PSEUDOPOTENTIAL TEST FOR Pt

- Flavour: **Troullier-Martins; tm2**

- Exchange-correlation: **Ceperley-Alder, relativistic; car**

- Number of core orbitals: **12**

- Number of valence orbitals: **4**

- Reference configuration: $6s^1, 5d^9, 6p^0, 5f^0$

- Cutoff radius:

    - $r_s = 2.35$ bohr
    - $r_p = 2.50$ bohr
    - $r_d = 1.24$ bohr
    - $r_f = 2.35$ bohr

- **Core corrections**: $r_{nlcc} = 1.7$

Configuration	Eigenvalues (Ry)		Total energies (Ry)	
	All electron	Pseudopotential	All electron	Pseudopotential
$6s^1, 6p^0, 5d^9, 5f^0$ (Reference)	$6s$ -0.4368 $6p \begin{cases} -0.1013 \\ -0.0615 \end{cases}$ $5d \begin{cases} -0.5319 \\ -0.4339 \end{cases}$	$6s$ -0.4368 $6p \begin{cases} -0.1013 \\ -0.0614 \end{cases}$ $5d \begin{cases} -0.5319 \\ -0.4339 \end{cases}$	-36798.3834	-56.8121
$6s^2, 6p^0, 5d^8, 5f^0$ (Pt neutral)	$6s$ -0.4964 $6p \begin{cases} -0.1327 \\ -0.0841 \end{cases}$ $5d \begin{cases} -0.6740 \\ -0.5695 \end{cases}$	$6s$ -0.4944 $6p \begin{cases} -0.1312 \\ -0.0829 \end{cases}$ $5d \begin{cases} -0.6786 \\ -0.5736 \end{cases}$	-36798.3087 $\Delta = 0.0747$ Ry	-56.7345 $\Delta = 0.0776$ Ry
$6s^0, 6p^0, 5d^{10}, 5f^0$ (Pt neutral)	$6s$ -0.3818 $6p \begin{cases} -0.0724 \\ -0.0403 \end{cases}$ $5d \begin{cases} -0.4067 \\ -0.3148 \end{cases}$	$6s$ -0.3845 $6p \begin{cases} -0.0742 \\ -0.0417 \end{cases}$ $5d \begin{cases} -0.4053 \\ -0.3140 \end{cases}$	-36798.3854 $\Delta = -0.0020$ Ry	-56.8121 $\Delta = 0.0000$ Ry
$6s^0, 6p^0, 5d^9, 5f^0$ (Pt^{+1})	$6s$ -0.9707 $6p \begin{cases} -0.5573 \\ -0.4824 \end{cases}$ $5d \begin{cases} -1.1358 \\ -1.0346 \end{cases}$	$6s$ -0.9724 $6p \begin{cases} -0.5588 \\ -0.4840 \end{cases}$ $5d \begin{cases} -1.1345 \\ -1.0338 \end{cases}$	-36797.6846 $\Delta = 0.6988$ Ry	-56.1125 $\Delta = 0.6996$ Ry
$6s^1, 6p^0, 5d^8, 5f^0$ (Pt^{+1})	$6s$ -1.0495 $6p \begin{cases} -0.6138 \\ -0.5308 \end{cases}$ $5d \begin{cases} -1.2991 \\ -1.1917 \end{cases}$	$6s$ -1.0485 $6p \begin{cases} -0.6126 \\ -0.5305 \end{cases}$ $5d \begin{cases} -1.3026 \\ -1.1949 \end{cases}$	-36797.5407 $\Delta = 0.8427$ Ry	-55.9681 $\Delta = 0.8440$ Ry