```
data_fig_2
_cell_length_a               7.13
_cell_length_b               7.13
_cell_length_c               10.0
_cell_angle_alpha             90.0
_cell_angle_beta              90.0
_cell_angle_gamma            120.0
_space_group_IT_number          1
_space_group_name_H-M_alt        P1
_space_group_name_Hall          'P 1'
loop_
 _atom_site_label
 _atom_site_Cartn_y
 _atom_site_Cartn_x
 _atom_site_Cartn_z
C417  6.175 13.5475235 0.0
X3  6.174999 14.973579 0.0
C199  6.1749983 16.399635 0.0
X142  7.4099994 12.8344965 0.0
C338  7.409999 14.2605505 0.0
C395  7.41 15.686606 0.0
X66  7.41 17.112661 0.0
C228  8.644999 12.1214695 0.0
C534  8.6449995 13.5475235 0.0
X107  8.6449995 14.973579 0.0
C303  8.644998 16.399635 0.0
C458  8.645 17.82569 0.0
X180  9.879999 12.8344965 0.0
C376  9.879998 14.2605505 0.0
C499  9.880001 15.686606 0.0
X67  9.879999 17.112661 0.0
C572  11.115001 13.5475235 0.0
X175  11.114999 14.973579 0.0
C371  11.114999 16.399635 0.0
X184  6.586665 11.408443 0.0
X74  4.5283318 14.973581 0.0
X14  6.586665 18.538717 0.0
```

X27 10.70333 18.538717 0.0
X125 12.761665 14.973581 0.0
X140 10.703332 11.408443 0.0
#jmolscript:{*}.radius=0.75