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Electronic Supplementary Information

for

Stability and Electronic Properties of Phosphorene Oxides: from 0-dimensional to Amorphous 2-dimensional Structures

Oleksandr I. Malyi[1], Kostiantyn V. Sopiha[2], Claudia Draxl[3], and Clas Persson[4]

1 – School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, 639798 Singapore, Singapore

2 – Engineering Product Development, Singapore University of Technology and Design, 8 Somapah Road, 487372 Singapore, Singapore

3 – Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, D-12489 Berlin, Germany

4 – Department of Physics, University of Oslo, P. O. Box 1048 Blindern, NO-0316 Oslo, Norway

Emails: oleksandrmalyi@gmail.com (O.I.M), kostiantyn.sopiha@gmail.com (K.V.S)

Screening details

1. First, we create the dataset of all interesting structures for further screening calculations. The structures are taken from the originally reported systems as well as the analysis of different group-15 and 16 compounds available in Materials Project database[1]. Here, our analysis is limited only to the binary structures containing P, As, N, O, S, and Se. The schematic illustration of the isolation of possible low-dimensional structures is shown in Figure S1. For 0d-P_xO_y, our dataset is limited to 0d-P_4O_6, 0d-P_4O_7, 0d-P_4O_8, 0d-P_4O_9, 0d-P_4O_{10} isolated directly from bulk structures available in Materials Project database as well as 0d-P_xO_y structures generated from bulk As_4S_3, AsS, As_8S_9, etc. For 2d-P_xO_y, based on preliminary analysis, we use blue and black phosphorene, layered P_4O_{10} structure, two P_4O_6 structures received by replacement of isovalent elements in As_2Se_3 and As_2O_3 structures. In addition, we also use 2d-P_4O_1, 2d-P_4O_2, 2d-P_4O_3, 2d-P_4O_4, and 2d-P_4O_{10} reported by Ziletti et al.[2] Other forms of phosphorene oxides reported before are only used for comparison due to their instability.

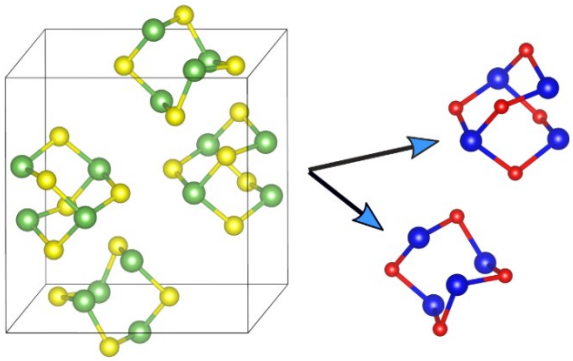

Figure S1. Schematic illustration for the isolation of different 0d building blocks from bulk As_8S_9 structure and formation of 0d-P_xO_y structures by replacements of isovalent elements.

2. For each structure in the dataset, we consider oxidation and reduction (see Fig. 1) to form a sequence of P_xO_y structures for all considered concentration range. For reduction, we consider remove of each unique O atom. For oxidation calculations, we screen different

adsorption configurations based on a random location of O atoms. In general, we generate over 500 structures for each system, which were further reduced to about 10-100 unique structures using structure matcher developed within pymatgen.[3] For simplicity, let us give an illustration for 0d-P_4O_6. Based on step-by-step oxidation of 0d-P_4O_6, we predict 0d-P_4O_7, 0d-P_4O_8, 0d-P_4O_9, 0d-P_4O_{10}, and 0d-P_4O_{11}. However, since the only the oxidation cannot provide sufficient information on structure stability, we also perform step-by-step reduction of 0d-P_4O_{11} to 0d-P_4O_6. Based on this, we find that both the oxidation of 0d-P_4O_6 and the reduction of 0d-P_4O_{11} can give the same structures for the intermediate region (see Fig. S2). To predict 0d-P_4O_1, 0d-P_4O_2, 0d-P_4O_3, 0d-P_4O_4, and 0d-P_4O_5 structures, we performed step-by-step reduction of 0d-P_4O_6. We use P_4 cluster obtained from the reduction of 0d-P_4O_1 for the step-by-step oxidation. We can reproduce all key structure based on the oxidation of P_4 cluster. However, during the screening calculations, we find 0d-P_4O_2 and 0d-P_4O_4 structures having higher stability than the corresponding structures found from the step-by-step reduction of 0d-P_4O_6. To ensure that the found lowest energy structures cannot stabilize other more stable 0d-P_4O_y structures, we performed both new step-by-step oxidation as well as step-by-step reduction of the lowest energy 0d-P_4O_2 and 0d-P_4O_4 structures. Since no lower energy structures can be found during both step-by-step oxidation and reduction of 0d-P_4O_4 and 0d-P_4O_2, we finish the screening calculations of 0d-P_4O_y.

