

```

data_global
 _chemical_name 'Diopside'
loop_
 _publ_author_name
'Downs R T'
'Thompson R M'
 _journal_name_full "American Mineralogist"
 _publ_section_title
;
  The crystal structure of diopside to 10 GPa
  Sample: P = .0001 GPa
;
 _chemical_formula_sum 'Ca Mg Si2 O6'
 _cell_length_a 9.7397
 _cell_length_b 8.9174
 _cell_length_c 5.2503
 _cell_angle_alpha 90
 _cell_angle_beta 105.866
 _cell_angle_gamma 90
 _cell_volume 438.631
 _symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
 _symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
 _atom_site_label
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_Uiso_or_equiv
CaM2  0.00000  0.30148  0.25000  0.00823
MgM1  0.00000  0.90808  0.25000  0.00393
SiT   0.28619  0.09319  0.22936  0.00431
O1    0.11554  0.08690  0.14186  0.00697
O2    0.36094  0.25019  0.31776  0.00785
O3    0.35073  0.01744  0.99543  0.00709
END
data_global
 _chemical_name 'Diopside'
loop_
 _publ_author_name
'Downs R T'
'Thompson R M'
 _journal_name_full "American Mineralogist"
 _publ_section_title
;

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The crystal structure of diopside to 10 GPa

Sample: P = .13 GPa

;

_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.7377
_cell_length_b 8.9151
_cell_length_c 5.2494
_cell_angle_alpha 90
_cell_angle_beta 105.851
_cell_angle_gamma 90
_cell_volume 438.386
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_

_symmetry_equiv_pos_as_xyz

'x,y,z'

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

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

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

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

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

'-x,-y,-z'

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

loop_

_atom_site_label

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_Uiso_or_equiv

CaM2 0.00000 0.30167 0.25000 0.01039

MgM1 0.00000 0.90811 0.25000 0.00583

SiT 0.28615 0.09324 0.22913 0.00646

O1 0.11566 0.08721 0.14245 0.00950

O2 0.36112 0.25050 0.31808 0.01013

O3 0.35099 0.01778 0.99527 0.00874

END

data_global

_chemical_name 'Diopside'

loop_

_publ_author_name

'Downs R T'

'Thompson R M'

_journal_name_full "American Mineralogist"

_publ_section_title

;

The crystal structure of diopside to 10 GPa

Sample: P = 2.32 GPa

;

_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.6808
_cell_length_b 8.8488
_cell_length_c 5.2180
_cell_angle_alpha 90
_cell_angle_beta 105.606
_cell_angle_gamma 90

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_cell_volume 430.513
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_Uiso_or_equiv
CaM2 0.00000 0.30270 0.25000 0.00912
MgM1 0.00000 0.90867 0.25000 0.00469
SiT 0.28626 0.09370 0.22834 0.00545
O1 0.11547 0.08705 0.14258 0.00785
O2 0.36079 0.25183 0.31872 0.00899
O3 0.35156 0.01943 0.99227 0.00760
END
data_global
_chemical_name 'Diopside'
loop_
_publ_author_name
'Downs R T'
'Thompson R M'
_journal_name_full "American Mineralogist"
_publ_section_title
;
The crystal structure of diopside to 10 GPa
Sample: P = 4.22 GPa
;
_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.6341
_cell_length_b 8.7948
_cell_length_c 5.1926
_cell_angle_alpha 90
_cell_angle_beta 105.421
_cell_angle_gamma 90
_cell_volume 424.129
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'

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'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_Uiso_or_equiv
CaM2  0.00000  0.30368  0.25000  0.01077
MgM1  0.00000  0.90951  0.25000  0.00621
SiT   0.28618  0.09426  0.22772  0.00747
O1    0.11512  0.08768  0.14162  0.00975
O2    0.36057  0.25337  0.31985  0.01140
O3    0.35221  0.02031  0.99045  0.00975
END
data_global
  _chemical_name 'Diopside'
loop_
  _publ_author_name
'Downs R T'
'Thompson R M'
  _journal_name_full "American Mineralogist"
  _publ_section_title
;
  The crystal structure of diopside to 10 GPa
  Sample: P = 5.11 GPa
;
  _chemical_formula_sum 'Ca Mg Si2 O6'
  _cell_length_a 9.6135
  _cell_length_b 8.7695
  _cell_length_c 5.1813
  _cell_angle_alpha 90
  _cell_angle_beta 105.337
  _cell_angle_gamma 90
  _cell_volume 421.256
  _symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
  _symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_Uiso_or_equiv
CaM2  0.00000  0.30411  0.25000  0.00849
MgM1  0.00000  0.90961  0.25000  0.00481

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SiT  0.28607  0.09451  0.22734  0.00595
