```
data_dia C2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia C2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diac2.cif.
;
_cell_length_a                      17.6347
_cell_length_b                      9.8367
_cell_length_c                      9.8784
_cell_angle_alpha                   90
_cell_angle_beta                    121.91
_cell_angle_gamma                   90
_cell_volume                        1454.622
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'C 2'
_symmetry_Int_Tables_number         5
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,-z
3 1/2+x,1/2+y,z
4 1/2-x,1/2+y,-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.15566 0.89354 0.67123 1
H2 H 4 0.27097 0.11608 0.78742 1
H3 H 4 0.24325 0.98321 0.35611 1
H4 H 2 0.50000 0.38418 0.00000 1
H5 H 2 0.50000 0.34528 0.50000 1
H6 H 4 0.44018 0.97766 0.83566 1
H7 H 4 0.56266 0.93917 0.45463 1
C1 C 4 0.18969 0.94629 0.62114 1
C2 C 4 0.24709 0.05673 0.67901 1
C3 C 4 0.23454 0.98956 0.45745 1
C4 C 4 0.47049 0.06250 0.91831 1
C5 C 2 0.50000 0.27318 0.00000 1
C6 C 4 0.53128 0.02412 0.47766 1
C7 C 2 0.50000 0.23426 0.50000 1
N1 N 4 0.18157 0.90403 0.47983 1
N2 N 4 0.27560 0.08363 0.57500 1
N3 N 4 0.45167 0.19647 0.86647 1
N4 N 4 0.55110 0.15797 0.46391 1
Zn1 Zn 4 0.37352 0.22411 0.62475 1
#End of data
```

```
data_dia Cc
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Cc
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diacc.cif.
;
_cell_length_a                      13.9069
_cell_length_b                      14.0549
_cell_length_c                      9.861
_cell_angle_alpha                   90
_cell_angle_beta                    133.64
_cell_angle_gamma                   90
_cell_volume                        1394.864
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'C c'
_symmetry_Int_Tables_number         9
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 x,-y,1/2+z
3 1/2+x,1/2+y,z
4 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.86774 0.55160 0.54822 1
H2 H 4 0.52487 0.57210 0.32725 1
H3 H 4 0.29878 0.68811 0.09763 1
H4 H 4 0.58333 0.81230 0.63612 1
H5 H 4 0.18191 0.09608 0.19009 1
H6 H 4 0.17444 0.20833 0.94995 1
C1 C 4 0.71653 0.36225 0.50640 1
C2 C 4 0.72043 0.41808 0.62615 1
C3 C 4 0.81614 0.49586 0.55440 1
C4 C 4 0.50392 0.63954 0.35728 1
C5 C 4 0.39176 0.69685 0.24353 1
C6 C 4 0.53667 0.76238 0.52048 1
N1 N 4 0.78424 0.50286 0.65670 1
N2 N 4 0.27730 0.91198 0.46104 1
N3 N 4 0.59562 0.68154 0.53295 1
N4 N 4 0.41309 0.77480 0.34802 1
Zn1 Zn 4 0.77626 0.62471 0.76051 1
#End of data
```

```
data_dia Fdd2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Fdd2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: dia_Fdd2SL.cif.
;
_cell_length_a                      14.0004
_cell_length_b                      14.2968
_cell_length_c                      14.418
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        2885.92
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'F d d 2'
_symmetry_Int_Tables_number         43
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/4-x,1/4+y,1/4+z
4 1/4+x,1/4-y,1/4+z
5 x,1/2+y,1/2+z
6 1/2+x,y,1/2+z
7 1/2+x,1/2+y,z
8 -x,1/2-y,1/2+z
9 1/2-x,-y,1/2+z
10 1/2-x,1/2-y,z
11 1/4-x,3/4+y,3/4+z
12 3/4-x,1/4+y,3/4+z
13 3/4-x,3/4+y,1/4+z
14 1/4+x,3/4-y,3/4+z
15 3/4+x,1/4-y,3/4+z
16 3/4+x,3/4-y,1/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 16 0.71886 0.53290 0.86929 1
H2 H 16 0.82828 0.65159 0.98002 1
H3 H 16 0.55834 0.61104 0.10586 1
C1 C 16 0.70167 0.56610 0.93531 1
C2 C 16 0.75599 0.62517 0.99031 1
C3 C 16 0.61715 0.60595 0.05635 1
N1 N 16 0.61341 0.55381 0.97762 1
N2 N 16 0.70205 0.65037 0.06703 1
Zn1 Zn 8 0.25000 0.75000 0.65935 1
#End of data
```

```
data_dia I4122
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I4122
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diai4122.cif.
;
_cell_length_a                      9.3279
_cell_length_b                      9.3279
_cell_length_c                      16.96
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1475.685
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'I 41 2 2'
_symmetry_Int_Tables_number         98
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 x,1/2-y,1/4-z
4 -x,1/2+y,1/4-z
5 -y,-x,-z
6 y,x,-z
7 y,1/2-x,1/4+z
8 -y,1/2+x,1/4+z
9 1/2+x,1/2+y,1/2+z
10 1/2-x,1/2-y,1/2+z
11 1/2+x,-y,3/4-z
12 1/2-x,y,3/4-z
13 1/2-y,1/2-x,1/2-z
14 1/2+y,1/2+x,1/2-z
15 1/2+y,-x,3/4+z
16 1/2-y,x,3/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 16 0.23417 0.64905 0.56452 1
H2 H 8 0.33732 0.25000 0.62500 1
C1 C 16 0.32360 0.69969 0.59509 1
C2 C 8 0.54568 0.75000 0.62500 1
N1 N 16 0.46493 0.66853 0.57565 1
Zn1 Zn 4 0.50000 0.50000 0.50000 1
#End of data
```

```
data_dia I41
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I41
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diai41.cif.
;
_cell_length_a                      10.0942
_cell_length_b                      10.0942
_cell_length_c                      15.2564
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1554.518
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'I 41'
_symmetry_Int_Tables_number         80
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 -y,1/2+x,1/4+z
4 y,1/2-x,1/4+z
5 1/2+x,1/2+y,1/2+z
6 1/2-x,1/2-y,1/2+z
7 1/2-y,x,3/4+z
8 1/2+y,-x,3/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.32766 0.24916 0.74528 1
H2 H 8 0.84073 0.97002 0.13638 1
H3 H 8 0.82299 0.10446 0.79220 1
C1 C 8 0.22704 0.96938 0.83262 1
C2 C 8 0.38709 0.26655 0.68682 1
C3 C 8 0.89317 0.87585 0.13240 1
N1 N 8 0.47513 0.17197 0.65536 1
N2 N 8 0.98420 0.85069 0.06609 1
Zn1 Zn 4 0.00000 0.50000 0.22212 1
#End of data
```

```
data_dia I-42d
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I-42d
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diai42d.cif.
;
_cell_length_a                      9.8488
_cell_length_b                      9.8488
_cell_length_c                      14.4373
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1400.402
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'I -4 2 d'
_symmetry_Int_Tables_number         122
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 x,1/2-y,1/4-z
4 -x,1/2+y,1/4-z
5 y,1/2+x,1/4+z
6 -y,1/2-x,1/4+z
7 -y,x,-z
8 y,-x,-z
9 1/2+x,1/2+y,1/2+z
10 1/2-x,1/2-y,1/2+z
11 1/2+x,-y,3/4-z
12 1/2-x,y,3/4-z
13 1/2+y,x,3/4+z
14 1/2-y,-x,3/4+z
15 1/2-y,1/2+x,1/2-z
16 1/2+y,1/2-x,1/2-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 16 0.63629 0.28600 0.81688 1
H2 H 8 0.88037 0.25000 0.12500 1
C1 C 16 0.69369 0.20141 0.84594 1
C2 C 8 0.99126 0.25000 0.12500 1
N1 N 16 0.65858 0.06765 0.82764 1
Zn1 Zn 4 0.00000 0.00000 0.00000 1
#End of data
```

```
data_dia Ima2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Ima2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diaima2.cif.
;
_cell_length_a                      10.4847
_cell_length_b                      14.9471
_cell_length_c                      10.5487
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1653.149
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'I m a 2'
_symmetry_Int_Tables_number         46
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/2-x,y,z
4 1/2+x,-y,z
5 1/2+x,1/2+y,1/2+z
6 1/2-x,1/2-y,1/2+z
7 -x,1/2+y,1/2+z
8 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.40860 0.43570 0.49058 1
H2 H 4 0.50000 0.50000 0.87020 1
H3 H 4 0.25000 0.16748 0.69729 1
H4 H 4 0.25000 0.05975 0.90619 1
H5 H 4 0.25000 0.33101 0.02238 1
C1 C 8 0.45137 0.46926 0.57086 1
C2 C 4 0.50000 0.50000 0.76674 1
C3 C 4 0.25000 0.18631 0.79664 1
C4 C 4 0.25000 0.13248 0.90284 1
C5 C 4 0.25000 0.27067 0.96444 1
N1 N 8 0.41801 0.44999 0.69501 1
N2 N 4 0.25000 0.27463 0.83549 1
N3 N 4 0.25000 0.18582 0.01138 1
Zn1 Zn 4 0.25000 0.37487 0.70470 1
#End of data
```

```
data_dia P212121
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P212121
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diap212121.cif.
;
_cell_length_a                      9.5495
_cell_length_b                      10.1421
_cell_length_c                      12.9073
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1250.098
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 21 21 21'
_symmetry_Int_Tables_number         19
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,-y,1/2+z
3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.44093 0.58970 0.12515 1
H2 H 4 0.66937 0.66878 0.24405 1
H3 H 4 0.73282 0.78646 0.93289 1
H4 H 4 0.22032 0.80491 0.28277 1
H5 H 4 0.90104 0.52812 0.21614 1
H6 H 4 0.27898 0.56884 0.38452 1
C1 C 4 0.53519 0.64292 0.10205 1
C2 C 4 0.64950 0.68128 0.16141 1
C3 C 4 0.68441 0.74396 0.00183 1
C4 C 4 0.19110 0.59523 0.33469 1
C5 C 4 0.16158 0.71266 0.28385 1
C6 C 4 0.99557 0.57160 0.24927 1
N1 N 4 0.55784 0.68352 0.00075 1
N2 N 4 0.74435 0.74506 0.09705 1
N3 N 4 0.08512 0.50609 0.31244 1
N4 N 4 0.03694 0.69710 0.22975 1
Zn1 Zn 4 0.93631 0.82097 0.12986 1
#End of data
```

```
data_P3121
_audit_creation_date                2010-03-02
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P3121
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diadfinalsym.cif.
;
_cell_length_a                      10.0927
_cell_length_b                      10.0927
_cell_length_c                      24.9858
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   120
_cell_volume                        2204.137
_cell_formula_units_Z               6
_symmetry_space_group_name_H-M      'P 31 2 1'
_symmetry_Int_Tables_number         152
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -y,x-y,1/3+z
3 -x+y,-x,2/3+z
4 x-y,-y,2/3-z
5 -x,-x+y,1/3-z
6 y,x,-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 6 0.08588 0.08043 0.94409 1
H2 H 3 0.52082 0.00000 0.33333 1
H3 H 6 0.84477 0.32776 0.17990 1
H4 H 3 0.00000 0.00950 0.16667 1
H5 H 6 0.88919 0.48382 0.90348 1
H6 H 6 0.18575 0.49533 0.78180 1
H7 H 6 0.04323 0.33740 0.93987 1
C1 C 6 0.16667 0.16511 0.97215 1
C2 C 3 0.62903 0.00000 0.33333 1
C3 C 6 0.92307 0.28434 0.17328 1
C4 C 3 0.00000 0.11770 0.16667 1
C5 C 6 0.97267 0.46357 0.88298 1
C6 C 6 0.04977 0.39125 0.90137 1
C7 C 6 0.12610 0.47198 0.82005 1
N1 N 6 0.29730 0.29571 0.95459 1
N2 N 6 0.87464 0.12968 0.17744 1
N3 N 6 0.02111 0.51458 0.83118 1
N4 N 6 0.14741 0.39682 0.86120 1
Zn1 Zn 6 0.97429 0.66391 0.79292 1
#End of data_P3121
```

```
data_dia P41212 - ..2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P41212 - ..2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diap41212sm.cif.
;
_cell_length_a                      10.3414
_cell_length_b                      10.3414
_cell_length_c                      11.8156
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1263.614
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 41 21 2'
_symmetry_Int_Tables_number         92
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,1/2+z
3 1/2+x,1/2-y,3/4-z
4 1/2-x,1/2+y,1/4-z
5 -y,-x,1/2-z
6 y,x,-z
7 1/2+y,1/2-x,3/4+z
8 1/2-y,1/2+x,1/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.81101 0.80041 0.78366 1
H2 H 8 0.76565 0.56437 0.89005 1
H3 H 8 0.71127 0.52123 0.53694 1
C1 C 8 0.78280 0.70762 0.74741 1
C2 C 8 0.75944 0.59038 0.80073 1
C3 C 8 0.73075 0.56512 0.61923 1
N1 N 8 0.76429 0.69118 0.63196 1
N2 N 8 0.72623 0.50021 0.71880 1
Zn1 Zn 4 0.80969 0.80969 0.50000 1
#End of data
```

```
data_dia P41212
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P41212
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: P41212_.cif.
;
_cell_length_a                      13.9293
_cell_length_b                      13.9293
_cell_length_c                      15.2321
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        2955.414
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'P 41 21 2'
_symmetry_Int_Tables_number         92
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,1/2+z
3 1/2+x,1/2-y,3/4-z
4 1/2-x,1/2+y,1/4-z
5 -y,-x,1/2-z
6 y,x,-z
7 1/2+y,1/2-x,3/4+z
8 1/2-y,1/2+x,1/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.61369 0.86003 0.46690 1
H2 H 8 0.52954 0.72884 0.35128 1
H3 H 8 0.57276 0.46920 0.93850 1
H4 H 4 0.72408 0.72408 0.00000 1
H5 H 8 0.45833 0.41428 0.28992 1
H6 H 4 0.68085 0.31915 0.75000 1
H7 H 8 0.67821 0.94088 0.20570 1
C1 C 8 0.61517 0.85708 0.39535 1
C2 C 8 0.57297 0.79226 0.33819 1
C3 C 8 0.64897 0.90051 0.26100 1
C4 C 8 0.58932 0.53760 0.96947 1
C5 C 4 0.66868 0.66868 0.00000 1
C6 C 8 0.44788 0.48848 0.26932 1
C7 C 4 0.62538 0.37462 0.75000 1
N1 N 8 0.66343 0.92560 0.34612 1
N2 N 8 0.59445 0.82009 0.25273 1
N3 N 8 0.67223 0.58852 0.94905 1
N4 N 8 0.36111 0.53550 0.28230 1
Zn1 Zn 8 0.52860 0.75195 0.15043 1
#End of data
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_citation_special_details
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_cell_length_c                      13.2008
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_cell_angle_gamma                   90
_cell_volume                        1285.746
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 41'
_symmetry_Int_Tables_number         76
_refine_ls_R_factor_all             0
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_symmetry_equiv_pos_as_xyz
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2 -x,-y,1/2+z
3 -y,x,1/4+z
4 y,-x,3/4+z
loop_
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_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.89431 0.54062 0.55826 1
H2 H 4 0.66427 0.60451 0.44438 1
H3 H 4 0.98999 0.85527 0.35246 1
H4 H 4 0.71256 0.58968 0.89865 1
H5 H 4 0.65606 0.82460 0.00975 1
H6 H 4 0.80948 0.52370 0.20717 1
C1 C 4 0.88001 0.61623 0.49898 1
C2 C 4 0.76599 0.64764 0.44221 1
C3 C 4 0.93222 0.77829 0.39326 1
C4 C 4 0.72463 0.61072 0.97928 1
C5 C 4 0.69625 0.72706 0.03448 1
C6 C 4 0.77565 0.57372 0.13782 1
N1 N 4 0.98522 0.69949 0.46765 1
N2 N 4 0.79972 0.75087 0.37525 1
N3 N 4 0.77498 0.51364 0.04534 1
N4 N 4 0.72899 0.70296 0.13513 1
Zn1 Zn 4 0.68268 0.81789 0.25893 1
#End of data
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dia P4322
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
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File: diap4322.cif.
