

σ -Aromaticity in Polyhydride Complexes of Ru, Ir, Os, and Pt

Elisa Jimenez-Izal¹ and Anastassia N. Alexandrova^{1,2,*}

¹Department of Chemistry and Biochemistry, and ²California NanoSystems Institute, University of California, Los Angeles, CA 90095-1569

Figure 1: First MOs of $\text{IrH}_5(\text{PPh}_3)_2$.

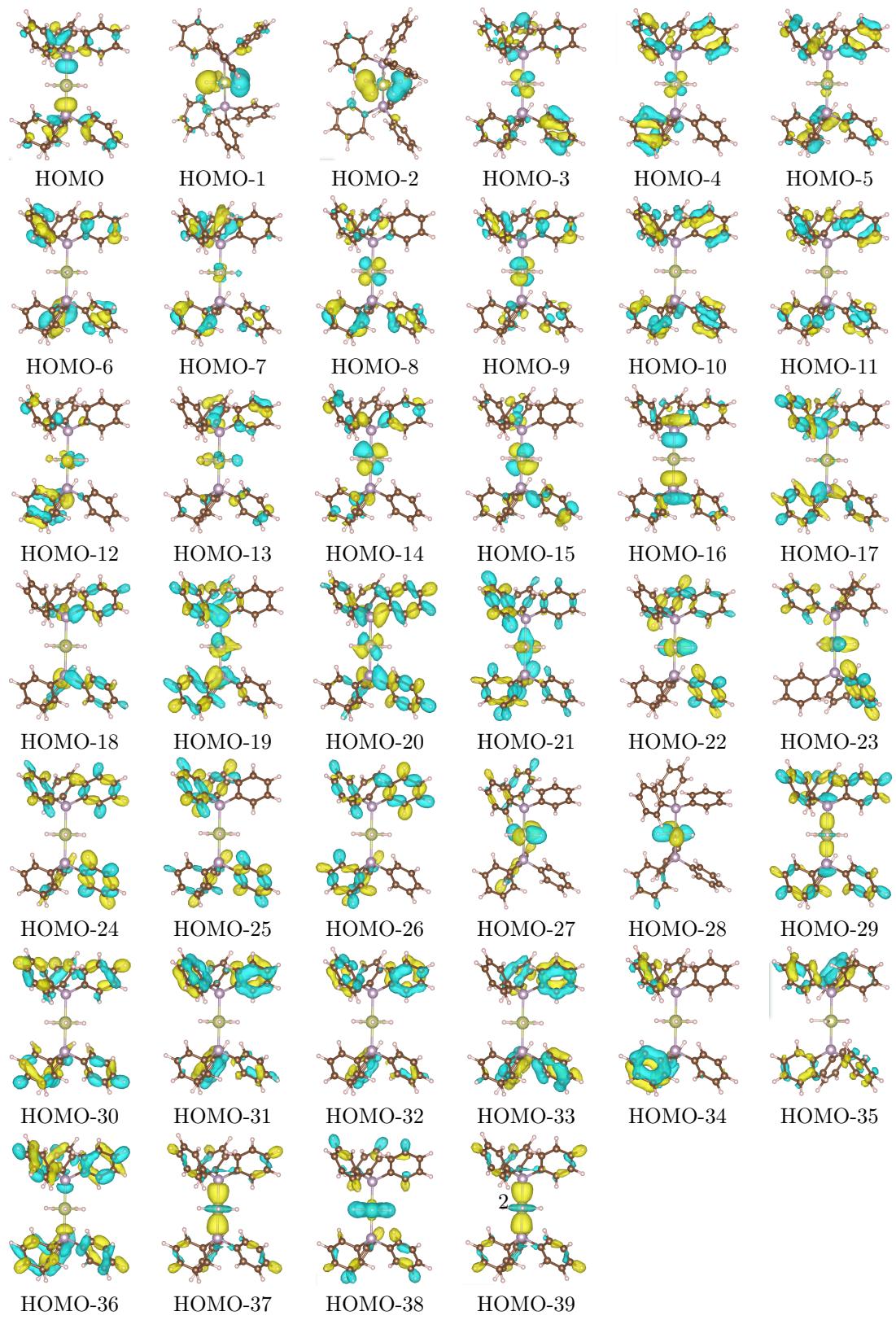


Figure 2: MOs of IrH_5 .