O1   0.11566  0.08821  0.14191  0.00811
O2   0.35967  0.25385  0.31975  0.00849
O3   0.35316  0.02091  0.99051  0.00836
END
data_global
  _chemical_name 'Diopside'
loop_
  _publ_author_name
    'Downs R T'
    'Thompson R M'
  _journal_name_full "American Mineralogist"
  _publ_section_title
    ;
    The crystal structure of diopside to 10 GPa
    Sample: P = 7.08 GPa
    ;
  _chemical_formula_sum 'Ca Mg Si2 O6'
  _cell_length_a 9.5731
  _cell_length_b 8.7197
  _cell_length_c 5.1580
  _cell_angle_alpha 90
  _cell_angle_beta 105.203
  _cell_angle_gamma 90
  _cell_volume 415.493
  _symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
  _symmetry_equiv_pos_as_xyz
    'x,y,z'
    '1/2+x,1/2+y,z'
    'x,-y,1/2+z'
    '1/2+x,1/2-y,1/2+z'
    '-x,y,1/2-z'
    '1/2-x,1/2+y,1/2-z'
    '-x,-y,-z'
    '1/2-x,1/2-y,-z'
loop_
  _atom_site_label
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_Uiso_or_equiv
CaM2  0.00000  0.30480  0.25000  0.00899
MgM1  0.00000  0.90984  0.25000  0.00507
SiT   0.28616  0.09503  0.22743  0.00608
O1    0.11519  0.08817  0.14212  0.00785
O2    0.35924  0.25493  0.32145  0.00912
O3    0.35263  0.02196  0.98889  0.00874
END
data_global
  _chemical_name 'Diopside'
loop_
  _publ_author_name
    'Downs R T'

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'Thompson R M'
_journal_name_full "American Mineralogist"
_publ_section_title
;
The crystal structure of diopside to 10 GPa
Sample: P = 8.01 GPa
;
_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.5557
_cell_length_b 8.6951
_cell_length_c 5.1474
_cell_angle_alpha 90
_cell_angle_beta 105.148
_cell_angle_gamma 90
_cell_volume 412.826
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_Uiso_or_equiv
CaM2 0.00000 0.30528 0.25000 0.00925
MgM1 0.00000 0.90998 0.25000 0.00519
SiT 0.28595 0.09523 0.22701 0.00646
O1 0.11494 0.08890 0.14173 0.00874
O2 0.35903 0.25554 0.32144 0.00975
O3 0.35425 0.02211 0.98887 0.00823
END
data_global
_chemical_name 'Diopside'
loop_
_publ_author_name
'Downs R T'
'Thompson R M'
_journal_name_full "American Mineralogist"
_publ_section_title
;
The crystal structure of diopside to 10 GPa
Sample: P = 8.88 GPa
;
_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.5391
_cell_length_b 8.6752

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_cell_length_c 5.1385
_cell_angle_alpha 90
_cell_angle_beta 105.106
_cell_angle_gamma 90
_cell_volume 410.536
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_Uiso_or_equiv
CaM2  0.00000  0.30559  0.25000  0.00874
MgM1  0.00000  0.91042  0.25000  0.00519
SiT   0.28632  0.09520  0.22734  0.00633
O1    0.11525  0.08839  0.14192  0.00735
O2    0.35930  0.25638  0.32204  0.00899
O3    0.35290  0.02239  0.98742  0.00849
END
data_global
_chemical_name 'Diopside'
loop_
_publ_author_name
'Downs R T'
'Thompson R M'
_journal_name_full "American Mineralogist"
_publ_section_title
;
The crystal structure of diopside to 10 GPa
Sample: P = 9.50 GPa
;
_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.5270
_cell_length_b 8.6587
_cell_length_c 5.1306
_cell_angle_alpha 90
_cell_angle_beta 105.067
_cell_angle_gamma 90
_cell_volume 408.681
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'

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'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_Uiso_or_equiv
CaM2 0.00000 0.30588 0.25000 0.00887
MgM1 0.00000 0.91060 0.25000 0.00494
SiT 0.28614 0.09547 0.22733 0.00633
O1 0.11520 0.08809 0.14222 0.00823
O2 0.35914 0.25645 0.32137 0.00861
O3 0.35342 0.02336 0.98756 0.00823
END
data_global
_chemical_name 'Diopside'
loop_
_publ_author_name
'Downs R T'
'Thompson R M'
_journal_name_full "American Mineralogist"
_publ_section_title
;
The crystal structure of diopside to 10 GPa
Sample: P = 10.16 GPa
;
_chemical_formula_sum 'Ca Mg Si2 O6'
_cell_length_a 9.5164
_cell_length_b 8.6449
_cell_length_c 5.1246
_cell_angle_alpha 90
_cell_angle_beta 105.033
_cell_angle_gamma 90
_cell_volume 407.164
_symmetry_space_group_name_H-M 'C 1 2/c 1'
loop_
_symmetry_equiv_pos_as_xyz
'x,y,z'
'1/2+x,1/2+y,z'
'x,-y,1/2+z'
'1/2+x,1/2-y,1/2+z'
'-x,y,1/2-z'
'1/2-x,1/2+y,1/2-z'
'-x,-y,-z'
'1/2-x,1/2-y,-z'
loop_
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y

```



```
_atom_site_fract_z
_atom_site_Uiso_or_equiv
CaM2  0.00000  0.30587  0.25000  0.00849
MgM1  0.00000  0.91075  0.25000  0.00557
SiT   0.28610  0.09554  0.22718  0.00595
O1    0.11538  0.08832  0.14178  0.00722
O2    0.35921  0.25714  0.32226  0.00861
O3    0.35409  0.02340  0.98725  0.00849
END
```