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_symmetry_Int_Tables_number         95
_refine_ls_R_factor_all             0
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_symmetry_equiv_pos_as_xyz
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3 x,-y,1/2-z
4 -x,y,-z
5 -y,-x,3/4-z
6 y,x,1/4-z
7 y,-x,1/4+z
8 -y,x,3/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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H2 H 8 0.99841 0.88596 0.69761 1
H3 H 4 0.59336 0.00000 0.75000 1
H4 H 8 0.00259 0.59819 0.68516 1
C1 C 8 0.91828 0.54840 0.71768 1
C2 C 4 0.70833 0.50000 0.75000 1
C3 C 8 0.91364 0.94273 0.72430 1
C4 C 4 0.70400 0.00000 0.75000 1
N1 N 8 0.78472 0.57881 0.69714 1
N2 N 8 0.78030 0.90702 0.70728 1
Zn1 Zn 4 0.74575 0.25425 0.87500 1
#End of data
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_chemical_formula_moiety
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dia Pna21
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
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File: diapna21.cif.
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_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1372.778
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P n a 21'
_symmetry_Int_Tables_number         33
_refine_ls_R_factor_all             0
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_symmetry_equiv_pos_as_xyz
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3 1/2-x,1/2+y,1/2+z
4 1/2+x,1/2-y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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H2 H 4 0.40280 0.13050 0.73649 1
H3 H 4 0.44173 0.23182 0.50298 1
H4 H 4 0.75994 0.81281 0.81272 1
H5 H 4 0.69240 0.54805 0.59169 1
H6 H 4 0.46326 0.66839 0.58865 1
C1 C 4 0.51872 0.99516 0.50274 1
C2 C 4 0.44058 0.10220 0.64439 1
C3 C 4 0.45989 0.15287 0.52824 1
C4 C 4 0.71040 0.75697 0.75153 1
C5 C 4 0.67247 0.62100 0.63717 1
C6 C 4 0.55914 0.68084 0.63525 1
N1 N 4 0.47839 0.00204 0.62780 1
N2 N 4 0.50937 0.08437 0.43836 1
N3 N 4 0.76809 0.66971 0.71124 1
N4 N 4 0.58379 0.76716 0.70806 1
Zn1 Zn 4 0.45511 0.88184 0.74915 1
#End of data
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;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: diapnc2.cif.
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_cell_volume                        1475.569
_cell_formula_units_Z               4
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_symmetry_Int_Tables_number         30
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_symmetry_equiv_pos_as_xyz
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3 -x,1/2+y,1/2+z
4 x,1/2-y,1/2+z
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_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
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H2 H 2 0.00000 0.50000 0.16862 1
H3 H 4 0.39759 0.56433 0.77060 1
H4 H 2 0.50000 0.50000 0.17013 1
H5 H 4 0.98672 0.24419 0.45124 1
H6 H 4 0.99230 0.35649 0.22895 1
H7 H 4 0.59804 0.25016 0.27525 1
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C2 C 2 0.00000 0.50000 0.05951 1
C3 C 4 0.44955 0.53223 0.85400 1
C4 C 2 0.50000 0.50000 0.06105 1
C5 C 4 0.90608 0.26276 0.38234 1
C6 C 4 0.90855 0.31900 0.27226 1
C7 C 4 0.70482 0.26423 0.29306 1
N1 N 4 0.91129 0.45211 0.98454 1
N2 N 4 0.41798 0.55271 0.98575 1
N3 N 4 0.77668 0.22798 0.39514 1
N4 N 4 0.78020 0.32023 0.21585 1
Zn1 Zn 4 0.74717 0.37316 0.03237 1
#End of data
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basis

Wyckoff positions compatible with the embeddings of the diamond net with one crystallographic kind of a node*

Space group	Wyckoff position	Space group	Wyckoff position
$P\bar{1}$	2*i*	$P4_12_12$	4*a* (..2)
*C*2	4*c*	$P4_12_12$	8*b*
Cc	4*a*	$P4_322$	4*c* (..2)
*P*2/*c*	4*g*	$P4_32_12$	4*a* (..2)
$P2_1/c$	4*e*	$P4_32_12$	8*b*
*C*2/*c*	4*e* (.2.)	$I4_122$	4*a* (2.22)
*C*2/*c*	8*f*	$I4_1md$	4*a* (2*mm*.)
*C*2/*m*	4*i* (.*m*.)	$I\bar{4}2d$	4*a* ($\bar{4}$..)
$P222_1$	4*e*	$I4_1/amd$	4*a* ($\bar{4}m2$)
$P2_12_12_1$	4*a*	$R\bar{3}$	6*c* (3.)
$I2_12_12_1$	4*a* (2..)	$P3_121$	6*c*
*Pnc*2	4*c*	$P3_221$	6*c*
$Pna2_1$	4*a*	*R*32	6*c* (3.)
*Fdd*2	8*a* (..2)	$R\bar{3}m$	6*c* (3*m*)
*Ima*2	4*b* (*m*..)	$R\bar{3}c$	12*c* (3.)
Pnna	4*c* (..2)	$Fd\bar{3}$	8*a* (23.)
Pnna	8*e*	$F4_132$	8*a* (23.)
Pmna	4*h* (*m*..)	$P4_332$	8*c* (.3.)
Pbcn	8*d*	$P4_132$	8*c* (.3.)
Pnma	4*c* (.*m*.)	$Fd\bar{3}m$	8*a* ($\bar{4}$3*m*)
Fddd	8*a* (222)		
Imma	4*e* (*mm*2)		
$P4_1$	4*a*		
$P4_3$	4*a*		
$I4_1$	4*a* (2..)		
$I4_1/a$	4*a* ($\bar{4}$..)		
$P4_122$	4*c* (..2)		

* Only one Wyckoff position out of a Wyckoff set is given; for enantiomorphic pairs of space groups information is given twice. For special positions oriented site-symmetry symbols are given in parentheses.

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_citation_special_details
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_symmetry_Int_Tables_number         1
_refine_ls_R_factor_all             0
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_symmetry_equiv_pos_as_xyz
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_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
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H2 H 1 0.33186 0.53296 0.69257 1
H3 H 1 0.23850 0.53739 0.92075 1
H4 H 1 0.50000 0.00000 0.66864 1
H5 H 1 0.55289 0.11208 0.30744 1
H6 H 1 0.50000 0.50000 0.66648 1
H7 H 1 0.44996 0.61347 0.30549 1
H8 H 1 0.55004 0.38653 0.30549 1
H9 H 1 0.05004 0.11347 0.30549 1
H10 H 1 0.94996 0.88653 0.30549 1
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H12 H 1 0.44711 0.88792 0.30744 1
H13 H 1 0.94711 0.61208 0.30744 1
H14 H 1 0.05289 0.38792 0.30744 1
H15 H 1 0.00000 0.50000 0.66864 1
H16 H 1 0.76150 0.46261 0.92075 1
H17 H 1 0.26150 0.03739 0.92075 1
H18 H 1 0.73849 0.96261 0.92074 1
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H20 H 1 0.16815 0.03296 0.69257 1
H21 H 1 0.83185 0.96704 0.69257 1
H22 H 1 0.74675 0.10260 0.77869 1
H23 H 1 0.24675 0.39740 0.77869 1
H24 H 1 0.75326 0.60260 0.77869 1
H25 H 1 0.75325 0.10260 0.27869 1
H26 H 1 0.24675 0.89740 0.27869 1
H27 H 1 0.74675 0.60260 0.27869 1
H28 H 1 0.83186 0.46704 0.19257 1
H29 H 1 0.16814 0.53296 0.19257 1
H30 H 1 0.66815 0.96704 0.19257 1
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H35 H 1 0.05289 0.88792 0.80744 1
H36 H 1 0.94711 0.11208 0.80744 1
H37 H 1 0.44711 0.38792 0.80744 1
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H40 H 1 0.05004 0.61347 0.80549 1
H41 H 1 0.55004 0.88653 0.80549 1
H42 H 1 0.44996 0.11347 0.80549 1
H43 H 1 0.50000 0.00000 0.16648 1
H44 H 1 0.55289 0.61208 0.80744 1
H45 H 1 0.50000 0.50000 0.16864 1
H46 H 1 0.23850 0.03739 0.42075 1
H47 H 1 0.33185 0.03296 0.19257 1
H48 H 1 0.25325 0.39740 0.27869 1
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C2 C 1 0.30079 0.60924 0.74444 1
C3 C 1 0.25416 0.61177 0.85724 1
C4 C 1 0.50000 0.00000 0.57012 1
C5 C 1 0.52656 0.05491 0.38238 1
C6 C 1 0.50000 0.50000 0.56784 1
C7 C 1 0.47560 0.55648 0.38083 1
C8 C 1 0.52441 0.44352 0.38083 1
C9 C 1 0.02441 0.05648 0.38083 1
C10 C 1 0.97560 0.94352 0.38083 1
C11 C 1 0.00000 0.00000 0.56784 1
C12 C 1 0.47344 0.94509 0.38238 1
C13 C 1 0.97344 0.55490 0.38238 1
C14 C 1 0.02656 0.44509 0.38238 1
C15 C 1 0.00000 0.50000 0.57012 1
C16 C 1 0.74584 0.38823 0.85724 1
C17 C 1 0.24584 0.11177 0.85724 1
C18 C 1 0.75416 0.88823 0.85724 1
C19 C 1 0.69921 0.39076 0.74443 1
C20 C 1 0.19921 0.10924 0.74444 1
C21 C 1 0.80079 0.89076 0.74443 1
C22 C 1 0.74070 0.20180 0.78590 1
C23 C 1 0.24070 0.29820 0.78591 1
C24 C 1 0.75930 0.70180 0.78591 1
C25 C 1 0.75930 0.20180 0.28591 1
C26 C 1 0.24070 0.79820 0.28591 1
C27 C 1 0.74070 0.70180 0.28591 1
C28 C 1 0.80079 0.39076 0.24444 1
C29 C 1 0.19921 0.60924 0.24444 1
C30 C 1 0.69921 0.89076 0.24444 1
C31 C 1 0.75416 0.38823 0.35724 1
C32 C 1 0.24584 0.61177 0.35724 1
C33 C 1 0.74584 0.88823 0.35724 1
C34 C 1 0.00000 0.00000 0.07012 1
C35 C 1 0.02656 0.94509 0.88238 1
C36 C 1 0.97344 0.05490 0.88238 1
C37 C 1 0.47344 0.44509 0.88238 1
C38 C 1 0.00000 0.50000 0.06784 1
C39 C 1 0.97560 0.44352 0.88083 1
C40 C 1 0.02441 0.55648 0.88083 1
C41 C 1 0.52440 0.94352 0.88083 1
C42 C 1 0.47559 0.05648 0.88083 1
C43 C 1 0.50000 0.00000 0.06784 1
C44 C 1 0.52656 0.55490 0.88238 1
C45 C 1 0.50000 0.50000 0.07012 1
C46 C 1 0.25416 0.11177 0.35724 1
C47 C 1 0.30079 0.10924 0.24444 1

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C48 C 1 0.25930 0.29820 0.28591 1
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N2 N 1 0.22631 0.73173 0.88320 1
N3 N 1 0.54416 0.08928 0.50164 1
N4 N 1 0.45919 0.59235 0.50014 1
N5 N 1 0.54081 0.40765 0.50014 1
N6 N 1 0.04081 0.09235 0.50014 1
N7 N 1 0.95919 0.90765 0.50014 1
N8 N 1 0.45584 0.91073 0.50164 1
N9 N 1 0.95584 0.58927 0.50164 1
N10 N 1 0.04416 0.41072 0.50164 1
N11 N 1 0.77369 0.26827 0.88320 1
N12 N 1 0.27369 0.23173 0.88320 1
N13 N 1 0.72631 0.76827 0.88320 1
N14 N 1 0.69513 0.27214 0.69927 1
N15 N 1 0.19513 0.22786 0.69927 1
N16 N 1 0.80487 0.77214 0.69927 1
N17 N 1 0.80487 0.27214 0.19927 1
N18 N 1 0.19513 0.72786 0.19927 1
N19 N 1 0.69513 0.77214 0.19927 1
N20 N 1 0.72631 0.26827 0.38320 1
N21 N 1 0.27369 0.73173 0.38320 1
N22 N 1 0.77369 0.76827 0.38320 1
N23 N 1 0.04416 0.91072 0.00164 1
N24 N 1 0.95584 0.08927 0.00164 1
N25 N 1 0.45584 0.41072 0.00164 1
N26 N 1 0.95919 0.40765 0.00014 1
N27 N 1 0.04081 0.59235 0.00014 1
N28 N 1 0.54081 0.90765 0.00014 1
N29 N 1 0.45919 0.09235 0.00014 1
N30 N 1 0.54416 0.58927 0.00164 1
N31 N 1 0.22631 0.23173 0.38320 1
N32 N 1 0.30487 0.22786 0.19927 1
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Zn2 Zn 1 0.62697 0.24562 0.53355 1
Zn3 Zn 1 0.12697 0.25438 0.53355 1
Zn4 Zn 1 0.87303 0.74562 0.53355 1
Zn5 Zn 1 0.87303 0.24562 0.03355 1
Zn6 Zn 1 0.12697 0.75438 0.03355 1
Zn7 Zn 1 0.62697 0.74562 0.03355 1
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_citation_special_details
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_symmetry_equiv_pos_as_xyz
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_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
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_atom_site_fract_z
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H2 H 1 0.65946 0.58102 0.10001 1
H3 H 1 0.11658 0.32112 0.66020 1
H4 H 1 0.79234 0.18622 0.14282 1
H5 H 1 0.00999 0.06521 0.36980 1
H6 H 1 0.39320 0.06522 0.57745 1
H7 H 1 0.60686 0.06523 0.92258 1
H8 H 1 0.60685 0.93479 0.42258 1
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H10 H 1 0.99005 0.06522 0.13022 1
H11 H 1 0.99005 0.93479 0.63022 1
H12 H 1 0.00999 0.93479 0.86980 1
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H14 H 1 0.20771 0.81379 0.85720 1