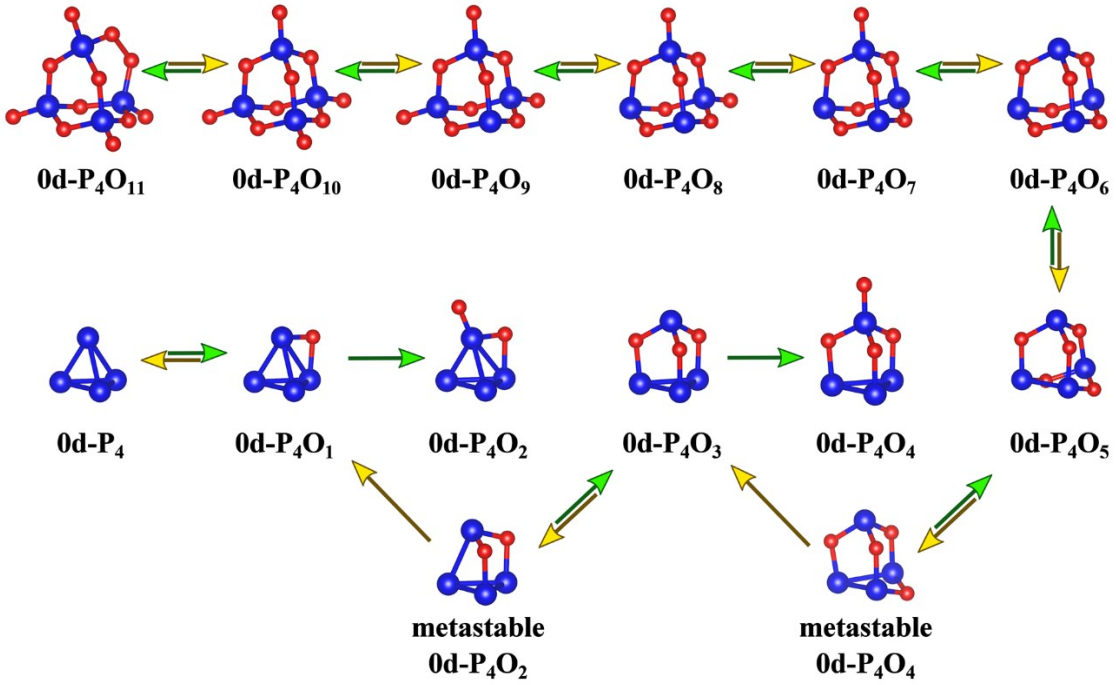

Figure S2. Schematic illustration of screening calculations used for the search of the lowest energy 0d-P_xO_y structures. Green and yellow arrows represent oxidation and reduction.