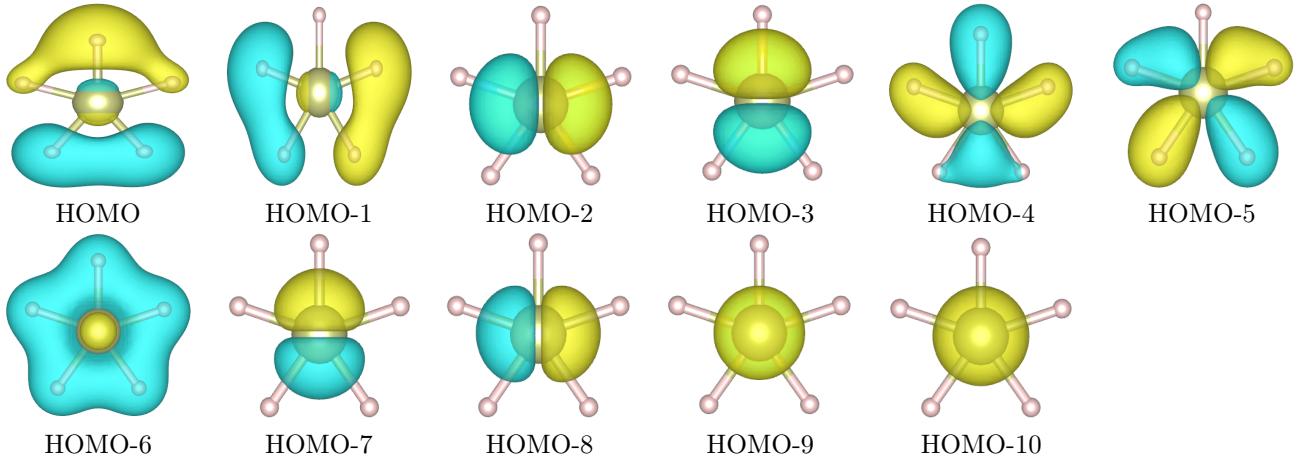


Figure 3: First MOs of $(\text{RuH}_5(\text{P}^i\text{Pr}_3)_2)^-$.