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H16 H 1 0.88346 0.32113 0.83982 1
H17 H 1 0.88346 0.67888 0.33982 1
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H19 H 1 0.34058 0.58102 0.40001 1
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H21 H 1 0.65944 0.41899 0.60000 1
H22 H 1 0.34462 0.67922 0.62912 1
H23 H 1 0.34462 0.32078 0.12912 1
H24 H 1 0.65541 0.32079 0.37088 1
H25 H 1 0.15540 0.82079 0.37086 1
H26 H 1 0.84463 0.82078 0.12913 1
H27 H 1 0.84464 0.17922 0.62914 1
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H29 H 1 0.84059 0.91899 0.90001 1
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H46 H 1 0.61658 0.82112 0.66020 1
H47 H 1 0.15945 0.08102 0.10000 1
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H26 H 1 0.47269 0.14490 0.96392 1
H27 H 1 0.52731 0.85510 0.46392 1
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H29 H 1 0.84028 0.75222 0.43041 1
H30 H 1 0.15972 0.24778 0.93041 1
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H32 H 1 0.34028 0.74779 0.31959 1
H33 H 1 0.24778 0.15972 0.06959 1
H34 H 1 0.75222 0.84028 0.56959 1
H35 H 1 0.74779 0.34028 0.68041 1
H36 H 1 0.72014 0.42191 0.27917 1
H37 H 1 0.27987 0.57808 0.77917 1
H38 H 1 0.77987 0.92191 0.97083 1
H39 H 1 0.22013 0.07809 0.47083 1
H40 H 1 0.57808 0.27987 0.22083 1
H41 H 1 0.42191 0.72014 0.72083 1
H42 H 1 0.07809 0.22013 0.52917 1
H43 H 1 0.92192 0.77987 0.02917 1
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H45 H 1 0.02731 0.64490 0.28608 1
H46 H 1 0.40220 0.97686 0.83381 1
H47 H 1 0.01741 0.90088 0.93001 1
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C11 C 1 0.05286 0.90333 0.60726 1
C12 C 1 0.40333 0.44714 0.35725 1
C13 C 1 0.59666 0.55286 0.85725 1
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C42 C 1 0.01727 0.25064 0.58553 1
C43 C 1 0.98273 0.74936 0.08553 1
C44 C 1 0.15058 0.68436 0.16433 1
C45 C 1 0.03846 0.67656 0.21694 1
C46 C 1 0.29594 0.98418 0.84394 1
C47 C 1 0.09667 0.94714 0.89275 1
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N2 N 1 0.57475 0.28160 0.55246 1
N3 N 1 0.07474 0.21840 0.19755 1
N4 N 1 0.92526 0.78160 0.69755 1
N5 N 1 0.28160 0.57475 0.44754 1
N6 N 1 0.71840 0.42525 0.94755 1
N7 N 1 0.78160 0.92526 0.30245 1
N8 N 1 0.59578 0.72584 0.14946 1
N9 N 1 0.40423 0.27415 0.64946 1
N10 N 1 0.90422 0.22585 0.10054 1
N11 N 1 0.09578 0.77415 0.60054 1
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N15 N 1 0.78109 0.43167 0.41667 1
N16 N 1 0.21891 0.56833 0.91667 1
N17 N 1 0.71891 0.93167 0.83333 1
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N20 N 1 0.43167 0.78109 0.58325 1
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N22 N 1 0.76893 0.61514 0.33065 1
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N24 N 1 0.73107 0.11514 0.91935 1
N25 N 1 0.26893 0.88486 0.41935 1
N26 N 1 0.38485 0.23107 0.16935 1
N27 N 1 0.61514 0.76893 0.66935 1
N28 N 1 0.88486 0.26893 0.58065 1
N29 N 1 0.11515 0.73107 0.08065 1
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N32 N 1 0.21840 0.07474 0.80245 1
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Zn2 Zn 1 0.24646 0.24336 0.72931 1
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H4 H 1 0.88061 0.88729 0.00945 1
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H6 H 1 0.88729 0.11939 0.50945 1
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C8 C 1 0.29013 0.03846 0.25018 1
C9 C 1 0.96154 0.29013 0.75018 1
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C11 C 1 0.14577 0.81654 0.63831 1
C12 C 1 0.30679 0.73816 0.87548 1
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N2 N 1 0.16455 0.31632 0.21834 1
N3 N 1 0.68368 0.16455 0.71834 1
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N5 N 1 0.34058 0.14041 0.40064 1
N6 N 1 0.85959 0.34058 0.90064 1
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N8 N 1 0.31632 0.83545 0.71834 1
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H4 H 1 0.50125 0.88381 0.49097 1
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C3 C 1 0.83729 0.37632 0.74947 1
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N9 N 1 0.07433 0.73982 0.28127 1
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N11 N 1 0.74223 0.10207 0.59988 1
N12 N 1 0.89791 0.74221 0.09988 1
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Zn2 Zn 1 0.75158 0.25151 0.40761 1
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_cell_angle_gamma                   90
_cell_volume                        764.2449
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 1'
_symmetry_Int_Tables_number         1
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 1 0.11928 0.91377 0.58030 1
H2 H 1 0.88072 0.08623 0.08030 1
H3 H 1 0.38072 0.91377 0.08031 1
H4 H 1 0.79793 0.26803 0.57678 1
H5 H 1 0.20207 0.73198 0.07678 1
H6 H 1 0.70206 0.26803 0.07678 1
H7 H 1 0.77811 0.03663 0.35713 1
H8 H 1 0.22189 0.96337 0.85713 1
H9 H 1 0.72189 0.03664 0.85713 1
H10 H 1 0.70945 0.40468 0.89370 1
H11 H 1 0.29055 0.59533 0.39370 1
H12 H 1 0.79055 0.40467 0.39370 1
H13 H 1 0.78139 0.81379 0.61265 1
H14 H 1 0.21861 0.18621 0.11265 1
H15 H 1 0.71861 0.81379 0.11265 1
H16 H 1 0.00556 0.60201 0.63624 1
H17 H 1 0.99444 0.39799 0.13625 1
H18 H 1 0.49444 0.60201 0.13625 1
H19 H 1 0.50556 0.39799 0.63625 1
H20 H 1 0.28139 0.18622 0.61265 1
H21 H 1 0.20945 0.59532 0.89369 1
H22 H 1 0.27811 0.96337 0.35713 1
H23 H 1 0.29794 0.73198 0.57678 1
H24 H 1 0.61928 0.08624 0.58031 1
C1 C 1 0.02862 0.97844 0.54887 1
C2 C 1 0.97138 0.02156 0.04887 1
C3 C 1 0.47138 0.97844 0.04887 1
C4 C 1 0.86164 0.15941 0.54417 1
C5 C 1 0.13836 0.84059 0.04418 1
C6 C 1 0.63836 0.15941 0.04418 1
```

```
C7 C 1 0.85301 0.04591 0.43479 1
C8 C 1 0.14699 0.95409 0.93479 1
C9 C 1 0.64698 0.04591 0.93480 1
C10 C 1 0.76113 0.48789 0.82173 1
C11 C 1 0.23887 0.51212 0.32173 1
C12 C 1 0.73887 0.48789 0.32172 1
C13 C 1 0.79987 0.69843 0.67617 1
C14 C 1 0.20013 0.30157 0.17617 1
C15 C 1 0.70013 0.69844 0.17617 1
C16 C 1 0.91130 0.59296 0.68741 1
C17 C 1 0.08870 0.40704 0.18742 1
C18 C 1 0.58869 0.59296 0.18742 1
C19 C 1 0.41130 0.40703 0.68741 1
C20 C 1 0.29987 0.30157 0.67617 1
C21 C 1 0.26112 0.51213 0.82173 1
C22 C 1 0.35302 0.95409 0.43480 1
C23 C 1 0.36164 0.84059 0.54418 1
C24 C 1 0.52861 0.02156 0.54887 1
N1 N 1 0.97342 0.11639 0.61608 1
N2 N 1 0.02658 0.88361 0.11608 1
N3 N 1 0.52658 0.11639 0.11609 1
N4 N 1 0.95970 0.93074 0.43809 1
N5 N 1 0.04030 0.06926 0.93809 1
N6 N 1 0.54030 0.93074 0.93810 1
N7 N 1 0.70476 0.63142 0.76178 1
N8 N 1 0.29525 0.36857 0.26178 1
N9 N 1 0.79524 0.63142 0.26178 1
N10 N 1 0.88667 0.45894 0.78006 1
N11 N 1 0.11333 0.54107 0.28006 1
N12 N 1 0.61333 0.45893 0.28006 1
N13 N 1 0.38667 0.54106 0.78006 1
N14 N 1 0.20476 0.36858 0.76178 1
N15 N 1 0.45970 0.06926 0.43810 1
N16 N 1 0.47342 0.88361 0.61609 1
Zn1 Zn 1 0.02173 0.25582 0.78943 1
Zn2 Zn 1 0.97827 0.74418 0.28942 1
Zn3 Zn 1 0.47827 0.25582 0.28943 1
Zn4 Zn 1 0.52173 0.74418 0.78943 1
#End of data
```

```
data_C6 H6 N4 Zn/Pc_Cc
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
C6 H6 N4 Zn/Pc_Cc
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: dia_Pcfin.cif.
;
_cell_length_a                      6.9018
_cell_length_b                      7.5408
_cell_length_c                      10.1759
_cell_angle_alpha                   90
_cell_angle_beta                    133.92
_cell_angle_gamma                   90
_cell_volume                        381.4798
_cell_formula_units_Z               2
_symmetry_space_group_name_H-M      'P 1'
_symmetry_Int_Tables_number         1
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 1 0.20892 0.69577 0.35685 1
H2 H 1 0.23782 0.90602 0.59511 1
H3 H 1 0.17861 0.40279 0.19078 1
H4 H 1 0.67382 0.54630 0.63587 1
H5 H 1 0.09905 0.78535 0.85173 1
H6 H 1 0.80098 0.90614 0.08112 1
H7 H 1 0.80098 0.09386 0.58112 1
H8 H 1 0.09905 0.21466 0.35173 1
H9 H 1 0.67382 0.45370 0.13587 1
H10 H 1 0.17861 0.59722 0.69078 1
H11 H 1 0.23783 0.09399 0.09511 1
H12 H 1 0.20892 0.30424 0.85685 1
C1 C 1 0.10040 0.47346 0.06864 1
C2 C 1 0.84390 0.54942 0.78313 1
C3 C 1 0.05663 0.66784 0.89059 1
C4 C 1 0.64413 0.98649 0.05299 1
C5 C 1 0.35108 0.08578 0.05695 1
C6 C 1 0.33660 0.19006 0.93813 1
C7 C 1 0.33660 0.80995 0.43813 1
C8 C 1 0.35108 0.91423 0.55695 1
C9 C 1 0.64413 0.01351 0.55298 1
C10 C 1 0.05663 0.33217 0.39059 1
C11 C 1 0.84390 0.45059 0.28313 1
C12 C 1 0.10040 0.52654 0.56864 1
N1 N 1 0.87126 0.42617 0.89635 1
N2 N 1 0.21946 0.61920 0.07201 1
N3 N 1 0.52402 0.12714 0.93650 1
N4 N 1 0.54601 0.95679 0.12957 1
N5 N 1 0.54600 0.04322 0.62958 1
N6 N 1 0.52402 0.87286 0.43650 1
```

```
N7 N 1 0.21946 0.38080 0.57201 1
N8 N 1 0.87126 0.57384 0.39635 1
Zn1 Zn 1 0.57382 0.75679 0.27989 1
Zn2 Zn 1 0.57382 0.24321 0.77989 1
#End of data
```

```
data_C6 H6 N4 Zn/Pnn2 Fdd2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
C6 H6 N4 Zn/Pnn2 Fdd2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: Pnn2.cif.
;
_cell_length_a                      6.5134
_cell_length_b                      7.8129
_cell_length_c                      7.7192
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        392.8189
_cell_formula_units_Z               2
_symmetry_space_group_name_H-M      'P 1'
_symmetry_Int_Tables_number         1
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 1 0.22772 0.11489 0.70454 1
H2 H 1 0.77228 0.88512 0.70454 1
H3 H 1 0.27228 0.61489 0.20453 1
H4 H 1 0.31442 0.59339 0.46279 1
H5 H 1 0.68558 0.40661 0.46279 1
H6 H 1 0.18558 0.09339 0.96279 1
H7 H 1 0.12114 0.36856 0.23135 1
H8 H 1 0.87886 0.63144 0.23135 1
H9 H 1 0.37886 0.86856 0.73135 1
H10 H 1 0.62114 0.13144 0.73135 1
H11 H 1 0.81442 0.90661 0.96279 1
H12 H 1 0.72772 0.38511 0.20453 1
C1 C 1 0.22892 0.21478 0.60681 1
C2 C 1 0.77108 0.78522 0.60681 1
C3 C 1 0.27108 0.71477 0.10681 1
C4 C 1 0.27037 0.45984 0.47810 1
C5 C 1 0.72963 0.54016 0.47811 1
C6 C 1 0.22963 0.95984 0.97810 1
C7 C 1 0.17420 0.34903 0.36373 1
C8 C 1 0.82580 0.65097 0.36373 1
C9 C 1 0.32580 0.84903 0.86373 1
C10 C 1 0.67421 0.15097 0.86373 1
C11 C 1 0.77037 0.04016 0.97810 1
C12 C 1 0.72891 0.28523 0.10681 1
N1 N 1 0.30792 0.37429 0.63210 1
N2 N 1 0.69208 0.62570 0.63210 1
N3 N 1 0.19209 0.87429 0.13209 1
N4 N 1 0.14617 0.19326 0.44622 1
N5 N 1 0.85383 0.80675 0.44621 1
N6 N 1 0.35382 0.69326 0.94623 1
```

```
N7 N 1 0.64618 0.30674 0.94623 1
N8 N 1 0.80791 0.12572 0.13209 1
Zn1 Zn 1 0.50000 0.50000 0.81581 1
Zn2 Zn 1 0.00000 0.00000 0.31581 1
#End of data
```

```
data_dia Aea2-Pnc2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Aea2-Pnc2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: aba2pnc2.cif.