3. All found lowest energy 2d-P_xO_y structures are used for BOMD simulations.

Electronic properties

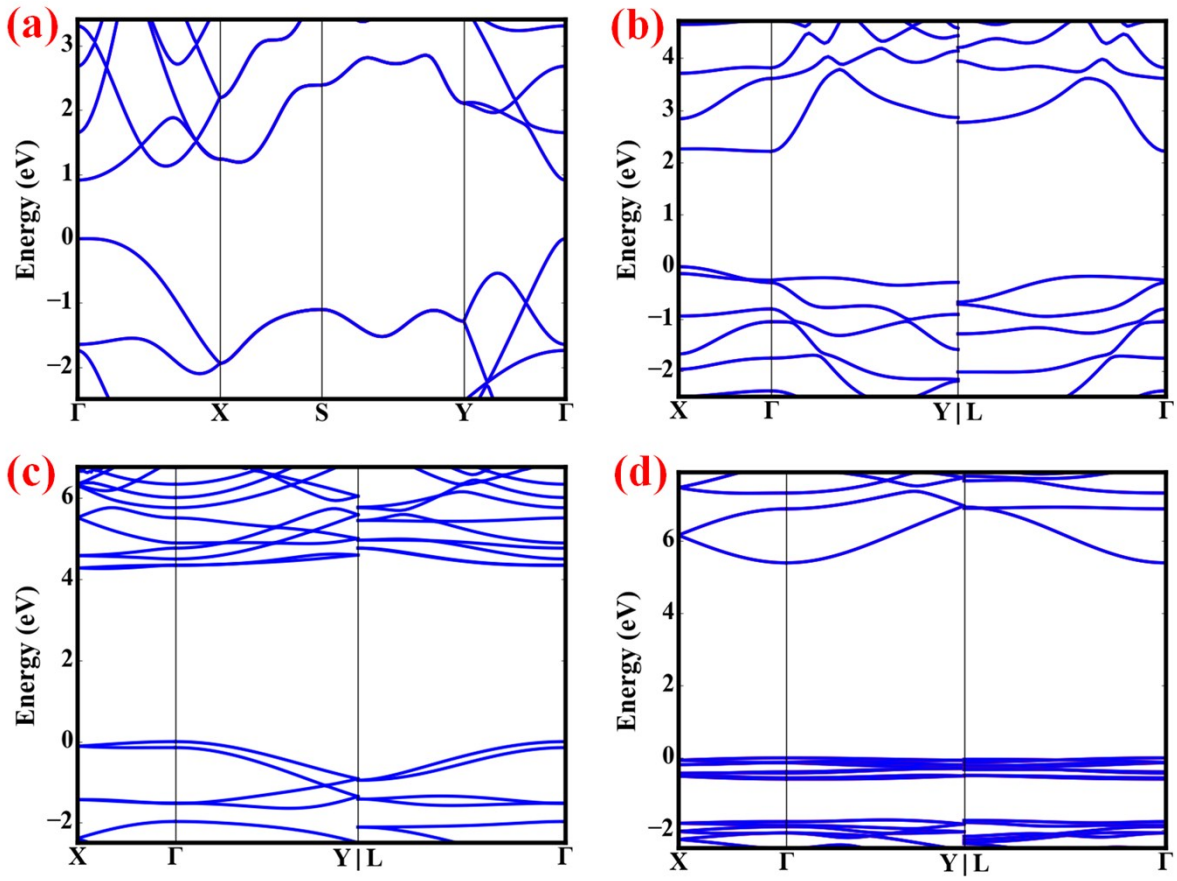

Figure S3. PBE band structures computed for (a) phosphorene, (b) 2d-P_4O_2, (c) 2d-P_4O_6, and (d) 2d-P_4O_{10}. The path along high symmetry lines in the Brillouin zone (BZ) is taken for standard primitive cells generated from 2d-P_xO_y structures by BZ paths features of AFLOW[4] as implemented in pymatgen.[3] **k**-path of the low-symmetry triclinic phase was used for all 2d-P_xO_y structures.

Table S1. Details on Monkhorst-Pack grids used in this work

Type of calculations	Size of supercell	Size of Γ-centered Monkhorst-Pack grids
Screening	1×1	8×8×1
Hybrid functional	1×1	8×8×1
	BOMD systems	2×2×1
BOMD	-	1×1×1

Table S2. Supercell sizes for modeled systems used in BOMD simulations

System	Supercell size
2d-P_4O_1	4×2
2d-P_4O_2	4×2
2d-P_4O_3	4×3
2d-P_4O_4	4×3
2d-P_4O_5	4×3
2d-P_4O_6	4×2
2d-P_4O_7	4×2
2d-P_4O_8	4×2
2d-P_4O_9	4×2
2d-P_4O_{10}	4×2
Surface form of P_4O_4 and planar form of P_4O_2	3×2

Lowest energy structures

0d-P_4O_1 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   26.93966000
_cell_length_b   27.23791200
_cell_length_c   26.93440300
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O
_chemical_formula_sum   'P4 O1'
_cell_volume   19763.9286141
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  P  P2  1  0.518480  0.460215  0.523131  1
  P  P3  1  0.525564  0.542377  0.523163  1
  P  P4  1  0.525584  0.501545  0.451344  1
  O  O5  1  0.455065  0.461426  0.522385  1
```

0d-P_4O_2 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   28.11198800
_cell_length_b   27.23585700
_cell_length_c   26.93821500
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O
_chemical_formula_sum   'P4 O2'
_cell_volume   20625.3543615
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  P  P2  1  0.469736  0.486854  0.514123  1
  P  P3  1  0.540302  0.508400  0.539682  1
  P  P4  1  0.528469  0.461806  0.467731  1
  O  O5  1  0.458899  0.537599  0.482461  1
  O  O6  1  0.429602  0.461377  0.538170  1
```

0d-P_4O_3 (screening)

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_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   27.16495800
_cell_length_b   27.49180700
_cell_length_c   27.52533700
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O3
_chemical_formula_sum   'P4 O3'
_cell_volume   20556.3010395
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 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.451402  0.499926  0.466583  1
  P  P2  1  0.524325  0.458898  0.466050  1
  P  P3  1  0.500245  0.499667  0.557796  1
  P  P4  1  0.523857  0.541764  0.466534  1
  O  O5  1  0.447155  0.499543  0.527982  1
  O  O6  1  0.526330  0.545308  0.527938  1
  O  O7  1  0.526846  0.454661  0.527406  1
```

0d-P_4O_4 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   PO
_chemical_formula_sum   'P4 O4'
_cell_volume   21584.7325774
_cell_formula_units_Z   4
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loop_
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 _atom_site_label
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 _atom_site_fract_z
 _atom_site_occupancy
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  P  P2  1  0.475843  0.541912  0.540539  1
  P  P3  1  0.549400  0.499854  0.539904  1
  P  P4  1  0.475781  0.457975  0.540384  1
  O  O5  1  0.473361  0.545427  0.482258  1
  O  O6  1  0.473285  0.454694  0.482082  1
  O  O7  1  0.499216  0.500219  0.405507  1
  O  O8  1  0.552875  0.499974  0.481573  1
```

0d-P_4O_5 (screening)

