

```

XTLGRF 200
DESCRP
REMARK Pt111_1x1x14_30.0_vac
FIXATOMS      7      8
CRYSTX      2.79121      2.79121      59.62720      90.00000      90.00000      60.00000
FORMAT ATOM      (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
HETATM      1 Pt      -0.00000      0.00000      -0.00117      Pt      1 0      0.00000
HETATM      2 Pt      0.80575      1.39561      2.28018      Pt      1 0      0.00000
HETATM      3 Pt      1.61151      2.79121      4.55805      Pt      1 0      0.00000
HETATM      4 Pt      0.00000      0.00000      6.83705      Pt      1 0      0.00000
HETATM      5 Pt      0.80575      1.39561      9.11606      Pt      1 0      0.00000
HETATM      6 Pt      1.61151      2.79121      11.39508      Pt      1 0      0.00000
HETATM      7 Pt      0.00000      0.00000      13.67409      Pt      1 0      0.00000
HETATM      8 Pt      0.80575      1.39561      15.95311      Pt      1 0      0.00000
HETATM      9 Pt      1.61151      2.79121      18.23212      Pt      1 0      0.00000
HETATM     10 Pt      0.00000      0.00000      20.51114      Pt      1 0      0.00000
HETATM     11 Pt      0.80575      1.39561      22.79015      Pt      1 0      0.00000
HETATM     12 Pt      1.61151      2.79121      25.06915      Pt      1 0      0.00000
HETATM     13 Pt      0.00000      0.00000      27.34702      Pt      1 0      0.00000
HETATM     14 Pt      0.80575      1.39561      29.62837      Pt      1 0      0.00000
UNIT ENERGY      kcal
ENERGY      -1830.353178
END

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XTLGRF 200
DESCRP
REMARK Pt100_1x1x14_30.0_vac
FIXATOMS      7      8
CRYSTX      2.79121      2.79121      55.65790      90.00000      90.00000      90.00000
FORMAT ATOM      (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
HETATM      1 Pt      0.00000      0.00000      -0.00963      Pt      1 0      0.00000
HETATM      2 Pt      1.39561      1.39561      1.97676      Pt      1 0      0.00000
HETATM      3 Pt      0.00000      0.00000      3.95060      Pt      1 0      0.00000
HETATM      4 Pt      1.39561      1.39561      5.92341      Pt      1 0      0.00000
HETATM      5 Pt      0.00000      0.00000      7.89590      Pt      1 0      0.00000
HETATM      6 Pt      1.39561      1.39561      9.86831      Pt      1 0      0.00000
HETATM      7 Pt      0.00000      0.00000      11.84211      Pt      1 0      0.00000
HETATM      8 Pt      1.39561      1.39561      13.81579      Pt      1 0      0.00000
HETATM      9 Pt      0.00000      0.00000      15.78959      Pt      1 0      0.00000
HETATM     10 Pt      1.39561      1.39561      17.76200      Pt      1 0      0.00000
HETATM     11 Pt      0.00000      0.00000      19.73450      Pt      1 0      0.00000
HETATM     12 Pt      1.39561      1.39561      21.70730      Pt      1 0      0.00000
HETATM     13 Pt      0.00000      0.00000      23.68114      Pt      1 0      0.00000
HETATM     14 Pt      1.39561      1.39561      25.66753      Pt      1 0      0.00000
UNIT ENERGY      kcal
ENERGY      -1820.620375
END

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XTLGRF 200
DESCRP
REMARK Pt110_1x1x14_30.0_vac
FIXATOMS      7      8
CRYSTX      3.94737      2.79121      48.14288      90.00000      90.00000      90.00000
FORMAT ATOM      (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
HETATM      1 Pt      -0.00000      0.00000      -0.00871      Pt      1 0      0.00000
HETATM      2 Pt      1.97369      1.39561      1.39890      Pt      1 0      0.00000
HETATM      3 Pt      -0.00001      0.00000      2.79245      Pt      1 0      0.00000
HETATM      4 Pt      1.97369      1.39561      4.18881      Pt      1 0      0.00000
HETATM      5 Pt      -0.00001      0.00000      5.58354      Pt      1 0      0.00000
HETATM      6 Pt      1.97369      1.39561      6.97895      Pt      1 0      0.00000
HETATM      7 Pt      0.00000      0.00000      8.37364      Pt      1 0      0.00000
HETATM      8 Pt      1.97368      1.39561      9.76924      Pt      1 0      0.00000
HETATM      9 Pt      -0.00001      0.00000      11.16393      Pt      1 0      0.00000

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HETATM      10 Pt          1.97369    1.39561   12.55934    Pt  1 0    0.00000
HETATM      11 Pt          -0.00001    0.00000   13.95407    Pt  1 0    0.00000
HETATM      12 Pt          1.97369    1.39561   15.35043    Pt  1 0    0.00000
HETATM      13 Pt          -0.00001    0.00000   16.74398    Pt  1 0    0.00000
HETATM      14 Pt          1.97368    1.39561   18.15159    Pt  1 0    0.00000
UNIT ENERGY      kcal
ENERGY            -1798.978178
END

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