

```

XTLGRF 200
DESCRP      B0090
REMARK      a-PtO2
CRYSTX      3.16017      3.16017      4.75548      90.00000      90.00000      120.00000
FORMAT ATOM  (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)
HETATM      1 Pt          -0.05652      -0.03263      0.00000      Pt  0 0  0.00000
HETATM      2 O           0.85747      1.54872      1.02456      O   0 0  0.00000
HETATM      3 O           1.76997      -0.03177      -1.02456      O   0 0  0.00000
UNIT ENERGY kcal
ENERGY      -290.067714
END

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XTLGRF 200
DESCRP      B0105
REMARK      b-PtO2
CRYSTX      4.58390      4.63850      3.23600      90.00000      90.00000      90.00000
FORMAT ATOM  (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)
HETATM      1 Pt          2.26761      2.29776      1.52855      Pt  0 0  0.00000
HETATM      2 Pt         -0.02552      -0.02155      -0.09787      Pt  0 0  0.00000
HETATM      3 O           1.24717      1.25821      -0.08809      O   0 0  0.00000
HETATM      4 O          -1.28797      -1.31127      -0.09025      O   0 0  0.00000
HETATM      5 O           0.99437      3.57682      1.52004      O   0 0  0.00000
HETATM      6 O           3.53018      1.00778      1.52043      O   0 0  0.00000
UNIT ENERGY kcal
ENERGY      -557.248505
END

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XTLGRF 200
DESCRP      B0126
REMARK      PtO
CRYSTX      3.25468      3.25468      5.33397      90.00000      90.00000      90.00000
FORMAT ATOM  (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)
HETATM      1 Pt         -0.08461      1.38140      2.59482      Pt  0 0  0.00000
HETATM      2 Pt          1.38037      -0.08609      -0.07218      Pt  0 0  0.00000
HETATM      3 O           0.10676      0.10600      3.92807      O   0 0  0.00000
HETATM      4 O           0.10574      0.10695      1.26140      O   0 0  0.00000
UNIT ENERGY kcal
ENERGY      -416.745891
END

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XTLGRF 200
DESCRP      B0150
REMARK      Pt3O4
CRYSTX      5.71200      5.71200      5.71200      90.00000      90.00000      90.00000
FORMAT ATOM  (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)
HETATM      1 Pt          1.35781      -0.05810      2.73009      Pt  1 1  0.00000
HETATM      2 Pt          4.26928      -0.02823      2.89594      Pt  1 1  0.00000
HETATM      3 Pt          2.73024      1.35786      -0.05778      Pt  1 1  0.00000
HETATM      4 Pt          2.89577      4.26918      -0.02858      Pt  1 1  0.00000
HETATM      5 Pt         -0.05800      2.73040      1.35780      Pt  1 1  0.00000
HETATM      6 Pt         -0.02836      2.89566      4.26930      Pt  1 1  0.00000
HETATM      7 O           1.40499      1.40575      1.40606      O   1 1  0.00000
HETATM      8 O           4.39105      3.95231      1.24419      O   1 1  0.00000
HETATM      9 O           3.95251      1.24471      4.39150      O   1 1  0.00000
HETATM     10 O           1.24555      4.39107      3.95216      O   1 1  0.00000
HETATM     11 O           4.22113      4.22027      4.22001      O   1 1  0.00000
HETATM     12 O           1.23461      1.67425      4.38270      O   1 1  0.00000
HETATM     13 O           1.67398      4.38215      1.23419      O   1 1  0.00000
HETATM     14 O           4.38144      1.23471      1.67443      O   1 1  0.00000
UNIT ENERGY kcal
ENERGY      -1353.705247
END

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