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_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O5
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 _atom_site_occupancy
  P  P1  1  0.533719  0.543477  0.472064  1
  P  P2  1  0.439277  0.499678  0.479932  1
  P  P3  1  0.508297  0.500392  0.562934  1
  P  P4  1  0.534014  0.456431  0.472556  1
  O  O5  1  0.474228  0.544960  0.460308  1
  O  O6  1  0.474538  0.454412  0.460811  1
  O  O7  1  0.534007  0.545580  0.532197  1
  O  O8  1  0.534308  0.455027  0.532712  1
  O  O9  1  0.453286  0.500062  0.538197  1
```

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```
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_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O3
_chemical_formula_sum   'P4 O6'
_cell_volume   21864.9276622
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 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.488261  0.437258  0.512334  1
  P  P2  1  0.488262  0.512326  0.437267  1
  P  P3  1  0.562182  0.513466  0.513466  1
  P  P4  1  0.461296  0.536932  0.536932  1
  O  O5  1  0.479791  0.456616  0.456615  1
  O  O6  1  0.456562  0.477790  0.542429  1
  O  O7  1  0.456567  0.542435  0.477784  1
  O  O8  1  0.543439  0.457572  0.522218  1
  O  O9  1  0.520203  0.543388  0.543390  1
  O  O10  1  0.543433  0.522215  0.457572  1
```

0d-P_4O_7 (screening)

```
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_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O7
_chemical_formula_sum   'P4 O7'
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  P  P3  1  0.472191  0.443654  0.519904  1
  P  P4  1  0.502880  0.493443  0.432212  1
  O  O5  1  0.451965  0.584931  0.535421  1
  O  O6  1  0.477685  0.538234  0.460577  1
  O  O7  1  0.528824  0.450285  0.535275  1
  O  O8  1  0.451567  0.495851  0.535214  1
  O  O9  1  0.555235  0.493134  0.459794  1
  O  O10  1  0.475811  0.450683  0.460811  1
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```

0d-P_4O_8 (screening)

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_symmetry_space_group_name_H-M   'P 1'
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_symmetry_Int_Tables_number   1
_chemical_formula_structural   PO2
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_cell_volume   23560.2363315
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  P  P2  1  0.537137  0.455345  0.536159  1
  P  P3  1  0.462863  0.455345  0.463842  1
  P  P4  1  0.534858  0.527134  0.464418  1
  O  O5  1  0.500006  0.429533  0.499994  1
  O  O6  1  0.500367  0.492467  0.562627  1
  O  O7  1  0.437178  0.492465  0.501119  1
  O  O8  1  0.499996  0.554242  0.499994  1
  O  O9  1  0.499628  0.492470  0.437375  1
  O  O10  1  0.436614  0.557113  0.564736  1
  O  O11  1  0.563395  0.557107  0.435267  1
  O  O12  1  0.562818  0.492470  0.498887  1
```

0d-P_4O_9 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
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_chemical_formula_structural   P4O9
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_cell_volume   24891.3730748
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  P  P2  1  0.528275  0.547099  0.514109  1
  P  P3  1  0.444133  0.500383  0.514110  1
  P  P4  1  0.527593  0.452518  0.514114  1
  O  O5  1  0.525296  0.542137  0.456552  1
  O  O6  1  0.450015  0.500339  0.456552  1
  O  O7  1  0.524684  0.457521  0.456557  1
  O  O8  1  0.475608  0.541980  0.530081  1
  O  O9  1  0.474999  0.458353  0.530084  1
  O  O10  1  0.549402  0.499661  0.530082  1
  O  O11  1  0.551484  0.585827  0.532420  1
  O  O12  1  0.398216  0.500692  0.532417  1
  O  O13  1  0.550290  0.413502  0.532430  1
```

0d-P_4O_{10} (screening)

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.00000000
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O5
_chemical_formula_sum   'P4 O10'
_cell_volume   23653.6133839
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 _atom_site_fract_x
 _atom_site_fract_y
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  P  P2  1  0.534910  0.535451  0.464923  1
  P  P3  1  0.464885  0.464877  0.464782  1
  P  P4  1  0.535392  0.464822  0.534883  1
  O  O5  1  0.500244  0.437817  0.499704  1
  O  O6  1  0.499740  0.562184  0.500284  1
  O  O7  1  0.435692  0.563705  0.564740  1
  O  O8  1  0.499835  0.500281  0.437817  1
  O  O9  1  0.435810  0.435820  0.435611  1
  O  O10  1  0.564708  0.435696  0.563744  1
  O  O11  1  0.563813  0.564805  0.435882  1
  O  O12  1  0.562189  0.500256  0.499838  1
  O  O13  1  0.437812  0.499755  0.500176  1
  O  O14  1  0.500179  0.499706  0.562183  1
```

2d-P_4O_1 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   3.28913042
_cell_length_b   6.90924689
_cell_length_c   27.75250034
_cell_angle_alpha   90.14041220
_cell_angle_beta   90.00994218
_cell_angle_gamma   89.32867359
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O
_chemical_formula_sum   'P4 O1'
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  P  P2  1  0.150815  0.319900  0.499207  1
  P  P3  1  0.640318  0.741764  0.520390  1
  P  P4  1  0.140814  0.717881  0.465572  1
  O  O5  1  0.146697  0.479648  0.453985  1
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2d-P_4O_2 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_length_b   6.80551718
_cell_length_c   27.56295700
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.67063228
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O
_chemical_formula_sum   'P4 O2'
_cell_volume   630.641871601
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.351774  0.432797  0.453507  1
  P  P2  1  0.849031  0.323748  0.500662  1
  P  P3  1  0.359977  0.741877  0.478826  1
  P  P4  1  0.859335  0.719728  0.535040  1
  O  O5  1  0.842978  0.112041  0.513836  1
  O  O6  1  0.853164  0.475595  0.546493  1
```

2d-P_4O_3 (BOMD)

