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The electronic structure of PrT2B2C (T=Co,Ni and Pt) : A Tight Binding - Extended Huckel D.H. GALVAN, C. SAMANIEGO, A. POSADA-AMARILLAS, A. DURAN, CCMC-UNAM, Mexico, F. MORALES, R. ESCUDERO, IIM-UNAM, Mexico — The calculations reported in this work were carried out by means of the tight-binding method within the Extended Huckel framework using YAeHMOP computer package with f-orbitals. The calculated energy bands indicate that the three compounds under investigation show metallic behavior mainly caused by the d-states of the **T**-atoms. For $\mathbf{PrNi_2B_2C}$ and $\mathbf{PrCo_2B_2C}$ compounds the Fermi level ($\mathbf{E_F}$) is located in a valley in the total density of states (**DOS**), while for $\mathbf{PrPt_3B_2C}$ the $\mathbf{E_F}$ is located in a crest. Our results predict the absence of superconductivity in $\mathbf{PrNi_2B_2C}$ and $\mathbf{PrCo_2B_2C}$ compounds, while the enhancement of **DOS** at the $\mathbf{E_F}$ in $\mathbf{PrPt_2B_2C}$ compound indicates the possibility of superconductivity. Moreover, the $\mathbf{PrNi_2B_2C}$ and $\mathbf{PrCo_2B_2C}$ compounds indicate strong and similar type of hybridization while different and reduced hybridization in $\mathbf{PrPt_2B_2C}$ compound is observed. Transport properties performed by our group confirms the existence of superconductivity in $\mathbf{PrPt_2B_2C}$ while the high value of Sommerfeld constant ($\gamma \approx$ 200-300 $\mathrm{mJ/mol - K^2}$) in $\mathbf{PrNi_2B_2C}$ and $\mathbf{PrCo_2B_2C}$ compounds might be connected by an enhancement of the hybridization observed here.

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