1/2
z,-x+1/2,y+1/2
-y,-z+1/2,-x+1/2
y,-z+1/2,x+1/2
-y,z+1/2,x+1/2
y,z+1/2,-x+1/2
-y,-x+1/2,z+1/2
y,x+1/2,z+1/2
-y,x+1/2,-z+1/2
y,-x+1/2,-z+1/2
-x,-z+1/2,y+1/2
x,-z+1/2,-y+1/2
x,z+1/2,y+1/2
-x,z+1/2,-y+1/2
-z,-y+1/2,x+1/2
-z,y+1/2,-x+1/2
z,-y+1/2,-x+1/2
z,y+1/2,x+1/2
x+1/2,y,z+1/2
-x+1/2,-y,z+1/2
-x+1/2,y,-z+1/2
x+1/2,-y,-z+1/2
z+1/2,x,y+1/2
z+1/2,-x,-y+1/2
-z+1/2,-x,y+1/2
-z+1/2,x,-y+1/2
y+1/2,z,x+1/2
-y+1/2,z,-x+1/2
y+1/2,-z,-x+1/2
-y+1/2,-z,x+1/2
y+1/2,x,-z+1/2
-y+1/2,-x,-z+1/2

y+1/2,-x,z+1/2
-y+1/2,x,z+1/2
x+1/2,z,-y+1/2
-x+1/2,z,y+1/2
-x+1/2,-z,-y+1/2
x+1/2,-z,y+1/2
z+1/2,y,-x+1/2
z+1/2,-y,x+1/2
-z+1/2,y,x+1/2
-z+1/2,-y,-x+1/2
-x+1/2,-y,-z+1/2
x+1/2,y,-z+1/2
x+1/2,-y,z+1/2
-x+1/2,y,z+1/2
-z+1/2,-x,-y+1/2
-z+1/2,x,y+1/2
z+1/2,x,-y+1/2
z+1/2,-x,y+1/2
-y+1/2,-z,-x+1/2
y+1/2,-z,x+1/2
-y+1/2,z,x+1/2
y+1/2,z,-x+1/2
-y+1/2,-x,z+1/2
y+1/2,x,z+1/2
-y+1/2,x,-z+1/2
y+1/2,-x,-z+1/2
-x+1/2,-z,y+1/2
x+1/2,-z,-y+1/2
x+1/2,z,y+1/2
-x+1/2,z,-y+1/2
-z+1/2,-y,x+1/2
-z+1/2,y,-x+1/2
z+1/2,-y,-x+1/2
z+1/2,y,x+1/2
x+1/2,y+1/2,z
-x+1/2,-y+1/2,z
-x+1/2,y+1/2,-z
x+1/2,-y+1/2,-z
z+1/2,x+1/2,y
z+1/2,-x+1/2,-y
-z+1/2,-x+1/2,y
-z+1/2,x+1/2,-y
y+1/2,z+1/2,x
-y+1/2,z+1/2,-x
y+1/2,-z+1/2,-x
-y+1/2,-z+1/2,x
y+1/2,x+1/2,-z
-y+1/2,-x+1/2,-z
y+1/2,-x+1/2,z
-y+1/2,x+1/2,z
x+1/2,z+1/2,-y
-x+1/2,z+1/2,y
-x+1/2,-z+1/2,-y
x+1/2,-z+1/2,y
z+1/2,y+1/2,-x
z+1/2,-y+1/2,x
-z+1/2,y+1/2,x
-z+1/2,-y+1/2,-x
-x+1/2,-y+1/2,-z
x+1/2,y+1/2,-z

```
  x+1/2,-y+1/2,z
  -x+1/2,y+1/2,z
  -z+1/2,-x+1/2,-y
  -z+1/2,x+1/2,y
  z+1/2,x+1/2,-y
  z+1/2,-x+1/2,y
  -y+1/2,-z+1/2,-x
  y+1/2,-z+1/2,x
  -y+1/2,z+1/2,x
  y+1/2,z+1/2,-x
  -y+1/2,-x+1/2,z
  y+1/2,x+1/2,z
  -y+1/2,x+1/2,-z
  y+1/2,-x+1/2,-z
  -x+1/2,-z+1/2,y
  x+1/2,-z+1/2,-y
  x+1/2,z+1/2,y
  -x+1/2,z+1/2,-y
  -z+1/2,-y+1/2,x
  -z+1/2,y+1/2,-x
  z+1/2,-y+1/2,-x
  z+1/2,y+1/2,x
_cell_length_a                 5.2226
_cell_length_b                 5.2226
_cell_length_c                 5.2226
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
Mg    Mg   0.00000   0.00000   0.00000   0.00000  Uiso   1.00
S     S    0.50000   0.50000   0.50000   0.00000  Uiso   1.00
```