```
_symmetry_space_group_name_H-M   'P 1'
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_cell_length_b   14.97410740
_cell_length_c   26.40509733
_cell_angle_alpha   88.49599257
_cell_angle_beta   86.83526719
_cell_angle_gamma   87.04427909
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O3
_chemical_formula_sum   'P48 O36'
_cell_volume   7252.76646533
_cell_formula_units_Z   12
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.167138  0.166249  0.537157  1
  P  P2  1  0.160733  0.511863  0.542903  1
  P  P3  1  0.181091  0.848405  0.532082  1
  P  P4  1  0.396532  0.177017  0.573830  1
  P  P5  1  0.426183  0.511858  0.549195  1
  P  P6  1  0.411947  0.856494  0.556901  1
  P  P7  1  0.657546  0.174922  0.530109  1
  P  P8  1  0.649948  0.523414  0.570239  1
  P  P9  1  0.675933  0.842426  0.529285  1
  P  P10  1  0.904460  0.198232  0.524690  1
  P  P11  1  0.911819  0.493733  0.538581  1
  P  P12  1  0.909473  0.840861  0.534917  1
  P  P13  1  0.035597  0.291072  0.551276  1
  P  P14  1  0.017226  0.605711  0.583134  1
  P  P15  1  0.035890  0.948486  0.548879  1
  P  P16  1  0.250596  0.273900  0.601647  1
  P  P17  1  0.287142  0.625470  0.554923  1
  P  P18  1  0.271977  0.958287  0.592245  1
  P  P19  1  0.527979  0.280077  0.584320  1
  P  P20  1  0.514004  0.624744  0.608695  1
  P  P21  1  0.543029  0.965167  0.541537  1
  P  P22  1  0.765641  0.270109  0.583916  1
  P  P23  1  0.787319  0.619944  0.570875  1
  P  P24  1  0.783167  0.977896  0.552537  1
  P  P25  1  0.127340  0.137724  0.621602  1
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P P26 1 0.201906 0.457919 0.619821 1
P P27 1 0.150441 0.812255 0.617148 1
P P28 1 0.441202 0.118345 0.646630 1
P P29 1 0.386733 0.495962 0.635175 1
P P30 1 0.478564 0.811022 0.626759 1
P P31 1 0.657239 0.119574 0.614057 1
P P32 1 0.715436 0.443484 0.630545 1
P P33 1 0.661739 0.863106 0.617213 1
P P34 1 0.954266 0.106031 0.586423 1
P P35 1 0.901930 0.469147 0.626681 1
P P36 1 0.956483 0.784925 0.608245 1
P P37 1 0.016739 0.208832 0.621037 1
P P38 1 0.982816 0.555423 0.654145 1
P P39 1 0.030472 0.892092 0.624350 1
P P40 1 0.174727 0.248034 0.660627 1
P P41 1 0.276663 0.567485 0.632948 1
P P42 1 0.225221 0.883244 0.655624 1
P P43 1 0.534019 0.188380 0.652782 1
P P44 1 0.437302 0.612035 0.668080 1
P P45 1 0.550494 0.928282 0.623150 1
P P46 1 0.723844 0.209795 0.651273 1
P P47 1 0.794826 0.546650 0.644130 1
P P48 1 0.722940 0.986050 0.626299 1
O O49 1 0.967189 0.273382 0.516492 1
O O50 1 0.975786 0.569882 0.536165 1
O O51 1 0.977370 0.907382 0.514213 1
O O52 1 0.231096 0.238276 0.547194 1
O O53 1 0.225305 0.579945 0.523545 1
O O54 1 0.246673 0.915430 0.539120 1
O O55 1 0.454188 0.256762 0.558026 1
O O56 1 0.490724 0.586367 0.555679 1
O O57 1 0.466895 0.928054 0.525957 1
O O58 1 0.725400 0.246955 0.534354 1
O O59 1 0.706327 0.603938 0.552429 1
O O60 1 0.739031 0.917296 0.515915 1
O O61 1 0.101577 0.240595 0.518718 1
O O62 1 0.102019 0.591103 0.568276 1
O O63 1 0.112282 0.933672 0.520554 1
O O64 1 0.333169 0.241917 0.607537 1
O O65 1 0.360658 0.580771 0.527308 1
O O66 1 0.359526 0.929513 0.589976 1
O O67 1 0.588270 0.247518 0.540144 1
O O68 1 0.595601 0.580259 0.613215 1
O O69 1 0.601256 0.897782 0.510739 1
O O70 1 0.850450 0.253966 0.569069 1
O O71 1 0.837591 0.560071 0.530386 1
O O72 1 0.853831 0.915700 0.566001 1
O O73 1 0.020715 0.054392 0.544975 1
O O74 1 0.043789 0.388602 0.556566 1
O O75 1 0.014252 0.712693 0.573510 1