;
_cell_length_a                      13.1893
_cell_length_b                      10.8884
_cell_length_c                      11.0019
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1579.987
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'A b a 2'
_symmetry_Int_Tables_number         41
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/2-x,1/2+y,z
4 1/2+x,1/2-y,z
5 x,1/2+y,1/2+z
6 -x,1/2-y,1/2+z
7 1/2-x,y,1/2+z
8 1/2+x,-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.24675 0.39740 0.22131 1
H2 H 8 0.16815 0.03296 0.30743 1
H3 H 8 0.26150 0.03739 0.07925 1
H4 H 4 0.00000 0.50000 0.33136 1
H5 H 8 0.94711 0.61208 0.69256 1
H6 H 4 0.00000 0.00000 0.33352 1
H7 H 8 0.05004 0.11347 0.69451 1
C1 C 8 0.24070 0.29820 0.21409 1
C2 C 8 0.19921 0.10924 0.25556 1
C3 C 8 0.24584 0.11177 0.14276 1
C4 C 4 0.00000 0.50000 0.42988 1
C5 C 8 0.97344 0.55490 0.61762 1
C6 C 4 0.00000 0.00000 0.43216 1
C7 C 8 0.02441 0.05648 0.61917 1
N1 N 8 0.19513 0.22786 0.30073 1
N2 N 8 0.27369 0.23173 0.11680 1
N3 N 8 0.95584 0.58927 0.49836 1
N4 N 8 0.04081 0.09235 0.49986 1
Zn1 Zn 8 0.12697 0.25438 0.46645 1
#End of data
```

```
data_dia C2/c Cc
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia C2/c Cc
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: C2c.cif.
;
_cell_length_a                      14.3357
_cell_length_b                      14.1537
_cell_length_c                      10.0918
_cell_angle_alpha                   90
_cell_angle_beta                    131.88
_cell_angle_gamma                   90
_cell_volume                        1524.573
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'C 2/c'
_symmetry_Int_Tables_number         15
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,y,1/2-z
3 -x,-y,-z
4 x,-y,1/2+z
5 1/2+x,1/2+y,z
6 1/2-x,1/2+y,1/2-z
7 1/2-x,1/2-y,-z
8 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.79364 0.07112 0.92710 1
H2 H 8 0.60051 0.93622 0.05822 1
H3 H 8 0.60983 0.81521 0.84988 1
H4 H 8 0.43427 0.81522 0.29113 1
H5 H 8 0.69058 0.33102 0.28117 1
H6 H 8 0.46550 0.42922 0.06013 1
C1 C 8 0.74082 0.01816 0.93273 1
C2 C 8 0.64248 0.94659 0.00073 1
C3 C 8 0.64668 0.88656 0.89622 1
C4 C 8 0.47383 0.76192 0.39469 1
C5 C 8 0.60456 0.68527 0.64592 1
C6 C 8 0.49236 0.63598 0.53564 1
N1 N 8 0.70313 0.02991 0.02487 1
N2 N 8 0.70813 0.93219 0.85210 1
N3 N 8 0.90936 0.18473 0.37602 1
N4 N 8 0.59282 0.76524 0.55602 1
Zn1 Zn 8 0.72976 0.86748 0.68825 1
#End of data
```

```
data_dia I41acd I4122
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I41cd I41
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: I41cd.cif.
;
_cell_length_a                      10.8324
_cell_length_b                      10.8324
_cell_length_c                      13.9715
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1639.428
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'I 41 c d'
_symmetry_Int_Tables_number         110
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 -y,1/2+x,1/4+z
4 y,1/2-x,1/4+z
5 -x,y,1/2+z
6 x,-y,1/2+z
7 1/2+y,x,1/4+z
8 1/2-y,-x,1/4+z
9 1/2+x,1/2+y,1/2+z
10 1/2-x,1/2-y,1/2+z
11 1/2-y,x,3/4+z
12 1/2+y,-x,3/4+z
13 1/2-x,1/2+y,z
14 1/2+x,1/2-y,z
15 y,1/2+x,3/4+z
16 -y,1/2-x,3/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 16 0.27768 0.36452 0.32922 1
H2 H 16 0.77771 0.63486 0.92059 1
H3 H 16 0.75027 0.35561 0.12549 1
C1 C 16 0.25000 0.54447 0.12533 1
C2 C 16 0.35414 0.30679 0.35265 1
C3 C 16 0.85415 0.69276 0.89738 1
N1 N 16 0.47547 0.34247 0.33662 1
N2 N 16 0.97547 0.65735 0.91381 1
Zn1 Zn 8 0.00000 0.00000 0.75026 1
#End of data
```

```
data_dia I41cd Fdd2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I41cd Fdd2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: i41cdfdd2.cif.
;
_cell_length_a                      9.9276
_cell_length_b                      9.9276
_cell_length_c                      15.2594
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1503.924
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'I 41 c d'
_symmetry_Int_Tables_number         110
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 -y,1/2+x,1/4+z
4 y,1/2-x,1/4+z
5 -x,y,1/2+z
6 x,-y,1/2+z
7 1/2+y,x,1/4+z
8 1/2-y,-x,1/4+z
9 1/2+x,1/2+y,1/2+z
10 1/2-x,1/2-y,1/2+z
11 1/2-y,x,3/4+z
12 1/2+y,-x,3/4+z
13 1/2-x,1/2+y,z
14 1/2+x,1/2-y,z
15 y,1/2+x,3/4+z
16 -y,1/2-x,3/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 16 0.24629 0.69092 0.62840 1
H2 H 16 0.02842 0.68426 0.74287 1
H3 H 16 0.33015 0.41760 0.83438 1
C1 C 16 0.23277 0.63373 0.68870 1
C2 C 16 0.12397 0.63028 0.74565 1
C3 C 16 0.27676 0.49093 0.79402 1
N1 N 16 0.32993 0.54519 0.71982 1
N2 N 16 0.15200 0.53950 0.81240 1
Zn1 Zn 8 0.50000 0.00000 0.40249 1
#End of data
```

```
data_dia I41/acd-I-42d
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia I41/acd-I-42d
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: i41acd_i42d.cif.
;
_cell_length_a                      10.9995
_cell_length_b                      10.9995
_cell_length_c                      12.616
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1526.397
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'I 41/a c d'
_symmetry_Int_Tables_number         142
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,1/2-y,z
3 x,-y,1/2-z
4 1/2-x,y,-z
5 1/4-y,1/4-x,1/4-z
6 3/4+y,1/4+x,1/4-z
7 1/4+y,1/4-x,3/4+z
8 1/4-y,3/4+x,1/4+z
9 -x,-y,-z
10 x,1/2+y,-z
11 -x,y,1/2+z
12 1/2+x,-y,z
13 1/4+y,1/4+x,1/4+z
14 3/4-y,1/4-x,1/4+z
15 1/4-y,1/4+x,3/4-z
16 1/4+y,3/4-x,1/4-z
17 1/2+x,1/2+y,1/2+z
18 1/2-x,-y,1/2+z
19 1/2+x,1/2-y,-z
20 -x,1/2+y,1/2-z
21 3/4-y,3/4-x,3/4-z
22 1/4+y,3/4+x,3/4-z
23 3/4+y,3/4-x,1/4+z
24 3/4-y,1/4+x,3/4+z
25 1/2-x,1/2-y,1/2-z
26 1/2+x,y,1/2-z
27 1/2-x,1/2+y,z
28 x,1/2-y,1/2+z
29 3/4+y,3/4+x,3/4+z
30 1/4-y,3/4-x,3/4+z
31 3/4-y,3/4+x,1/4-z
32 3/4+y,1/4-x,3/4-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
```

```
_atom_site_occupancy
H1 H 32 0.86475 0.98407 0.04911 1
H2 H 16 0.75000 0.62307 0.00000 1
C1 C 32 0.80645 0.90907 0.02462 1
C2 C 16 0.75000 0.72168 0.00000 1
N1 N 32 0.84211 0.78982 0.04083 1
Zn1 Zn 8 0.50000 0.75000 0.87500 1
#End of data
```

```
data_dia P21212-P212121
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P21212-P212121
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: p21212p212121.cif.
;
_cell_length_a                      10.116
_cell_length_b                      10.939
_cell_length_c                      7.1148
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        787.3161
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 21 21 2'
_symmetry_Int_Tables_number         18
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/2+x,1/2-y,-z
4 1/2-x,1/2+y,-z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.83395 0.93597 0.97157 1
H2 H 4 0.03922 0.90946 0.71103 1
H3 H 4 0.07825 0.64183 0.13532 1
H4 H 4 0.35710 0.99898 0.12436 1
H5 H 4 0.36003 0.77753 0.30990 1
H6 H 4 0.20449 0.04992 0.67132 1
C1 C 4 0.91264 0.86819 0.96343 1
C2 C 4 0.01694 0.85807 0.83808 1
C3 C 4 0.03863 0.71717 0.05182 1
C4 C 4 0.32252 0.97714 0.26535 1
C5 C 4 0.32553 0.86625 0.35915 1
C6 C 4 0.24513 0.00505 0.54747 1
N1 N 4 0.92554 0.77785 0.09801 1
N2 N 4 0.09762 0.76302 0.89465 1
N3 N 4 0.27082 0.06536 0.38451 1
N4 N 4 0.27653 0.88364 0.53925 1
Zn1 Zn 4 0.26481 0.73921 0.72411 1
#End of data
```

```
data_dia P41212 P212121
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P41212 P212121
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: P41212.cif.
;
_cell_length_a                      10.6306
_cell_length_b                      10.6306
_cell_length_c                      13.5254
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1528.501
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'P 41 21 2'
_symmetry_Int_Tables_number         92
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,1/2+z
3 1/2+x,1/2-y,3/4-z
4 1/2-x,1/2+y,1/4-z
5 -y,-x,1/2-z
6 y,x,-z
7 1/2+y,1/2-x,3/4+z
8 1/2-y,1/2+x,1/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.21540 0.44927 0.39370 1
H2 H 8 0.00198 0.47194 0.51005 1
H3 H 8 0.97300 0.14472 0.33397 1
H4 H 8 0.49769 0.60938 0.67848 1
H5 H 8 0.52228 0.38298 0.57470 1
H6 H 8 0.88219 0.53842 0.62298 1
C1 C 8 0.13388 0.38768 0.39904 1
C2 C 8 0.02579 0.40003 0.45586 1
C3 C 8 0.00979 0.23081 0.36630 1
C4 C 8 0.58121 0.56117 0.65140 1
C5 C 8 0.59333 0.44940 0.59964 1
C6 C 8 0.78035 0.52691 0.62296 1
N1 N 8 0.12406 0.27956 0.34219 1
N2 N 8 0.94631 0.30017 0.43459 1
N3 N 8 0.70035 0.61000 0.66639 1
N4 N 8 0.71958 0.42763 0.58108 1
Zn1 Zn 8 0.77216 0.27186 0.50212 1
#End of data
```

```
data_dia P41212 P41
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P41212 P41
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: p41212p41.cif.
;
_cell_length_a                      10.1602
_cell_length_b                      10.1602
_cell_length_c                      14.9787
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1546.246
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'P 41 21 2'
_symmetry_Int_Tables_number         92
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,1/2+z
3 1/2+x,1/2-y,3/4-z
4 1/2-x,1/2+y,1/4-z
5 -y,-x,1/2-z
6 y,x,-z
7 1/2+y,1/2-x,3/4+z
8 1/2-y,1/2+x,1/4+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.89088 0.99225 0.18864 1
H2 H 8 0.09912 0.98259 0.06999 1
H3 H 8 0.02314 0.59780 0.16620 1
H4 H 8 0.35510 0.97269 0.71392 1
H5 H 8 0.34028 0.74778 0.81959 1
H6 H 8 0.22014 0.07809 0.97083 1
C1 C 8 0.94875 0.90812 0.16648 1
C2 C 8 0.05286 0.90334 0.10725 1
C3 C 8 0.01582 0.70406 0.15606 1
C4 C 8 0.32344 0.96154 0.78306 1
C5 C 8 0.31564 0.84942 0.83567 1
C6 C 8 0.25065 0.01727 0.91447 1
N1 N 8 0.92525 0.78160 0.19755 1
N2 N 8 0.09578 0.77415 0.10054 1
N3 N 8 0.28109 0.06833 0.83333 1
N4 N 8 0.26893 0.88486 0.91935 1
Zn1 Zn 8 0.25354 0.74337 0.02069 1
#End of data
```

```
data_dia P42 I41
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P42 I41
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: p42i41.cif.
;
_cell_length_a                      7.3214
_cell_length_b                      7.3214
_cell_length_c                      7.3889
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        396.0665
_cell_formula_units_Z               2
_symmetry_space_group_name_H-M      'P 42'
_symmetry_Int_Tables_number         77
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,1/2+z
4 y,-x,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.22492 0.92125 0.53062 1
H2 H 4 0.38061 0.61271 0.99055 1
H3 H 4 0.16567 0.39762 0.76684 1
C1 C 4 0.23816 0.80679 0.62452 1
C2 C 4 0.31654 0.64577 0.86169 1
C3 C 4 0.20987 0.53846 0.74982 1
N1 N 4 0.33545 0.81632 0.78166 1
N2 N 4 0.15942 0.64041 0.59936 1
Zn1 Zn 2 0.50000 0.00000 0.90761 1
#End of data
```

```
data_dia P42 P41
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia P42 P41
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: p42p41.cif.
;
_cell_length_a                      10.354
_cell_length_b                      10.354
_cell_length_c                      7.3889
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        792.1294
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 42'
_symmetry_Int_Tables_number         77
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 -y,x,1/2+z
4 y,-x,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.21570 0.38657 0.26625 1
H2 H 4 0.00122 0.38384 0.49097 1
H3 H 4 0.92610 0.15169 0.03070 1
H4 H 4 0.88407 0.49423 0.99007 1
H5 H 4 0.88115 0.27862 0.76751 1
H6 H 4 0.65200 0.57215 0.53053 1
C1 C 4 0.12365 0.33729 0.24947 1
C2 C 4 0.01693 0.33568 0.36186 1
C3 C 4 0.97627 0.21595 0.12451 1
C4 C 4 0.83505 0.47896 0.86150 1
C5 C 4 0.83391 0.37167 0.75020 1
C6 C 4 0.71538 0.52103 0.62454 1
N1 N 4 0.09833 0.26105 0.09890 1
N2 N 4 0.92277 0.25906 0.28200 1
N3 N 4 0.76014 0.57432 0.78128 1
N4 N 4 0.75776 0.39790 0.59988 1
Zn1 Zn 4 0.74841 0.24846 0.40761 1
#End of data
```

```
data_dia Pbca P212121
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Pbca P212121
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: pbcap212121.cif.