S2. CIF for the CSP-predicted wurtzite form of MgS

```
data_MgS_wurtzite
_audit_creation_date              2016-12-16
_audit_creation_method            ' Crystal structure prediction (USPEX interfaced with Quantum Espresso)'
_symmetry_space_group_name_H-M    'P63MC'
_symmetry_Int_Tables_number       186
_symmetry_cell_setting            hexagonal
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
_cell_length_a                 4.0484
_cell_length_b                 4.0484
_cell_length_c                 6.4863
_cell_angle_alpha               90.0000
_cell_angle_beta                90.0000
_cell_angle_gamma              120.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
Mg    Mg    0.33333   0.66667  -0.34506   0.00000  Uiso   1.00
S     S     0.33333   0.66667   0.03576   0.00000  Uiso   1.00
```

S3. CIF for the CSP-predicted zinc-blende form of MgS

```
data_MgS_zinc-blende
_audit_creation_date              2016-12-16
_audit_creation_method           'Crystal structure prediction (USPEX interfaced with Quantum Espresso)'
_symmetry_space_group_name_H-M    'F-43M'
_symmetry_Int_Tables_number       216
_symmetry_cell_setting            cubic
loop_
_symmetry_equiv_pos_as_xyz
 x,y,z
 -x,-y,z
 -x,y,-z
 x,-y,-z
 z,x,y
 z,-x,-y
 -z,-x,y
 -z,x,-y
 y,z,x
 -y,z,-x
 y,-z,-x
 -y,-z,x
 y,x,z
 -y,-x,z
 y,-x,-z
 -y,x,-z
 x,z,y
 -x,z,-y
 -x,-z,y
 x,-z,-y
 z,y,x
 z,-y,-x
 -z,y,-x
 -z,-y,x
 x,y+1/2,z+1/2
 -x,-y+1/2,z+1/2
 -x,y+1/2,-z+1/2
 x,-y+1/2,-z+1/2
```

z,x+1/2,y+1/2
z,-x+1/2,-y+1/2
-z,-x+1/2,y+1/2
-z,x+1/2,-y+1/2
y,z+1/2,x+1/2
-y,z+1/2,-x+1/2
y,-z+1/2,-x+1/2
-y,-z+1/2,x+1/2
y,x+1/2,z+1/2
-y,-x+1/2,z+1/2
y,-x+1/2,-z+1/2
-y,x+1/2,-z+1/2
x,z+1/2,y+1/2
-x,z+1/2,-y+1/2
-x,-z+1/2,y+1/2
x,-z+1/2,-y+1/2
z,y+1/2,x+1/2
z,-y+1/2,-x+1/2
-z,y+1/2,-x+1/2
-z,-y+1/2,x+1/2
x+1/2,y,z+1/2
-x+1/2,-y,z+1/2
-x+1/2,y,-z+1/2
x+1/2,-y,-z+1/2
z+1/2,x,y+1/2
z+1/2,-x,-y+1/2
-z+1/2,-x,y+1/2
-z+1/2,x,-y+1/2
y+1/2,z,x+1/2
-y+1/2,z,-x+1/2
y+1/2,-z,-x+1/2
-y+1/2,-z,x+1/2
y+1/2,x,z+1/2
-y+1/2,-x,z+1/2
y+1/2,-x,-z+1/2
-y+1/2,x,-z+1/2
x+1/2,z,y+1/2
-x+1/2,z,-y+1/2
-x+1/2,-z,y+1/2
x+1/2,-z,-y+1/2
z+1/2,y,x+1/2
z+1/2,-y,-x+1/2
-z+1/2,y,-x+1/2
-z+1/2,-y,x+1/2
x+1/2,y+1/2,z
-x+1/2,-y+1/2,z
-x+1/2,y+1/2,-z
x+1/2,-y+1/2,-z
z+1/2,x+1/2,y
z+1/2,-x+1/2,-y
-z+1/2,-x+1/2,y
-z+1/2,x+1/2,-y
y+1/2,z+1/2,x
-y+1/2,z+1/2,-x
y+1/2,-z+1/2,-x
-y+1/2,-z+1/2,x
y+1/2,x+1/2,z
-y+1/2,-x+1/2,z
y+1/2,-x+1/2,-z
-y+1/2,x+1/2,-z

```
  x+1/2,z+1/2,y
  -x+1/2,z+1/2,-y
  -x+1/2,-z+1/2,y
  x+1/2,-z+1/2,-y
  z+1/2,y+1/2,x
  z+1/2,-y+1/2,-x
  -z+1/2,y+1/2,-x
  -z+1/2,-y+1/2,x
_cell_length_a                 5.6919
_cell_length_b                 5.6919
_cell_length_c                 5.6919
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma              90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
Mg    Mg   0.75000   0.75000   0.75000   0.00000  Uiso   1.00
S     S    0.50000   0.50000   0.50000   0.00000  Uiso   1.00
```