O	O76	1	0.266555	0.058198	0.589023	1
O	O77	1	0.262189	0.379646	0.592163	1
O	O78	1	0.283207	0.724552	0.549494	1
O	O79	1	0.551112	0.060669	0.527069	1
O	O80	1	0.532925	0.377079	0.593661	1
O	O81	1	0.534017	0.727836	0.597373	1
O	O82	1	0.801926	0.064778	0.528175	1
O	O83	1	0.763205	0.377445	0.585721	1
O	O84	1	0.803389	0.716295	0.568477	1

2d-P_4O_4 (BOMD)

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_cell_angle_beta   89.07990762
_cell_angle_gamma   85.54143687
_symmetry_Int_Tables_number   1
_chemical_formula_structural   PO
_chemical_formula_sum   'P48 O48'
_cell_volume   7281.67983006
_cell_formula_units_Z   48
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 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
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 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  P  P2  1  0.187708  0.513723  0.422413  1
  P  P3  1  0.180118  0.825840  0.624172  1
  P  P4  1  0.405557  0.187875  0.608002  1
  P  P5  1  0.425474  0.505117  0.484083  1
  P  P6  1  0.427621  0.855175  0.578209  1
  P  P7  1  0.688822  0.198731  0.580033  1
  P  P8  1  0.685974  0.577599  0.554173  1
  P  P9  1  0.630337  0.923066  0.629784  1
  P  P10  1  0.887057  0.263437  0.520831  1
  P  P11  1  0.950710  0.665215  0.509353  1
  P  P12  1  0.921560  0.898186  0.682123  1
  P  P13  1  0.037608  0.287410  0.554652  1
  P  P14  1  0.026138  0.546311  0.440161  1
  P  P15  1  0.027629  0.875390  0.596622  1
  P  P16  1  0.247238  0.210957  0.579500  1
  P  P17  1  0.275415  0.582164  0.501019  1
  P  P18  1  0.264964  0.939981  0.563956  1
  P  P19  1  0.530638  0.270709  0.567324  1
  P  P20  1  0.520303  0.577086  0.564950  1
  P  P21  1  0.489131  0.879046  0.678663  1
  P  P22  1  0.783710  0.328973  0.600841  1
  P  P23  1  0.796688  0.700951  0.542266  1
  P  P24  1  0.768216  0.975124  0.687328  1
  P  P25  1  0.092301  0.083860  0.578812  1
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P P26 1 0.242138 0.392168 0.456248 1
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P P29 1 0.382000 0.397272 0.530376 1
P P30 1 0.433797 0.723184 0.613058 1
P P31 1 0.732712 0.151763 0.656103 1
P P32 1 0.716484 0.584961 0.637030 1
P P33 1 0.626176 0.789729 0.600643 1
P P34 1 0.898930 0.151853 0.576842 1
P P35 1 0.957106 0.746575 0.438957 1
P P36 1 0.968192 0.022845 0.688819 1
P P37 1 0.008301 0.184588 0.610646 1
P P38 1 0.012818 0.662477 0.390174 1
P P39 1 0.059879 0.988463 0.639894 1
P P40 1 0.183343 0.123347 0.630513 1
P P41 1 0.262127 0.451113 0.532719 1
P P42 1 0.258977 0.005076 0.640199 1
P P43 1 0.504423 0.344744 0.638406 1
P P44 1 0.402791 0.425674 0.612988 1
P P45 1 0.537603 0.750090 0.657883 1
P P46 1 0.840598 0.218549 0.643651 1
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P P48 1 0.704575 0.722079 0.658846 1
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O O50 1 0.988498 0.571268 0.495708 1
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O O66 1 0.339408 0.875203 0.566444 1
O O67 1 0.598430 0.201143 0.584937 1
O O68 1 0.599598 0.616424 0.546607 1
O O69 1 0.559318 0.936802 0.670633 1
O O70 1 0.819651 0.328039 0.543346 1
O O71 1 0.863063 0.641749 0.513151 1
O O72 1 0.837058 0.916600 0.658892 1
O O73 1 0.015900 0.891556 0.541521 1
O O74 1 0.080003 0.353497 0.576936 1
O O75 1 0.001748 0.467281 0.419123 1

O	O76	1	0.257042	0.995678	0.517962	1
O	O77	1	0.244070	0.294831	0.604389	1
O	O78	1	0.240778	0.653835	0.530452	1
O	O79	1	0.451622	0.888214	0.728984	1
O	O80	1	0.545675	0.321344	0.520520	1
O	O81	1	0.469462	0.669533	0.562579	1
O	O82	1	0.764265	0.052493	0.642327	1
O	O83	1	0.784531	0.409864	0.627892	1
O	O84	1	0.794710	0.792296	0.528107	1
O	O85	1	0.164883	0.342587	0.472155	1
O	O86	1	0.174885	0.517979	0.366764	1
O	O87	1	0.229737	0.753445	0.642663	1
O	O88	1	0.426987	0.114232	0.642160	1
O	O89	1	0.434228	0.479420	0.430310	1
O	O90	1	0.479504	0.876524	0.536386	1
O	O91	1	0.724830	0.165249	0.532734	1
O	O92	1	0.701746	0.491257	0.534245	1
O	O93	1	0.630550	0.991178	0.590172	1
O	O94	1	0.880939	0.241351	0.466830	1
O	O95	1	0.977824	0.699708	0.557263	1
O	O96	1	0.923367	0.843475	0.728825	1