;
_cell_length_a                      10.3908
_cell_length_b                      9.8596
_cell_length_c                      14.353
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        1470.452
_cell_formula_units_Z               8
_symmetry_space_group_name_H-M      'P b c a'
_symmetry_Int_Tables_number         61
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 1/2-x,-y,1/2+z
3 1/2+x,1/2-y,-z
4 -x,1/2+y,1/2-z
5 -x,-y,-z
6 1/2+x,y,1/2-z
7 1/2-x,1/2+y,z
8 x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 8 0.21486 0.23545 0.27814 1
H2 H 8 0.19378 0.02554 0.40683 1
H3 H 8 0.88854 0.99743 0.21270 1
H4 H 8 0.22432 0.53975 0.65434 1
H5 H 8 0.99860 0.58333 0.55569 1
H6 H 8 0.28876 0.84226 0.45064 1
C1 C 8 0.14314 0.15495 0.28337 1
C2 C 8 0.13504 0.04764 0.34580 1
C3 C 8 0.97588 0.03248 0.24736 1
C4 C 8 0.20484 0.61059 0.59769 1
C5 C 8 0.09227 0.63125 0.54763 1
C6 C 8 0.23973 0.76678 0.49316 1
N1 N 8 0.04154 0.14523 0.22113 1
N2 N 8 0.02891 0.96942 0.32240 1
N3 N 8 0.29831 0.69721 0.56277 1
N4 N 8 0.11478 0.73010 0.48060 1
Zn1 Zn 8 0.98152 0.78769 0.38354 1
#End of data
```

```
data_dia Pca21 Pna21
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Pca21 Pna21
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: pca21pna21.cif.
;
_cell_length_a                      10.1762
_cell_length_b                      7.4976
_cell_length_c                      10.0167
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        764.2449
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P c a 21'
_symmetry_Int_Tables_number         29
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,1/2+z
3 1/2-x,y,1/2+z
4 1/2+x,-y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.38072 0.58624 0.58031 1
H2 H 4 0.70206 0.23198 0.57678 1
H3 H 4 0.72189 0.46337 0.35713 1
H4 H 4 0.79055 0.09532 0.89369 1
H5 H 4 0.71861 0.68621 0.61265 1
H6 H 4 0.49444 0.89799 0.63625 1
C1 C 4 0.47139 0.52156 0.54887 1
C2 C 4 0.63836 0.34059 0.54418 1
C3 C 4 0.64698 0.45409 0.43480 1
C4 C 4 0.73888 0.01212 0.82173 1
C5 C 4 0.70013 0.80157 0.67617 1
C6 C 4 0.58870 0.90703 0.68741 1
N1 N 4 0.52658 0.38361 0.61609 1
N2 N 4 0.54030 0.56926 0.43810 1
N3 N 4 0.79524 0.86858 0.76178 1
N4 N 4 0.61333 0.04106 0.78006 1
Zn1 Zn 4 0.47827 0.24418 0.78943 1
#End of data
```

```
data_dia Pc Cc
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Pc Cc
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: PcCC.cif.
;
_cell_length_a                      6.9018
_cell_length_b                      7.5408
_cell_length_c                      9.961
_cell_angle_alpha                   90
_cell_angle_beta                    132.62
_cell_angle_gamma                   90
_cell_volume                        381.4859
_cell_formula_units_Z               2
_symmetry_space_group_name_H-M      'P c'
_symmetry_Int_Tables_number         7
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 x,-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 2 0.79705 0.09721 0.80922 1
H2 H 2 0.40208 0.95370 0.36413 1
H3 H 2 0.39559 0.71465 0.14827 1
H4 H 2 0.63874 0.59386 0.91888 1
H5 H 2 0.04761 0.59399 0.40489 1
H6 H 2 0.49522 0.80423 0.64315 1
C1 C 2 0.96312 0.02654 0.93136 1
C2 C 2 0.27764 0.95059 0.21687 1
C3 C 2 0.27545 0.83217 0.10941 1
C4 C 2 0.53816 0.51351 0.94702 1
C5 C 2 0.23718 0.41422 0.94305 1
C6 C 2 0.46034 0.30994 0.06187 1
N1 N 2 0.07856 0.07384 0.10365 1
N2 N 2 0.07544 0.88080 0.92799 1
N3 N 2 0.65102 0.37286 0.06350 1
N4 N 2 0.28685 0.54322 0.87042 1
Zn1 Zn 2 0.01404 0.74321 0.72011 1
#End of data
```

```
data_dia Pnn2  Fdd2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
dia Pnn2  Fdd2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: pnn2fdd2.cif.
;
_cell_length_a                      6.5134
_cell_length_b                      7.8129
_cell_length_c                      7.7192
_cell_angle_alpha                   90
_cell_angle_beta                    90
_cell_angle_gamma                   90
_cell_volume                        392.8189
_cell_formula_units_Z               2
_symmetry_space_group_name_H-M      'P n n 2'
_symmetry_Int_Tables_number         34
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,-y,z
3 1/2-x,1/2+y,1/2+z
4 1/2+x,1/2-y,1/2+z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 4 0.27228 0.38511 0.70453 1
H2 H 4 0.18558 0.90661 0.46279 1
H3 H 4 0.37886 0.13144 0.23135 1
C1 C 4 0.27109 0.28523 0.60681 1
C2 C 4 0.22963 0.04016 0.47810 1
C3 C 4 0.32579 0.15097 0.36373 1
N1 N 4 0.19209 0.12571 0.63209 1
N2 N 4 0.35382 0.30674 0.44623 1
Zn1 Zn 2 0.00000 0.00000 0.81581 1
#End of data
```

```
data_C6 H6 N4 Zn/C2
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
C6 H6 N4 Zn/C2
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: dia_C2
;
_cell_length_a                      18.2479
_cell_length_b                      9.8367
_cell_length_c                      9.8784
_cell_angle_alpha                   90
_cell_angle_beta                    124.88
_cell_angle_gamma                   90
_cell_volume                        1454.618
_cell_formula_units_Z               4
_symmetry_space_group_name_H-M      'P 1'
_symmetry_Int_Tables_number         1
_refine_ls_R_factor_all             0
loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
H1 H 1 0.65566 0.10646 0.14009 1
H2 H 1 0.77097 0.88393 0.25453 1
H3 H 1 0.74325 0.01679 0.63040 1
H4 H 1 0.94018 0.02233 0.54470 1
H5 H 1 0.00000 0.61582 0.50000 1
H6 H 1 0.06266 0.06084 0.17069 1
H7 H 1 0.00000 0.65472 0.00000 1
H8 H 1 0.93734 0.06084 0.82931 1
H9 H 1 0.05982 0.02234 0.45530 1
H10 H 1 0.25674 0.01679 0.36960 1
H11 H 1 0.22902 0.88392 0.74547 1
H12 H 1 0.34434 0.10646 0.85991 1
H13 H 1 0.84434 0.60646 0.85991 1
H14 H 1 0.72902 0.38392 0.74547 1
H15 H 1 0.75674 0.51679 0.36960 1
H16 H 1 0.55982 0.52234 0.45529 1
H17 H 1 0.43734 0.56083 0.82931 1
H18 H 1 0.50000 0.15472 0.00000 1
H19 H 1 0.56266 0.56083 0.17069 1
H20 H 1 0.50000 0.11582 0.50000 1
H21 H 1 0.44018 0.52234 0.54470 1
H22 H 1 0.24325 0.51679 0.63040 1
H23 H 1 0.27097 0.38392 0.25453 1
H24 H 1 0.15566 0.60646 0.14009 1
C1 C 1 0.68969 0.05372 0.25825 1
C2 C 1 0.74709 0.94327 0.31517 1
C3 C 1 0.73454 0.01044 0.51164 1
C4 C 1 0.97049 0.93750 0.52267 1
C5 C 1 0.00000 0.72682 0.50000 1
C6 C 1 0.03128 0.97588 0.08490 1
```

```
C7 C 1 0.00000 0.76574 0.00000 1
C8 C 1 0.96872 0.97588 0.91509 1
C9 C 1 0.02951 0.93750 0.47734 1
C10 C 1 0.26545 0.01044 0.48836 1
C11 C 1 0.25291 0.94327 0.68483 1
C12 C 1 0.31030 0.05371 0.74175 1
C13 C 1 0.81030 0.55371 0.74175 1
C14 C 1 0.75291 0.44327 0.68483 1
C15 C 1 0.76546 0.51044 0.48837 1
C16 C 1 0.52951 0.43750 0.47733 1
C17 C 1 0.46872 0.47588 0.91509 1
C18 C 1 0.50000 0.26574 0.00000 1
C19 C 1 0.53128 0.47588 0.08490 1
C20 C 1 0.50000 0.22683 0.50000 1
C21 C 1 0.47049 0.43750 0.52267 1
C22 C 1 0.23454 0.51044 0.51163 1
C23 C 1 0.24709 0.44327 0.31517 1
C24 C 1 0.18969 0.55371 0.25825 1
N1 N 1 0.68157 0.09597 0.38331 1
N2 N 1 0.77560 0.91637 0.47620 1
N3 N 1 0.95167 0.80352 0.53687 1
N4 N 1 0.05110 0.84203 0.13829 1
N5 N 1 0.94890 0.84203 0.86171 1
N6 N 1 0.04833 0.80352 0.46313 1
N7 N 1 0.22440 0.91637 0.52380 1
N8 N 1 0.31843 0.09597 0.61669 1
N9 N 1 0.81843 0.59597 0.61669 1
N10 N 1 0.72440 0.41637 0.52380 1
N11 N 1 0.54833 0.30353 0.46313 1
N12 N 1 0.44890 0.34203 0.86171 1
N13 N 1 0.55110 0.34203 0.13829 1
N14 N 1 0.45167 0.30353 0.53687 1
N15 N 1 0.27560 0.41637 0.47620 1
N16 N 1 0.18157 0.59597 0.38331 1
Zn1 Zn 1 0.87352 0.77589 0.62229 1
Zn2 Zn 1 0.12648 0.77589 0.37771 1
Zn3 Zn 1 0.62648 0.27589 0.37771 1
Zn4 Zn 1 0.37352 0.27589 0.62229 1
#End of data
```

```
data_C6 H6 N4 Zn/Cc
_audit_creation_date                2009-12-07
_audit_creation_method              'Igor Baburin'
_chemical_formula_moiety
;
C6 H6 N4 Zn/Cc
;
_chemical_formula_sum               'C6 H6 N4 Zn1'
_citation_special_details
;
File: dia_Cc
;
_cell_length_a                      13.9069
_cell_length_b                      14.0549
_cell_length_c                      10.0678
_cell_angle_alpha                   90
_cell_angle_beta                    134.86
_cell_angle_gamma                   90
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H2 H 1 0.00818 0.65393 0.19009 1
H3 H 1 0.77551 0.54167 0.94995 1
H4 H 1 0.80238 0.17789 0.32726 1
H5 H 1 0.79885 0.06189 0.09764 1
H6 H 1 0.05273 0.93770 0.63613 1
H7 H 1 0.05273 0.06230 0.13613 1
H8 H 1 0.79885 0.93811 0.59763 1
H9 H 1 0.80238 0.82211 0.82725 1
H10 H 1 0.77551 0.45833 0.44994 1
H11 H 1 0.00818 0.34607 0.69010 1
H12 H 1 0.68048 0.80160 0.04823 1
H13 H 1 0.18048 0.30160 0.04823 1
H14 H 1 0.50818 0.84607 0.69010 1
H15 H 1 0.27551 0.95833 0.44995 1
H16 H 1 0.30238 0.32211 0.82724 1
H17 H 1 0.29885 0.43811 0.59763 1
H18 H 1 0.55273 0.56230 0.13612 1
H19 H 1 0.55273 0.43770 0.63611 1
H20 H 1 0.29885 0.56189 0.09763 1
H21 H 1 0.30238 0.67790 0.32725 1
H22 H 1 0.27551 0.04167 0.94995 1
H23 H 1 0.50818 0.15392 0.19009 1
H24 H 1 0.18048 0.69840 0.54822 1
C1 C 1 0.78987 0.38775 0.50639 1
C2 C 1 0.90572 0.33192 0.62615 1
C3 C 1 0.73826 0.25415 0.55440 1
C4 C 1 0.85336 0.11046 0.35729 1
C5 C 1 0.85177 0.05315 0.24354 1
C6 C 1 0.98381 0.98762 0.52049 1
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C9 C 1 0.85336 0.88954 0.85728 1
C10 C 1 0.73826 0.74586 0.05440 1
C11 C 1 0.90573 0.66808 0.12614 1
C12 C 1 0.78987 0.61225 0.00640 1
C13 C 1 0.28987 0.11225 0.00640 1
C14 C 1 0.40572 0.16807 0.12615 1
C15 C 1 0.23826 0.24586 0.05441 1
C16 C 1 0.35336 0.38954 0.85728 1
C17 C 1 0.35178 0.44685 0.74353 1
C18 C 1 0.48381 0.51238 0.02048 1
C19 C 1 0.48381 0.48762 0.52048 1
C20 C 1 0.35177 0.55315 0.24353 1
C21 C 1 0.35336 0.61046 0.35728 1
C22 C 1 0.23826 0.75414 0.55440 1
C23 C 1 0.40572 0.83192 0.62615 1
C24 C 1 0.28987 0.88775 0.50640 1
N1 N 1 0.87246 0.24714 0.65670 1
N2 N 1 0.18374 0.83802 0.46104 1
N3 N 1 0.93733 0.06847 0.53296 1
N4 N 1 0.93493 0.97520 0.34803 1
N5 N 1 0.93493 0.02480 0.84803 1
N6 N 1 0.93733 0.93154 0.03295 1
N7 N 1 0.18374 0.16198 0.96105 1
N8 N 1 0.87246 0.75286 0.15670 1
N9 N 1 0.37246 0.25286 0.15670 1
N10 N 1 0.68374 0.66198 0.96104 1
N11 N 1 0.43733 0.43154 0.03295 1
N12 N 1 0.43493 0.52480 0.84803 1
N13 N 1 0.43493 0.47520 0.34802 1
N14 N 1 0.43733 0.56846 0.53295 1
N15 N 1 0.68374 0.33802 0.46104 1
N16 N 1 0.37246 0.74714 0.65670 1
Zn1 Zn 1 0.98425 0.12529 0.76052 1
Zn2 Zn 1 0.98425 0.87471 0.26051 1