S4. CIF for the CSP-predicted form of MgS_2

```
data_MgS2
_audit_creation_date              2016-12-16
_audit_creation_method            'Crystal structure prediction (USPEX interfaced with Quantum Espresso)'
_symmetry_space_group_name_H-M    'PA-3'
_symmetry_Int_Tables_number       205
_symmetry_cell_setting            cubic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,-y,z+1/2
  -x,y+1/2,-z+1/2
  x+1/2,-y+1/2,-z
  z,x,y
  z+1/2,-x+1/2,-y
  -z+1/2,-x,y+1/2
  -z,x+1/2,-y+1/2
  y,z,x
  -y,z+1/2,-x+1/2
  y+1/2,-z+1/2,-x
  -y+1/2,-z,x+1/2
  -x,-y,-z
  x+1/2,y,-z+1/2
  x,-y+1/2,z+1/2
  -x+1/2,y+1/2,z
  -z,-x,-y
  -z+1/2,x+1/2,y
  z+1/2,x,-y+1/2
  z,-x+1/2,y+1/2
  -y,-z,-x
  y,-z+1/2,x+1/2
  -y+1/2,z+1/2,x
```

```
  y+1/2,z,-x+1/2
_cell_length_a                 6.1319
_cell_length_b                 6.1319
_cell_length_c                 6.1319
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma              90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
Mg    Mg   0.00000   0.00000   0.00000   0.00000  Uiso   1.00
S     S   -0.40119  -0.40119  -0.40119   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
S     S      2.099   13_444 D
```

S5. CIF for the CSP-predicted form of Mg_2S_3

```
data_Mg2S3
_audit_creation_date              2016-12-16
_audit_creation_method            'Crystal structure prediction (USPEX interfaced with Quantum Espresso)'
_symmetry_space_group_name_H-M    'PMN21'
_symmetry_Int_Tables_number       31
_symmetry_cell_setting            orthorhombic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,-y,z+1/2
  x+1/2,-y,z+1/2
  -x,y,z
_cell_length_a                 3.7383
_cell_length_b                 8.4672
_cell_length_c                 6.1324
_cell_angle_alpha              90.0000
_cell_angle_beta               90.0000
_cell_angle_gamma              90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
Mg1   Mg   0.00000   0.34400  -0.31290   0.00000  Uiso   1.00
Mg2   Mg   0.00000  -0.07800  -0.28590   0.00000  Uiso   1.00
S3    S    0.00000   0.46310   0.30280   0.00000  Uiso   1.00
```

```
S4    S    0.00000  -0.12460   0.11610   0.00000  Uiso   1.00
S5    S    0.00000   0.26460   0.10020   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
S3    S5     2.090   .     D
```