2d-P_4O_5 (BOMD)

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_cell_angle_gamma   87.42224582
_symmetry_Int_Tables_number   1
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_chemical_formula_sum   'P48 O60'
_cell_volume   7501.47482293
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 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
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  P  P2  1  0.009807  0.424820  0.527820  1
  P  P3  1  0.001981  0.711763  0.586222  1
  P  P4  1  0.256314  0.072031  0.515895  1
  P  P5  1  0.261623  0.379020  0.540181  1
  P  P6  1  0.241387  0.728790  0.521992  1
  P  P7  1  0.531467  0.043979  0.516158  1
  P  P8  1  0.532420  0.416470  0.494391  1
  P  P9  1  0.484944  0.730166  0.524179  1
  P  P10  1  0.761554  0.141003  0.431036  1
  P  P11  1  0.760959  0.407085  0.542415  1
  P  P12  1  0.776348  0.704790  0.521145  1
  P  P13  1  0.120743  0.167235  0.540592  1
  P  P14  1  0.136245  0.460686  0.593935  1
  P  P15  1  0.139685  0.796481  0.605942  1
  P  P16  1  0.396136  0.123374  0.564634  1
  P  P17  1  0.399584  0.461030  0.562009  1
  P  P18  1  0.357779  0.817651  0.577415  1
  P  P19  1  0.663748  0.132984  0.528538  1
  P  P20  1  0.625575  0.498118  0.570613  1
  P  P21  1  0.634470  0.795945  0.545625  1
  P  P22  1  0.887153  0.181570  0.501743  1
  P  P23  1  0.886680  0.466923  0.601863  1
  P  P24  1  0.867060  0.816552  0.580275  1
  P  P25  1  0.054748  0.291734  0.608864  1
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P P30 1 0.306989 0.974926 0.617101 1
P P31 1 0.543207 0.335022 0.604304 1
P P32 1 0.565788 0.639893 0.618096 1
P P33 1 0.641218 0.954645 0.590541 1
P P34 1 0.805335 0.303524 0.641605 1
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O O67 1 0.709943 0.171653 0.480566 1
O O68 1 0.712395 0.485265 0.562262 1
O O69 1 0.699313 0.760843 0.510692 1
O O70 1 0.962905 0.209468 0.475764 1
O O71 1 0.964895 0.476734 0.572296 1
O O72 1 0.923440 0.745166 0.606955 1
O O73 1 0.127173 0.247208 0.573945 1
O O74 1 0.136341 0.554211 0.606957 1
O O75 1 0.157131 0.879233 0.617588 1

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O O77 1 0.378393 0.540970 0.581357 1
O O78 1 0.361714 0.912239 0.576753 1
O O79 1 0.635130 0.191180 0.567706 1
O O80 1 0.622373 0.594653 0.572516 1
O O81 1 0.635859 0.889345 0.537002 1
O O82 1 0.856735 0.240579 0.539905 1
O O83 1 0.860982 0.541786 0.626930 1
O O84 1 0.907060 0.887326 0.561943 1
O O85 1 0.234163 0.042019 0.463691 1
O O86 1 0.222903 0.346303 0.494607 1
O O87 1 0.234347 0.704935 0.466165 1
O O88 1 0.501022 0.986681 0.479628 1
O O89 1 0.533111 0.398898 0.437168 1
O O90 1 0.457244 0.690484 0.477039 1
O O91 1 0.733874 0.162215 0.377007 1
O O92 1 0.739858 0.377688 0.489889 1
O O93 1 0.786344 0.647691 0.478198 1
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O O99 1 0.022659 0.647566 0.634768 1
O O100 1 0.253779 0.011173 0.566088 1
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O O102 1 0.266572 0.660300 0.564844 1
O O103 1 0.563898 0.009241 0.573522 1
O O104 1 0.544143 0.342182 0.535656 1
O O105 1 0.499339 0.673945 0.577206 1
O O106 1 0.774007 0.046979 0.443582 1
O O107 1 0.752319 0.346525 0.593081 1
O O108 1 0.765447 0.669202 0.580519 1