Zn3 Zn 1 0.48424 0.37471 0.26050 1
Zn4 Zn 1 0.48425 0.62529 0.76051 1
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H3 H 1 0.21886 0.53290 0.36929 1
H4 H 1 0.82828 0.65159 0.98002 1
H5 H 1 0.82828 0.15159 0.48002 1
H6 H 1 0.32828 0.65159 0.48002 1
H7 H 1 0.55834 0.61104 0.10586 1
H8 H 1 0.55834 0.11105 0.60585 1
H9 H 1 0.05834 0.61105 0.60585 1
H10 H 1 0.44166 0.38896 0.10586 1
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H12 H 1 0.94166 0.38896 0.60585 1
H13 H 1 0.69169 0.86104 0.35585 1
H14 H 1 0.69169 0.36104 0.85585 1
H15 H 1 0.19169 0.86104 0.85585 1
H16 H 1 0.80831 0.63896 0.35585 1
H17 H 1 0.80831 0.13896 0.85585 1
H18 H 1 0.30831 0.63896 0.85585 1
H19 H 1 0.17172 0.34841 0.98002 1
H20 H 1 0.17173 0.84841 0.48002 1
H21 H 1 0.67172 0.34841 0.48002 1
H22 H 1 0.42173 0.90159 0.23007 1
H23 H 1 0.42173 0.40159 0.73007 1
H24 H 1 0.92173 0.90159 0.73007 1
H25 H 1 0.07827 0.59841 0.23007 1
H26 H 1 0.07827 0.09841 0.73007 1
H27 H 1 0.57827 0.59841 0.73007 1
H28 H 1 0.28114 0.46710 0.86929 1
H29 H 1 0.28114 0.96710 0.36929 1
H30 H 1 0.78114 0.46710 0.36929 1
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H32 H 1 0.53113 0.28293 0.61930 1
H33 H 1 0.03113 0.78293 0.61930 1
H34 H 1 0.96887 0.71707 0.11930 1
H35 H 1 0.96887 0.21707 0.61930 1
H36 H 1 0.46887 0.71707 0.61930 1
H37 H 1 0.46887 0.21707 0.11930 1
H38 H 1 0.03113 0.28293 0.11930 1
H39 H 1 0.78114 0.96710 0.86929 1
H40 H 1 0.57827 0.09841 0.23007 1
H41 H 1 0.92173 0.40159 0.23007 1
H42 H 1 0.67172 0.84841 0.98002 1
H43 H 1 0.30831 0.13896 0.35585 1
H44 H 1 0.19169 0.36104 0.35585 1
H45 H 1 0.94166 0.88896 0.10586 1
H46 H 1 0.05834 0.11104 0.10586 1
H47 H 1 0.32827 0.15159 0.98002 1
H48 H 1 0.21886 0.03290 0.86929 1
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C2 C 1 0.70168 0.06610 0.43531 1
C3 C 1 0.20168 0.56610 0.43531 1
C4 C 1 0.75599 0.62517 0.99031 1
C5 C 1 0.75599 0.12517 0.49031 1
C6 C 1 0.25598 0.62517 0.49031 1
C7 C 1 0.61715 0.60595 0.05635 1
C8 C 1 0.61715 0.10595 0.55634 1
C9 C 1 0.11715 0.60595 0.55634 1
C10 C 1 0.38285 0.39405 0.05635 1
C11 C 1 0.38285 0.89405 0.55635 1
C12 C 1 0.88286 0.39405 0.55635 1
C13 C 1 0.63288 0.85595 0.30635 1
C14 C 1 0.63287 0.35595 0.80635 1
C15 C 1 0.13287 0.85595 0.80635 1
C16 C 1 0.86713 0.64405 0.30635 1
C17 C 1 0.86713 0.14405 0.80635 1
C18 C 1 0.36713 0.64405 0.80635 1
C19 C 1 0.24401 0.37483 0.99031 1
C20 C 1 0.24402 0.87483 0.49031 1
C21 C 1 0.74402 0.37483 0.49031 1
C22 C 1 0.49402 0.87518 0.24034 1
C23 C 1 0.49402 0.37518 0.74034 1
C24 C 1 0.99402 0.87518 0.74034 1
C25 C 1 0.00598 0.62482 0.24034 1
C26 C 1 0.00598 0.12482 0.74034 1
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C29 C 1 0.29833 0.93390 0.43531 1
C30 C 1 0.79833 0.43390 0.43531 1
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C32 C 1 0.54832 0.31611 0.68532 1
C33 C 1 0.04832 0.81611 0.68532 1
C34 C 1 0.95168 0.68389 0.18532 1
C35 C 1 0.95168 0.18389 0.68532 1
C36 C 1 0.45167 0.68389 0.68532 1
C37 C 1 0.45167 0.18389 0.18532 1
C38 C 1 0.04832 0.31611 0.18532 1
C39 C 1 0.79833 0.93390 0.93531 1
C40 C 1 0.50598 0.12482 0.24034 1
C41 C 1 0.99402 0.37518 0.24034 1
C42 C 1 0.74401 0.87483 0.99031 1
C43 C 1 0.36713 0.14405 0.30635 1
C44 C 1 0.13287 0.35595 0.30635 1
C45 C 1 0.88285 0.89405 0.05635 1
C46 C 1 0.11715 0.10595 0.05635 1
C47 C 1 0.25598 0.12517 0.99031 1
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C48 C 1 0.20167 0.06610 0.93531 1
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N2 N 1 0.61341 0.05381 0.47762 1
N3 N 1 0.11341 0.55381 0.47762 1
N4 N 1 0.70205 0.65037 0.06703 1
N5 N 1 0.70205 0.15037 0.56703 1
N6 N 1 0.20206 0.65038 0.56703 1
N7 N 1 0.29794 0.34963 0.06703 1
N8 N 1 0.29794 0.84963 0.56703 1
N9 N 1 0.79795 0.34963 0.56703 1
N10 N 1 0.54797 0.90037 0.31705 1
N11 N 1 0.54797 0.40037 0.81705 1
N12 N 1 0.04797 0.90037 0.81705 1
N13 N 1 0.95204 0.59963 0.31705 1
N14 N 1 0.95203 0.09963 0.81705 1
N15 N 1 0.45203 0.59963 0.81705 1
N16 N 1 0.38659 0.44619 0.97762 1
N17 N 1 0.38660 0.94619 0.47762 1
N18 N 1 0.88660 0.44619 0.47762 1
N19 N 1 0.63660 0.80382 0.22762 1
N20 N 1 0.63660 0.30382 0.72762 1
N21 N 1 0.13660 0.80382 0.72762 1
N22 N 1 0.86340 0.69618 0.22762 1
N23 N 1 0.86340 0.19618 0.72762 1
N24 N 1 0.36340 0.69617 0.72762 1
N25 N 1 0.36340 0.19617 0.22762 1
N26 N 1 0.13660 0.30382 0.22762 1
N27 N 1 0.88659 0.94619 0.97762 1
N28 N 1 0.45204 0.09963 0.31705 1
N29 N 1 0.04797 0.40037 0.31705 1
N30 N 1 0.79795 0.84963 0.06703 1
N31 N 1 0.20205 0.15037 0.06703 1
N32 N 1 0.11341 0.05381 0.97762 1
Zn1 Zn 1 0.25000 0.75000 0.65935 1
Zn2 Zn 1 0.75000 0.25000 0.65935 1
Zn3 Zn 1 0.00000 0.00000 0.90937 1
Zn4 Zn 1 0.50000 0.50000 0.90937 1
Zn5 Zn 1 0.50000 0.00000 0.40937 1
Zn6 Zn 1 0.00000 0.50000 0.40937 1
Zn7 Zn 1 0.75000 0.75000 0.15935 1
Zn8 Zn 1 0.25000 0.25000 0.15935 1
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H2 H 1 0.73390 0.14892 0.56435 1
H3 H 1 0.26557 0.64943 0.68547 1
H4 H 1 0.73398 0.35052 0.68552 1
H5 H 1 0.14914 0.73420 0.43552 1
H6 H 1 0.85038 0.26570 0.43555 1
H7 H 1 0.85091 0.23412 0.81436 1
H8 H 1 0.14884 0.76589 0.81438 1
H9 H 1 0.16245 0.25016 0.62461 1
H10 H 1 0.83706 0.74983 0.62465 1
H11 H 1 0.33707 0.24973 0.12464 1
H12 H 1 0.66248 0.75000 0.12468 1
H13 H 1 0.74987 0.83728 0.37469 1
H14 H 1 0.24959 0.16263 0.37463 1
H15 H 1 0.74956 0.66260 0.87470 1
H16 H 1 0.64873 0.26584 0.31437 1
H17 H 1 0.35077 0.73406 0.31437 1
H18 H 1 0.35055 0.76566 0.93552 1
H19 H 1 0.64926 0.23412 0.93553 1
H20 H 1 0.23397 0.85041 0.18550 1
H21 H 1 0.76556 0.14935 0.18548 1
H22 H 1 0.23392 0.64884 0.06432 1
H23 H 1 0.76562 0.35101 0.06432 1
H24 H 1 0.24980 0.33727 0.87463 1
C1 C 1 0.17617 0.80042 0.59486 1
C2 C 1 0.95408 0.75000 0.62470 1
C3 C 1 0.04544 0.25000 0.62468 1
C4 C 1 0.82335 0.19960 0.59487 1
C5 C 1 0.17615 0.69995 0.65483 1
C6 C 1 0.82339 0.30005 0.65485 1
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C7 C 1 0.19966 0.82357 0.40486 1
C8 C 1 0.79984 0.17632 0.40489 1
C9 C 1 0.80021 0.32355 0.84490 1
C10 C 1 0.19947 0.67641 0.84490 1
C11 C 1 0.69939 0.17637 0.34489 1
C12 C 1 0.30012 0.82351 0.34489 1
C13 C 1 0.29995 0.67630 0.90487 1
C14 C 1 0.69975 0.32355 0.90489 1
C15 C 1 0.32339 0.79994 0.15485 1
C16 C 1 0.67615 0.19987 0.15484 1
C17 C 1 0.32336 0.69950 0.09486 1
C18 C 1 0.74978 0.95427 0.37473 1
C19 C 1 0.24972 0.04562 0.37472 1
C20 C 1 0.24980 0.45427 0.87471 1
C21 C 1 0.74973 0.54561 0.87477 1
C22 C 1 0.54546 0.75000 0.12472 1
C23 C 1 0.45409 0.24986 0.12471 1
C24 C 1 0.67619 0.30032 0.09486 1
N1 N 1 0.03483 0.83153 0.57538 1
N2 N 1 0.96467 0.16849 0.57537 1
N3 N 1 0.03482 0.66855 0.67413 1
N4 N 1 0.96473 0.33144 0.67413 1
N5 N 1 0.16830 0.96491 0.42415 1
N6 N 1 0.83118 0.03497 0.42417 1
N7 N 1 0.83131 0.46489 0.82543 1
N8 N 1 0.16827 0.53510 0.82540 1
N9 N 1 0.66824 0.03504 0.32540 1
N10 N 1 0.33127 0.96482 0.32540 1
N11 N 1 0.33127 0.53492 0.92415 1
N12 N 1 0.66835 0.46489 0.92420 1
N13 N 1 0.46473 0.83132 0.17415 1
N14 N 1 0.53482 0.16848 0.17414 1
N15 N 1 0.46469 0.66838 0.07539 1
N16 N 1 0.53487 0.33141 0.07538 1
Zn1 Zn 1 0.99976 0.00000 0.49974 1
Zn2 Zn 1 0.99980 0.50000 0.74974 1
Zn3 Zn 1 0.49978 0.49988 0.99976 1
Zn4 Zn 1 0.49979 0.00000 0.24976 1
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H3 H 1 0.67686 0.39560 0.79215 1
H4 H 1 0.32291 0.60446 0.79222 1
H5 H 1 0.60470 0.17715 0.04221 1
H6 H 1 0.39536 0.82295 0.04222 1
H7 H 1 0.34067 0.47001 0.13639 1
H8 H 1 0.47017 0.15944 0.38635 1
H9 H 1 0.53003 0.84067 0.38631 1
H10 H 1 0.82768 0.74921 0.74526 1
H11 H 1 0.74919 0.67254 0.99527 1
H12 H 1 0.25074 0.32749 0.99527 1
H13 H 1 0.75088 0.82747 0.49527 1
H14 H 1 0.24932 0.17251 0.49528 1
H15 H 1 0.32778 0.24915 0.24531 1
H16 H 1 0.02988 0.34056 0.88634 1
H17 H 1 0.97003 0.65932 0.88632 1
H18 H 1 0.84097 0.97014 0.63642 1
H19 H 1 0.89536 0.32285 0.54220 1
H20 H 1 0.10471 0.67705 0.54221 1
H21 H 1 0.82324 0.10440 0.29217 1
H22 H 1 0.17715 0.89555 0.29222 1
H23 H 1 0.15939 0.02999 0.63639 1
H24 H 1 0.67236 0.75081 0.24527 1
C1 C 1 0.27287 0.53056 0.83263 1
C2 C 1 0.11293 0.23346 0.68682 1
C3 C 1 0.60673 0.62406 0.13244 1
C4 C 1 0.39316 0.37587 0.13240 1
C5 C 1 0.37603 0.10694 0.38239 1
C6 C 1 0.62426 0.89305 0.38235 1
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C7 C 1 0.88718 0.76659 0.68682 1
C8 C 1 0.76647 0.61309 0.93678 1
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C11 C 1 0.46927 0.77293 0.08264 1
C12 C 1 0.53078 0.22715 0.08264 1
C13 C 1 0.03079 0.72707 0.58263 1
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C15 C 1 0.22721 0.96946 0.33263 1
C16 C 1 0.73358 0.88690 0.43678 1
C17 C 1 0.26671 0.11307 0.43681 1
C18 C 1 0.38714 0.26652 0.18682 1
C19 C 1 0.12403 0.39306 0.88239 1
C20 C 1 0.87580 0.60695 0.88235 1
C21 C 1 0.89333 0.87593 0.63244 1
C22 C 1 0.10690 0.12413 0.63240 1
C23 C 1 0.61289 0.73341 0.18683 1
C24 C 1 0.77313 0.03054 0.33260 1
N1 N 1 0.02484 0.32798 0.65537 1
N2 N 1 0.51573 0.64925 0.06612 1
N3 N 1 0.48420 0.35074 0.06609 1
N4 N 1 0.35086 0.01593 0.31607 1
N5 N 1 0.64948 0.98408 0.31605 1
N6 N 1 0.97517 0.67198 0.65535 1
N7 N 1 0.67187 0.52507 0.90533 1
N8 N 1 0.32795 0.47497 0.90536 1
N9 N 1 0.82819 0.97493 0.40533 1
N10 N 1 0.17212 0.02505 0.40536 1
N11 N 1 0.47524 0.17201 0.15537 1
N12 N 1 0.14920 0.48408 0.81607 1
N13 N 1 0.85058 0.51591 0.81605 1
N14 N 1 0.98433 0.85074 0.56612 1
N15 N 1 0.01586 0.14926 0.56610 1
N16 N 1 0.52489 0.82801 0.15536 1
Zn1 Zn 1 0.50020 0.00000 0.22212 1
Zn2 Zn 1 0.00000 0.00000 0.47213 1
Zn3 Zn 1 0.50000 0.50000 0.97213 1
Zn4 Zn 1 0.99989 0.50000 0.72211 1
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H6 H 1 0.63601 0.21369 0.93249 1
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H9 H 1 0.28529 0.36386 0.68246 1
H10 H 1 0.71326 0.63636 0.68260 1
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H15 H 1 0.13601 0.71379 0.43269 1
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H17 H 1 0.13606 0.78592 0.81641 1
H18 H 1 0.37967 0.74952 0.12438 1
H19 H 1 0.61907 0.24952 0.12410 1
H20 H 1 0.24948 0.11946 0.37459 1
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H22 H 1 0.24920 0.38015 0.87449 1
H23 H 1 0.74920 0.61941 0.87434 1
H24 H 1 0.86343 0.21385 0.81657 1
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C2 C 1 0.00807 0.75000 0.62471 1
C3 C 1 0.99061 0.25000 0.62449 1
C4 C 1 0.69333 0.20104 0.34552 1