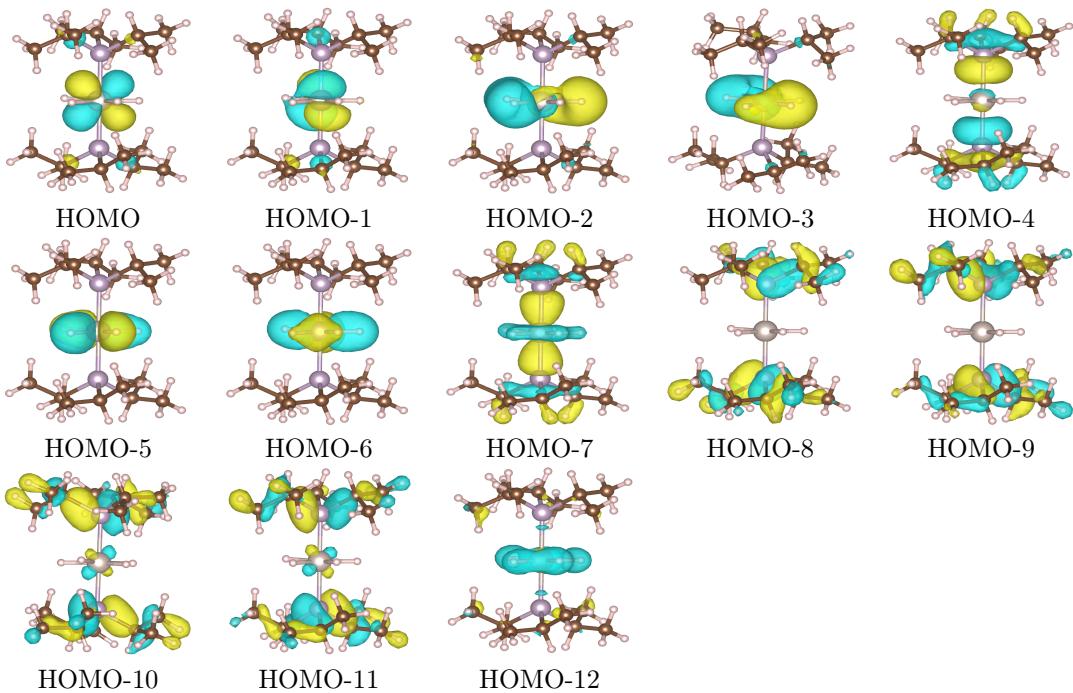


Figure 4: $(\text{TMH}_5\text{L}_2)^{0,-1}$ ($\text{L} = \text{PMe}_3$, PPh_3 , and P^iPr_3) structures not shown in the manuscript. The pink, turquoise, green, blue orange, gray, and white spheres represent Ir, Ru, Os, Pt, P, C, and H atoms respectively.