2d-P_4O_6 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.46227400
_cell_length_b   8.34103717
_cell_length_c   26.67229200
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   90.08946376
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O3
_chemical_formula_sum   'P4 O6'
_cell_volume   992.741319024
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.036125  0.698519  0.468651  1
  P  P2  1  0.536042  0.846313  0.530939  1
  P  P3  1  0.041063  0.346206  0.469113  1
  P  P4  1  0.541315  0.198530  0.531349  1
  O  O5  1  0.834487  0.740011  0.520414  1
  O  O6  1  0.843074  0.302982  0.521169  1
  O  O7  1  0.334570  0.805467  0.479054  1
  O  O8  1  0.342948  0.242598  0.479454  1
  O  O9  1  0.664312  0.022206  0.510550  1
  O  O10  1  0.164352  0.523236  0.489412  1
```

2d-P_4O_7 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.49919200
_cell_length_b   7.85656944
_cell_length_c   27.33746100
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   89.72967966
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O7
_chemical_formula_sum   'P4 O7'
_cell_volume   966.319676999
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.952923  0.568298  0.457248  1
  P  P2  1  0.456284  0.669392  0.528233  1
  P  P3  1  0.654494  0.989837  0.476147  1
  P  P4  1  0.145836  0.232512  0.499676  1
  O  O5  1  0.021408  0.358482  0.458105  1
  O  O6  1  0.528011  0.876769  0.522034  1
  O  O7  1  0.769901  0.583101  0.510198  1
  O  O8  1  0.268164  0.648955  0.474386  1
  O  O9  1  0.871262  0.111863  0.511321  1
  O  O10  1  0.367083  0.117751  0.466595  1
  O  O11  1  0.278184  0.312829  0.542752  1
```

2d-P_4O_8 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.47710700
_cell_length_b   7.92059294
_cell_length_c   27.92705900
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   89.97213550
_symmetry_Int_Tables_number   1
_chemical_formula_structural   PO2
_chemical_formula_sum   'P4 O8'
_cell_volume   990.330875399
_cell_formula_units_Z   4
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.911554  0.062272  0.465333  1
  P  P2  1  0.411649  0.158892  0.534906  1
  P  P3  1  0.594808  0.491499  0.490194  1
  P  P4  1  0.094882  0.729138  0.509746  1
  O  O5  1  0.962252  0.849265  0.469768  1
  O  O6  1  0.462265  0.371847  0.530279  1
  O  O7  1  0.737430  0.089678  0.518220  1
  O  O8  1  0.237418  0.131040  0.482073  1
  O  O9  1  0.824707  0.602707  0.521892  1
  O  O10  1  0.324698  0.618034  0.477943  1
  O  O11  1  0.226905  0.806178  0.552405  1
  O  O12  1  0.726756  0.413883  0.447595  1
```

2d-P_4O_9 (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.68431367
_cell_length_b   7.89711051
_cell_length_c   29.04593561
_cell_angle_alpha   90.00168513
_cell_angle_beta   90.01382343
_cell_angle_gamma   93.80335704
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P4O9
_chemical_formula_sum   'P4 O9'
_cell_volume   1072.11652271
_cell_formula_units_Z   1
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.481378  0.630277  0.524954  1
  P  P2  1  0.995399  0.781788  0.477210  1
  P  P3  1  0.495924  0.281922  0.562469  1
  P  P4  1  0.976030  0.134533  0.511438  1
  O  O5  1  0.673126  0.701226  0.482320  1
  O  O6  1  0.659603  0.139530  0.531974  1
  O  O7  1  0.035498  0.220370  0.467839  1
  O  O8  1  0.164401  0.642648  0.504803  1
  O  O9  1  0.537930  0.710640  0.569624  1
  O  O10  1  0.166839  0.199835  0.555304  1
  O  O11  1  0.013962  0.933705  0.514456  1
  O  O12  1  0.511544  0.431737  0.521291  1
  O  O13  1  0.083184  0.821345  0.430385  1
```

2d-P_4O_{10} (screening)

```
_symmetry_space_group_name_H-M   'P 1'
_cell_length_a   4.71465400
_cell_length_b   7.77139242
_cell_length_c   30.20437700
_cell_angle_alpha   90.00000000
_cell_angle_beta   90.00000000
_cell_angle_gamma   93.93872686
_symmetry_Int_Tables_number   1
_chemical_formula_structural   P2O5
_chemical_formula_sum   'P4 O10'
_cell_volume   1104.05717649
_cell_formula_units_Z   2
loop_
 _symmetry_equiv_pos_site_id
 _symmetry_equiv_pos_as_xyz
  1  'x, y, z'
loop_
 _atom_site_type_symbol
 _atom_site_label
 _atom_site_symmetry_multiplicity
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
  P  P1  1  0.565633  0.657765  0.505288  1
  P  P2  1  0.080691  0.801826  0.458699  1
  P  P3  1  0.582318  0.302008  0.541299  1
  P  P4  1  0.067913  0.157571  0.494715  1
  O  O5  1  0.762433  0.717056  0.463607  1
  O  O6  1  0.755878  0.161065  0.515702  1
  O  O7  1  0.120614  0.252134  0.453640  1
  O  O8  1  0.253923  0.660144  0.484108  1
  O  O9  1  0.616329  0.752673  0.546354  1
  O  O10  1  0.264380  0.216510  0.536471  1
  O  O11  1  0.099332  0.953990  0.495283  1
  O  O12  1  0.599333  0.454443  0.504800  1
  O  O13  1  0.667808  0.346751  0.586153  1
  O  O14  1  0.165790  0.846796  0.413847  1
```

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