C5 C 1 0.30597 0.70116 0.90324 1
C6 C 1 0.69327 0.29832 0.90336 1
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C11 C 1 0.29802 0.19346 0.15326 1
C12 C 1 0.70071 0.80604 0.15319 1
C13 C 1 0.70073 0.69337 0.09544 1
C14 C 1 0.29801 0.30595 0.09535 1
C15 C 1 0.19328 0.79840 0.40354 1
C16 C 1 0.80595 0.20104 0.40332 1
C17 C 1 0.19332 0.70125 0.84547 1
C18 C 1 0.49056 0.74963 0.12436 1
C19 C 1 0.50819 0.24960 0.12417 1
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C22 C 1 0.24940 0.49104 0.87443 1
C23 C 1 0.74933 0.50852 0.87437 1
C24 C 1 0.80593 0.29840 0.84559 1
N1 N 1 0.34089 0.93217 0.32730 1
N2 N 1 0.65814 0.06728 0.32725 1
N3 N 1 0.34097 0.56737 0.92155 1
N4 N 1 0.65794 0.43207 0.92155 1
N5 N 1 0.93174 0.84141 0.57748 1
N6 N 1 0.06704 0.15857 0.57736 1
N7 N 1 0.06698 0.34160 0.67161 1
N8 N 1 0.93159 0.65851 0.67184 1
N9 N 1 0.43179 0.15826 0.17149 1
N10 N 1 0.56694 0.84117 0.17149 1
N11 N 1 0.56697 0.65815 0.07721 1
N12 N 1 0.43176 0.34100 0.07695 1
N13 N 1 0.15814 0.93216 0.42186 1
N14 N 1 0.84108 0.06729 0.42164 1
N15 N 1 0.15799 0.56752 0.82725 1
N16 N 1 0.84092 0.43219 0.82726 1
Zn1 Zn 1 0.99962 0.99988 0.49972 1
Zn2 Zn 1 0.99933 0.50000 0.74951 1
Zn3 Zn 1 0.49946 0.99975 0.24937 1
Zn4 Zn 1 0.49942 0.49966 0.99933 1
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H3 H 1 0.75000 0.33253 0.69728 1
H4 H 1 0.75000 0.44026 0.90619 1
H5 H 1 0.75000 0.16899 0.02238 1
H6 H 1 0.25000 0.83100 0.02238 1
H7 H 1 0.25000 0.55973 0.90617 1
H8 H 1 0.25000 0.66748 0.69729 1
H9 H 1 0.00000 0.00000 0.87020 1
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H12 H 1 0.09142 0.93570 0.49058 1
H13 H 1 0.59140 0.43569 0.99058 1
H14 H 1 0.40859 0.56429 0.99058 1
H15 H 1 0.90860 0.43569 0.99058 1
H16 H 1 0.50000 0.50000 0.37019 1
H17 H 1 0.75000 0.16747 0.19728 1
H18 H 1 0.75000 0.05973 0.40617 1
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H21 H 1 0.25000 0.94024 0.40620 1
H22 H 1 0.25000 0.83252 0.19729 1
H23 H 1 0.00000 0.50000 0.37020 1
H24 H 1 0.09140 0.56429 0.99058 1
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C2 C 1 0.50000 0.00000 0.76674 1
C3 C 1 0.75000 0.31369 0.79664 1
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C6 C 1 0.25000 0.77066 0.96445 1
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C8 C 1 0.25000 0.68631 0.79665 1
C9 C 1 0.00000 0.00000 0.76674 1
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C11 C 1 0.95139 0.03075 0.57086 1
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C13 C 1 0.54861 0.46924 0.07086 1
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C17 C 1 0.75000 0.18630 0.29664 1
C18 C 1 0.75000 0.13247 0.40283 1
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C22 C 1 0.25000 0.81368 0.29664 1
C23 C 1 0.00000 0.50000 0.26674 1
C24 C 1 0.04863 0.53073 0.07086 1
N1 N 1 0.58199 0.05001 0.69500 1
N2 N 1 0.75000 0.22537 0.83548 1
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N6 N 1 0.41801 0.94999 0.69500 1
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N12 N 1 0.75000 0.27462 0.33548 1
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Zn3 Zn 1 0.75000 0.37485 0.20470 1
Zn4 Zn 1 0.25000 0.62512 0.20471 1
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H4 H 1 0.80044 0.82168 0.27818 1
H5 H 1 0.14380 0.70627 0.15637 1
H6 H 1 0.97805 0.33114 0.59407 1
H7 H 1 0.85998 0.41360 0.84055 1
H8 H 1 0.73899 0.30519 0.18693 1
H9 H 1 0.35307 0.48577 0.00409 1
H10 H 1 0.49391 0.80028 0.86330 1
H11 H 1 0.37261 0.14541 0.75337 1
H12 H 1 0.45807 0.99493 0.38549 1
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C2 C 1 0.29012 0.67005 0.58980 1
C3 C 1 0.49246 0.46896 0.50742 1
C4 C 1 0.88786 0.70185 0.32579 1
C5 C 1 0.05864 0.64450 0.26533 1
C6 C 1 0.97612 0.44953 0.49136 1
C7 C 1 0.73654 0.41171 0.92561 1
C8 C 1 0.67604 0.35864 0.09794 1
C9 C 1 0.47507 0.45117 0.00671 1
C10 C 1 0.46756 0.89191 0.74802 1
C11 C 1 0.40750 0.06285 0.69361 1
C12 C 1 0.45135 0.98855 0.50126 1
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N2 N 1 0.45486 0.57640 0.57354 1
N3 N 1 0.83594 0.57763 0.46950 1
N4 N 1 0.11419 0.48378 0.37091 1
N5 N 1 0.60844 0.46986 0.86823 1
N6 N 1 0.50982 0.38428 0.14883 1
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N7 N 1 0.49493 0.84546 0.62548 1
N8 N 1 0.39748 0.12364 0.53670 1
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H4 H 1 0.58123 0.41932 0.99402 1
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H6 H 1 0.08118 0.08058 0.00593 1
H7 H 1 0.46352 0.48279 0.68287 1
H8 H 1 0.03644 0.51718 0.18286 1
H9 H 1 0.96351 0.01714 0.31709 1
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H17 H 1 0.77811 0.34892 0.46612 1
H18 H 1 0.22184 0.84893 0.03385 1
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H22 H 1 0.53644 0.98280 0.81710 1
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H24 H 1 0.33970 0.69091 0.62483 1
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C2 C 1 0.89288 0.71479 0.35201 1
C3 C 1 0.10705 0.21477 0.14793 1
C4 C 1 0.56872 0.39947 0.91138 1
C5 C 1 0.93125 0.60048 0.41138 1
C6 C 1 0.06869 0.10046 0.08858 1
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C7 C 1 0.50602 0.43439 0.75181 1
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C9 C 1 0.00602 0.06556 0.24815 1
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C11 C 1 0.84522 0.05887 0.58468 1
C12 C 1 0.15474 0.55888 0.91530 1
C13 C 1 0.53731 0.91157 0.03383 1
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C18 C 1 0.17837 0.75440 0.00072 1
C19 C 1 0.32159 0.24555 0.50073 1
C20 C 1 0.46264 0.41156 0.46615 1
C21 C 1 0.34521 0.44109 0.41531 1
C22 C 1 0.49395 0.93440 0.74817 1
C23 C 1 0.43127 0.89949 0.58858 1
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N2 N 1 0.93349 0.69212 0.25070 1
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N12 N 1 0.05287 0.71303 0.02024 1
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N14 N 1 0.25607 0.33510 0.43756 1
N15 N 1 0.49505 0.99433 0.65294 1
N16 N 1 0.43351 0.80783 0.74924 1
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Zn2 Zn 1 0.07096 0.31365 0.37980 1
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Zn4 Zn 1 0.57095 0.18629 0.62012 1
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H4 H 1 0.77123 0.68538 0.76581 1
H5 H 1 0.57428 0.65470 0.66012 1
H6 H 1 0.21905 0.22857 0.21905 1
H7 H 1 0.11746 0.10794 0.10794 1
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H12 H 1 0.38581 0.05807 0.90280 1
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H14 H 1 0.16028 0.48803 0.00501 1
H15 H 1 0.56603 0.16069 0.67688 1
H16 H 1 0.45465 0.34380 0.93846 1
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H23 H 1 0.32522 0.28202 0.61941 1
H24 H 1 0.83757 0.17497 0.88077 1
H25 H 1 0.05267 0.36229 0.86696 1
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H27 H 1 0.25118 0.75585 0.94156 1
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H30 H 1 0.50767 0.19806 0.01235 1
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H38	H	1	0.20377	0.28961	0.28420	1
H39	H	1	0.72864	0.64821	0.73405	1
H40	H	1	0.10456	0.01872	0.09915	1
H41	H	1	0.90761	0.98803	0.99345	1
H42	H	1	0.55238	0.56190	0.55238	1
H43	H	1	0.45079	0.44127	0.44127	1
H44	H	1	0.95833	0.43751	0.43751	1
H45	H	1	0.65974	0.65974	0.18052	1
H46	H	1	0.01391	0.49692	0.16918	1
H47	H	1	0.61362	0.45833	0.94137	1
H48	H	1	0.71915	0.39140	0.23614	1
H49	H	1	0.78279	0.93806	0.26581	1
H50	H	1	0.49361	0.82136	0.33835	1
H51	H	1	0.89936	0.49402	0.01021	1
H52	H	1	0.78799	0.67713	0.27180	1
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H55	H	1	0.51893	0.00274	0.40808	1
H56	H	1	0.39634	0.69054	0.35315	1
H57	H	1	0.79759	0.84078	0.13498	1
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H59	H	1	0.65855	0.61535	0.95275	1
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H61	H	1	0.38601	0.69562	0.20030	1
H62	H	1	0.64474	0.83045	0.14006	1
H63	H	1	0.58451	0.08918	0.27490	1
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H65	H	1	0.79013	0.28545	0.97584	1
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H67	H	1	0.73052	0.43633	0.39313	1
H68	H	1	0.55829	0.96363	0.07448	1
H69	H	1	0.37692	0.89390	0.04917	1
H70	H	1	0.21529	0.73608	0.21529	1
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H72	H	1	0.54359	0.54901	0.46316	1
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H74	H	1	0.53710	0.62295	0.61753	1
H75	H	1	0.06197	0.98155	0.06739	1
H76	H	1	0.43790	0.35205	0.43248	1
H77	H	1	0.24094	0.32137	0.32678	1
H78	H	1	0.88572	0.89524	0.88572	1
H79	H	1	0.78412	0.77460	0.77460	1
H80	H	1	0.29167	0.77085	0.77085	1
H81	H	1	0.99307	0.99307	0.51385	1
H82	H	1	0.34725	0.83026	0.50252	1
H83	H	1	0.94695	0.79167	0.27470	1
H84	H	1	0.05248	0.72474	0.56947	1
H85	H	1	0.11612	0.27139	0.59914	1
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H88	H	1	0.12132	0.01047	0.60513	1
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H92	H	1	0.72967	0.02387	0.68648	1
H93	H	1	0.13092	0.17412	0.46831	1
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C38 C 1 0.98850 0.94787 0.23067 1
C39 C 1 0.62533 0.62533 0.50000 1
C40 C 1 0.37466 0.37466 0.00000 1
C41 C 1 0.12540 0.87460 0.25000 1
C42 C 1 0.87460 0.12540 0.75000 1
C43 C 1 0.01150 0.05213 0.73067 1
C44 C 1 0.83132 0.83132 0.00000 1
C45 C 1 0.96240 0.91067 0.03053 1
C46 C 1 0.59946 0.85104 0.73899 1
C47 C 1 0.70773 0.92704 0.66181 1
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C48 C 1 0.64292 0.88484 0.60465 1
N1 N 1 0.66346 0.07446 0.90393 1
N2 N 1 0.33654 0.92554 0.40393 1
N3 N 1 0.83659 0.57440 0.34614 1
N4 N 1 0.16341 0.42560 0.84614 1
N5 N 1 0.92554 0.33654 0.59607 1
N6 N 1 0.07445 0.66347 0.09608 1
N7 N 1 0.42561 0.16341 0.15386 1
N8 N 1 0.59452 0.18004 0.99726 1
N9 N 1 0.40548 0.81995 0.49726 1
N10 N 1 0.90557 0.67988 0.25273 1
N11 N 1 0.09443 0.32012 0.75273 1
N12 N 1 0.81996 0.40548 0.50274 1
N13 N 1 0.18004 0.59452 0.00275 1
N14 N 1 0.32013 0.09443 0.24727 1
N15 N 1 0.67221 0.41150 0.30096 1
N16 N 1 0.32779 0.58850 0.80097 1
N17 N 1 0.82774 0.91149 0.94905 1
N18 N 1 0.17226 0.08851 0.44906 1
N19 N 1 0.58851 0.32780 0.19903 1
N20 N 1 0.41149 0.67219 0.69904 1
N21 N 1 0.08852 0.17225 0.55095 1
N22 N 1 0.36114 0.46457 0.96776 1
N23 N 1 0.63886 0.53543 0.46776 1
N24 N 1 0.13890 0.96448 0.28232 1
N25 N 1 0.86110 0.03552 0.78231 1
N26 N 1 0.53543 0.63885 0.53224 1
N27 N 1 0.46457 0.36114 0.03224 1
N28 N 1 0.03552 0.86111 0.21769 1
N29 N 1 0.96448 0.13890 0.71769 1
N30 N 1 0.91148 0.82776 0.05095 1
N31 N 1 0.67988 0.90556 0.74727 1
N32 N 1 0.57439 0.83658 0.65387 1
Zn1 Zn 1 0.52861 0.24810 0.09955 1
Zn2 Zn 1 0.47139 0.75189 0.59957 1
Zn3 Zn 1 0.97140 0.74805 0.15042 1
Zn4 Zn 1 0.02860 0.25195 0.65042 1
Zn5 Zn 1 0.75190 0.47139 0.40045 1
Zn6 Zn 1 0.24810 0.52861 0.90046 1
Zn7 Zn 1 0.25197 0.02859 0.34958 1
Zn8 Zn 1 0.74804 0.97140 0.84957 1
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_atom_site_symmetry_multiplicity
_atom_site_fract_x
_atom_site_fract_y
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H2 H 1 0.60558 0.04075 0.94170 1
H3 H 1 0.95944 0.60576 0.19175 1
H4 H 1 0.16432 0.89569 0.55557 1
H5 H 1 0.83572 0.10435 0.05557 1
H6 H 1 0.89545 0.83577 0.30563 1
H7 H 1 0.48994 0.64472 0.64754 1
H8 H 1 0.51010 0.35532 0.14755 1
H9 H 1 0.64476 0.51002 0.39755 1
H10 H 1 0.21257 0.91036 0.10137 1
H11 H 1 0.78748 0.08968 0.60138 1
H12 H 1 0.91033 0.78745 0.85134 1
H13 H 1 0.15606 0.67547 0.99025 1
H14 H 1 0.84399 0.32457 0.49025 1
H15 H 1 0.67541 0.84394 0.74025 1
H16 H 1 0.30952 0.97637 0.79284 1
H17 H 1 0.69052 0.02366 0.29285 1
H18 H 1 0.97631 0.69056 0.54282 1
H19 H 1 0.02373 0.30948 0.04282 1
H20 H 1 0.32463 0.15608 0.24025 1
H21 H 1 0.08970 0.21257 0.35134 1
H22 H 1 0.35528 0.49003 0.89754 1
H23 H 1 0.10459 0.16427 0.80563 1
H24 H 1 0.04060 0.39428 0.69175 1
C1 C 1 0.38004 0.88375 0.50100 1
C2 C 1 0.62000 0.11630 0.00101 1
C3 C 1 0.88381 0.62002 0.25102 1
C4 C 1 0.26601 0.85246 0.55778 1
C5 C 1 0.73405 0.14758 0.05778 1
C6 C 1 0.85236 0.73403 0.30779 1
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C7 C 1 0.43217 0.72171 0.60675 1
C8 C 1 0.56787 0.27833 0.10675 1
C9 C 1 0.72175 0.56779 0.35674 1
C10 C 1 0.22464 0.88931 0.02073 1
C11 C 1 0.77540 0.11072 0.52074 1
C12 C 1 0.88930 0.77539 0.77071 1
C13 C 1 0.19626 0.77300 0.96552 1
C14 C 1 0.80378 0.22704 0.46552 1
C15 C 1 0.77296 0.80376 0.71553 1
C16 C 1 0.27568 0.92632 0.86219 1
C17 C 1 0.72436 0.07372 0.36220 1
C18 C 1 0.92630 0.72438 0.61217 1
C19 C 1 0.07374 0.27565 0.11217 1
C20 C 1 0.22708 0.19627 0.21552 1
C21 C 1 0.11073 0.22464 0.27071 1
C22 C 1 0.27829 0.43226 0.85674 1
C23 C 1 0.14768 0.26601 0.80779 1
C24 C 1 0.11623 0.38002 0.75102 1
N1 N 1 0.48520 0.80045 0.53233 1
N2 N 1 0.51484 0.19960 0.03233 1
N3 N 1 0.80057 0.51479 0.28235 1
N4 N 1 0.29969 0.74920 0.62476 1
N5 N 1 0.70036 0.25083 0.12476 1
N6 N 1 0.74914 0.70030 0.37475 1
N7 N 1 0.27500 0.98639 0.95468 1
N8 N 1 0.72504 0.01365 0.45469 1
N9 N 1 0.98637 0.72504 0.70465 1
N10 N 1 0.22899 0.79708 0.86488 1
N11 N 1 0.77105 0.20295 0.36488 1
N12 N 1 0.79706 0.77102 0.61488 1
N13 N 1 0.20298 0.22901 0.11487 1
N14 N 1 0.01366 0.27499 0.20466 1
N15 N 1 0.25091 0.29975 0.87475 1
N16 N 1 0.19947 0.48525 0.78235 1
Zn1 Zn 1 0.18269 0.68216 0.74102 1
Zn2 Zn 1 0.81736 0.31788 0.24103 1
Zn3 Zn 1 0.68213 0.81734 0.49109 1
Zn4 Zn 1 0.31791 0.18270 0.99109 1
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_symmetry_Int_Tables_number         1
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H2 H 1 0.99751 0.09824 0.56476 1
H3 H 1 0.00250 0.09823 0.93519 1
H4 H 1 0.59778 0.00000 0.00000 1
H5 H 1 0.99847 0.61395 0.05239 1
H6 H 1 0.00153 0.38605 0.55239 1
H7 H 1 0.99847 0.38603 0.94758 1
H8 H 1 0.59342 0.50000 0.00000 1
H9 H 1 0.40192 0.50291 0.68510 1
H10 H 1 0.59808 0.49709 0.18510 1
H11 H 1 0.40191 0.49711 0.31487 1
H12 H 1 0.50000 0.90187 0.25000 1
H13 H 1 0.88595 0.49854 0.80233 1
H14 H 1 0.11404 0.50147 0.30233 1
H15 H 1 0.88595 0.50146 0.19764 1
H16 H 1 0.00000 0.90656 0.25000 1
H17 H 1 0.00000 0.09344 0.75000 1
H18 H 1 0.11405 0.49854 0.69764 1
H19 H 1 0.50000 0.09813 0.75000 1
H20 H 1 0.59808 0.50289 0.81487 1
H21 H 1 0.40657 0.50000 0.50000 1
H22 H 1 0.00153 0.61397 0.44758 1
H23 H 1 0.40221 0.00000 0.50000 1
H24 H 1 0.99749 0.90177 0.43519 1
C1 C 1 0.91818 0.95160 0.03227 1
C2 C 1 0.08181 0.04840 0.53227 1
C3 C 1 0.91819 0.04840 0.96768 1
C4 C 1 0.70833 0.00000 0.00000 1
C5 C 1 0.91370 0.55720 0.02570 1
C6 C 1 0.08629 0.44281 0.52570 1
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C7 C 1 0.91370 0.44278 0.97428 1
C8 C 1 0.70406 0.50000 0.00000 1
C9 C 1 0.45165 0.41859 0.71765 1
C10 C 1 0.54834 0.58141 0.21765 1
C11 C 1 0.45165 0.58142 0.28232 1
C12 C 1 0.50000 0.79131 0.25000 1
C13 C 1 0.94274 0.41376 0.77565 1
C14 C 1 0.05725 0.58624 0.27565 1
C15 C 1 0.94274 0.58623 0.22432 1
C16 C 1 0.00000 0.79590 0.25000 1
C17 C 1 0.00000 0.20410 0.75000 1
C18 C 1 0.05725 0.41377 0.72432 1
C19 C 1 0.50000 0.20869 0.75000 1
C20 C 1 0.54834 0.41858 0.78232 1
C21 C 1 0.29594 0.50000 0.50000 1
C22 C 1 0.08629 0.55722 0.47428 1
C23 C 1 0.29167 0.00000 0.50000 1
C24 C 1 0.08180 0.95161 0.46768 1
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N2 N 1 0.21536 0.07883 0.55282 1
N3 N 1 0.78463 0.07882 0.94715 1
N4 N 1 0.78037 0.59289 0.04274 1
N5 N 1 0.21962 0.40712 0.54274 1
N6 N 1 0.78037 0.40710 0.95723 1
N7 N 1 0.42127 0.28501 0.69710 1
N8 N 1 0.57872 0.71499 0.19711 1
N9 N 1 0.42127 0.71500 0.30287 1
N10 N 1 0.90699 0.28040 0.79265 1
N11 N 1 0.09301 0.71960 0.29265 1
N12 N 1 0.90698 0.71959 0.20732 1
N13 N 1 0.09301 0.28041 0.70732 1
N14 N 1 0.57872 0.28501 0.80287 1
N15 N 1 0.21962 0.59290 0.45723 1
N16 N 1 0.21536 0.92118 0.44715 1
Zn1 Zn 1 0.74570 0.24584 0.87500 1
Zn2 Zn 1 0.25429 0.75416 0.37500 1
Zn3 Zn 1 0.74568 0.75413 0.12500 1
Zn4 Zn 1 0.25432 0.24587 0.62500 1
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H2 H 1 0.96324 0.16837 0.08868 1
H3 H 1 0.46324 0.33162 0.08866 1
H4 H 1 0.94550 0.57510 0.45942 1
H5 H 1 0.05441 0.42489 0.95940 1
H6 H 1 0.55444 0.07511 0.95941 1
H7 H 1 0.09724 0.36949 0.73650 1
H8 H 1 0.90283 0.63052 0.23653 1
H9 H 1 0.40280 0.86950 0.23649 1
H10 H 1 0.05830 0.26820 0.50297 1
H11 H 1 0.94176 0.73181 0.00300 1
H12 H 1 0.44172 0.76817 0.00298 1
H13 H 1 0.74006 0.68721 0.81275 1
H14 H 1 0.25993 0.31282 0.31271 1
H15 H 1 0.75992 0.18720 0.31272 1
H16 H 1 0.80758 0.95194 0.59166 1
H17 H 1 0.19238 0.04804 0.09170 1
H18 H 1 0.69238 0.45195 0.09169 1
H19 H 1 0.30759 0.54805 0.59170 1
H20 H 1 0.24005 0.81282 0.81272 1
H21 H 1 0.55826 0.23183 0.50297 1
H22 H 1 0.59720 0.13050 0.73648 1
H23 H 1 0.44553 0.92488 0.45941 1
H24 H 1 0.53673 0.66839 0.58865 1
C1 C 1 0.98126 0.50483 0.50275 1
C2 C 1 0.01869 0.49516 0.00273 1
C3 C 1 0.51871 0.00484 0.00274 1
C4 C 1 0.05945 0.39780 0.64440 1
C5 C 1 0.94059 0.60220 0.14441 1
C6 C 1 0.44058 0.89780 0.14439 1
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C7 C 1 0.04013 0.34714 0.52825 1
C8 C 1 0.95990 0.65287 0.02826 1
C9 C 1 0.45988 0.84712 0.02823 1
C10 C 1 0.78960 0.74304 0.75154 1
C11 C 1 0.21039 0.25697 0.25153 1
C12 C 1 0.71039 0.24304 0.25153 1
C13 C 1 0.82751 0.87899 0.63715 1
C14 C 1 0.17246 0.12100 0.13718 1
C15 C 1 0.67246 0.37900 0.13717 1
C16 C 1 0.94085 0.81915 0.63523 1
C17 C 1 0.05912 0.18082 0.13527 1
C18 C 1 0.55913 0.31916 0.13525 1
C19 C 1 0.44086 0.68084 0.63525 1
C20 C 1 0.32752 0.62100 0.63717 1
C21 C 1 0.28959 0.75697 0.75153 1
C22 C 1 0.54011 0.15287 0.52824 1
C23 C 1 0.55941 0.10220 0.64438 1
C24 C 1 0.48128 0.99516 0.50273 1
N1 N 1 0.02161 0.49796 0.62781 1
N2 N 1 0.97838 0.50203 0.12781 1
N3 N 1 0.47838 0.99797 0.12780 1
N4 N 1 0.99061 0.41564 0.43837 1
N5 N 1 0.00936 0.58436 0.93837 1
N6 N 1 0.50936 0.91563 0.93835 1
N7 N 1 0.73190 0.83029 0.71124 1
N8 N 1 0.26807 0.16972 0.21123 1
N9 N 1 0.76808 0.33029 0.21125 1
N10 N 1 0.91621 0.73284 0.70806 1
N11 N 1 0.08377 0.26715 0.20807 1
N12 N 1 0.58377 0.23284 0.20806 1
N13 N 1 0.41620 0.76717 0.70806 1
N14 N 1 0.23190 0.66971 0.71124 1
N15 N 1 0.49062 0.08437 0.43836 1
N16 N 1 0.52161 0.00204 0.62780 1
Zn1 Zn 1 0.04486 0.61815 0.74914 1
Zn2 Zn 1 0.95513 0.38185 0.24913 1
Zn3 Zn 1 0.45506 0.11817 0.24918 1
Zn4 Zn 1 0.54488 0.88184 0.74915 1
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_atom_site_fract_x
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H2 H 1 0.39164 0.94005 0.76959 1
H3 H 1 0.39168 0.55992 0.26960 1
H4 H 1 0.50000 0.00000 0.16862 1
H5 H 1 0.10239 0.93563 0.77059 1
H6 H 1 0.89758 0.06430 0.77060 1
H7 H 1 0.89761 0.43563 0.27059 1
H8 H 1 0.00000 0.00000 0.17013 1
H9 H 1 0.51328 0.25579 0.45123 1
H10 H 1 0.48673 0.74418 0.45124 1
H11 H 1 0.48673 0.75579 0.95123 1
H12 H 1 0.50769 0.14348 0.22894 1
H13 H 1 0.49230 0.85648 0.22895 1
H14 H 1 0.49231 0.64349 0.72894 1
H15 H 1 0.90196 0.24982 0.27525 1
H16 H 1 0.09805 0.75014 0.27526 1
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H18 H 1 0.90196 0.25014 0.77525 1
H19 H 1 0.50771 0.35648 0.72895 1
H20 H 1 0.51328 0.24418 0.95124 1
H21 H 1 0.00000 0.50000 0.67013 1
H22 H 1 0.10242 0.56431 0.27060 1
H23 H 1 0.50000 0.50000 0.66862 1
H24 H 1 0.60836 0.44005 0.26959 1
C1 C 1 0.55430 0.02938 0.85298 1
C2 C 1 0.44566 0.97058 0.85298 1
C3 C 1 0.44570 0.52938 0.35298 1
C4 C 1 0.50000 0.00000 0.05951 1
C5 C 1 0.05044 0.96773 0.85400 1
C6 C 1 0.94955 0.03221 0.85400 1
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C7 C 1 0.94957 0.46773 0.35400 1
C8 C 1 0.00000 0.00000 0.06105 1
C9 C 1 0.59393 0.23722 0.38234 1
C10 C 1 0.40609 0.76275 0.38234 1
C11 C 1 0.40608 0.73722 0.88234 1
C12 C 1 0.59144 0.18098 0.27226 1
C13 C 1 0.40855 0.81899 0.27226 1
C14 C 1 0.40857 0.68098 0.77226 1
C15 C 1 0.79518 0.23574 0.29305 1
C16 C 1 0.20483 0.76422 0.29306 1
C17 C 1 0.20483 0.73575 0.79305 1
C18 C 1 0.79518 0.26421 0.79306 1
C19 C 1 0.59146 0.31899 0.77226 1
C20 C 1 0.59392 0.26275 0.88234 1
C21 C 1 0.00000 0.50000 0.56105 1
C22 C 1 0.05046 0.53221 0.35400 1
C23 C 1 0.50000 0.50000 0.55951 1
C24 C 1 0.55434 0.47058 0.35298 1
N1 N 1 0.58870 0.04787 0.98454 1
N2 N 1 0.41129 0.95210 0.98454 1
N3 N 1 0.41131 0.54787 0.48454 1
N4 N 1 0.08200 0.94726 0.98575 1
N5 N 1 0.91798 0.05269 0.98575 1
N6 N 1 0.91801 0.44726 0.48575 1
N7 N 1 0.72333 0.27200 0.39514 1
N8 N 1 0.27669 0.72797 0.39514 1
N9 N 1 0.27668 0.77199 0.89514 1
N10 N 1 0.71979 0.17975 0.21585 1
N11 N 1 0.28020 0.82021 0.21585 1
N12 N 1 0.28021 0.67975 0.71585 1
N13 N 1 0.71980 0.32021 0.71585 1
N14 N 1 0.72332 0.22797 0.89514 1
N15 N 1 0.08203 0.55269 0.48575 1
N16 N 1 0.58872 0.45210 0.48454 1
Zn1 Zn 1 0.75283 0.12682 0.03239 1
Zn2 Zn 1 0.24718 0.87315 0.03237 1
Zn3 Zn 1 0.24717 0.62682 0.53238 1
Zn4 Zn 1 0.75284 0.37315 0.53237 1
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