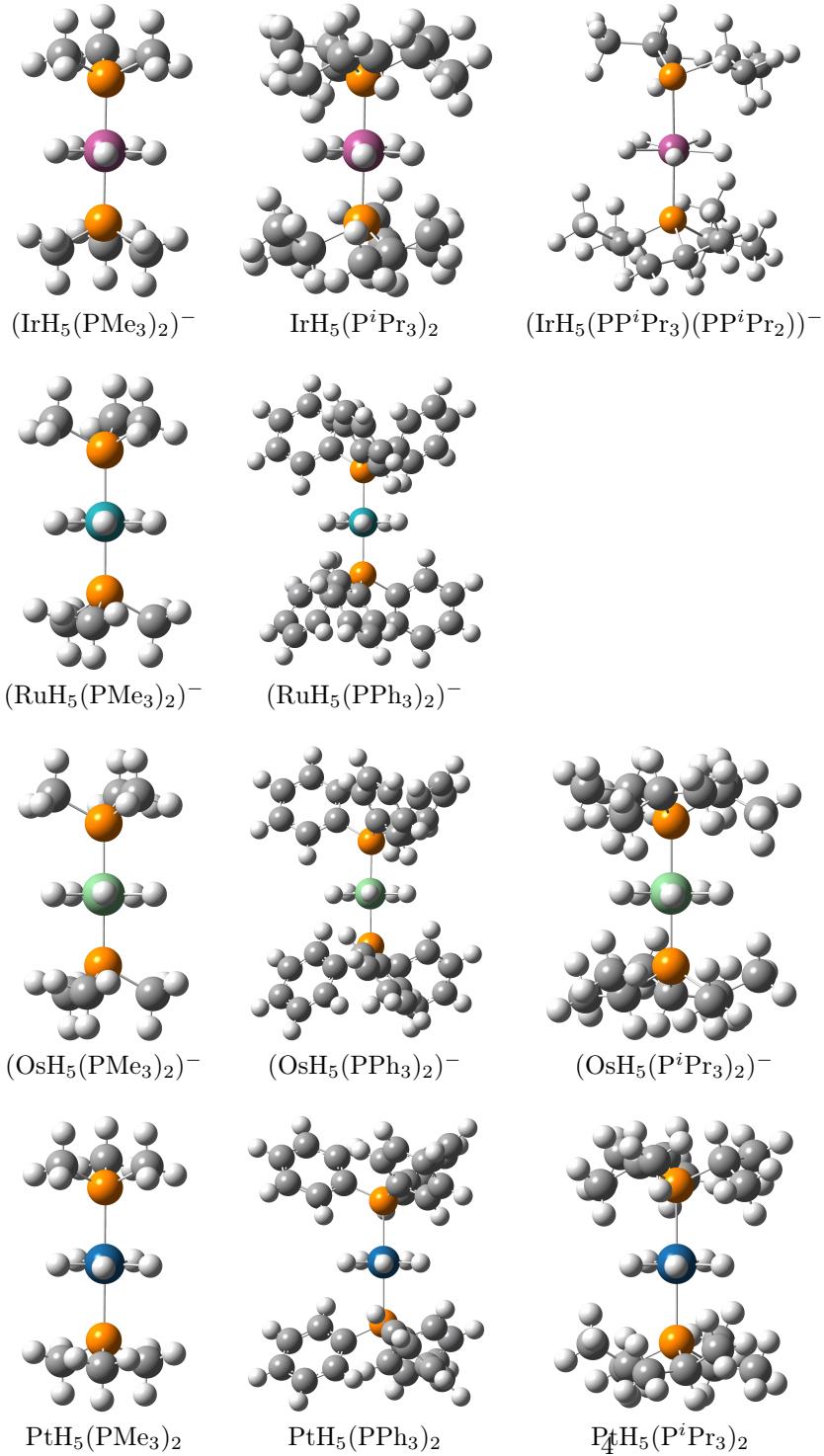


Figure 5: $(\text{TMH}_4\text{L}_3)^{0,-1}$ ($\text{L} = \text{PMe}_3$, and Me_2Ph) structures not shown in the manuscript. The green, turquoise, orange, gray, and white spheres represent Os, Ru, P, C, and H atoms respectively.

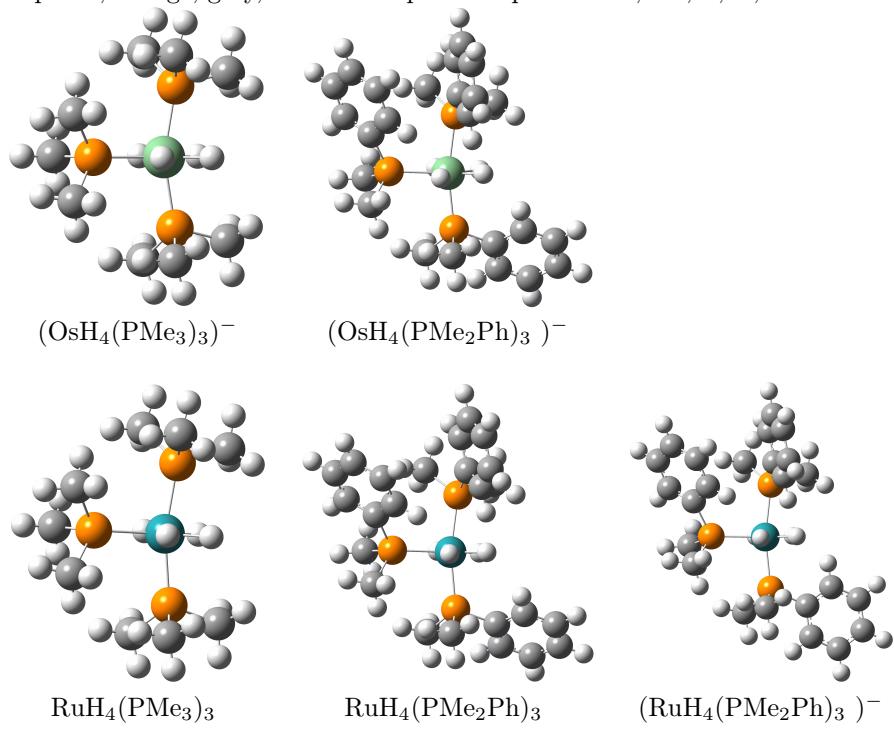


Figure 6: First MOs of $\text{OsH}_4(\text{PPhMe}_2)_3$.

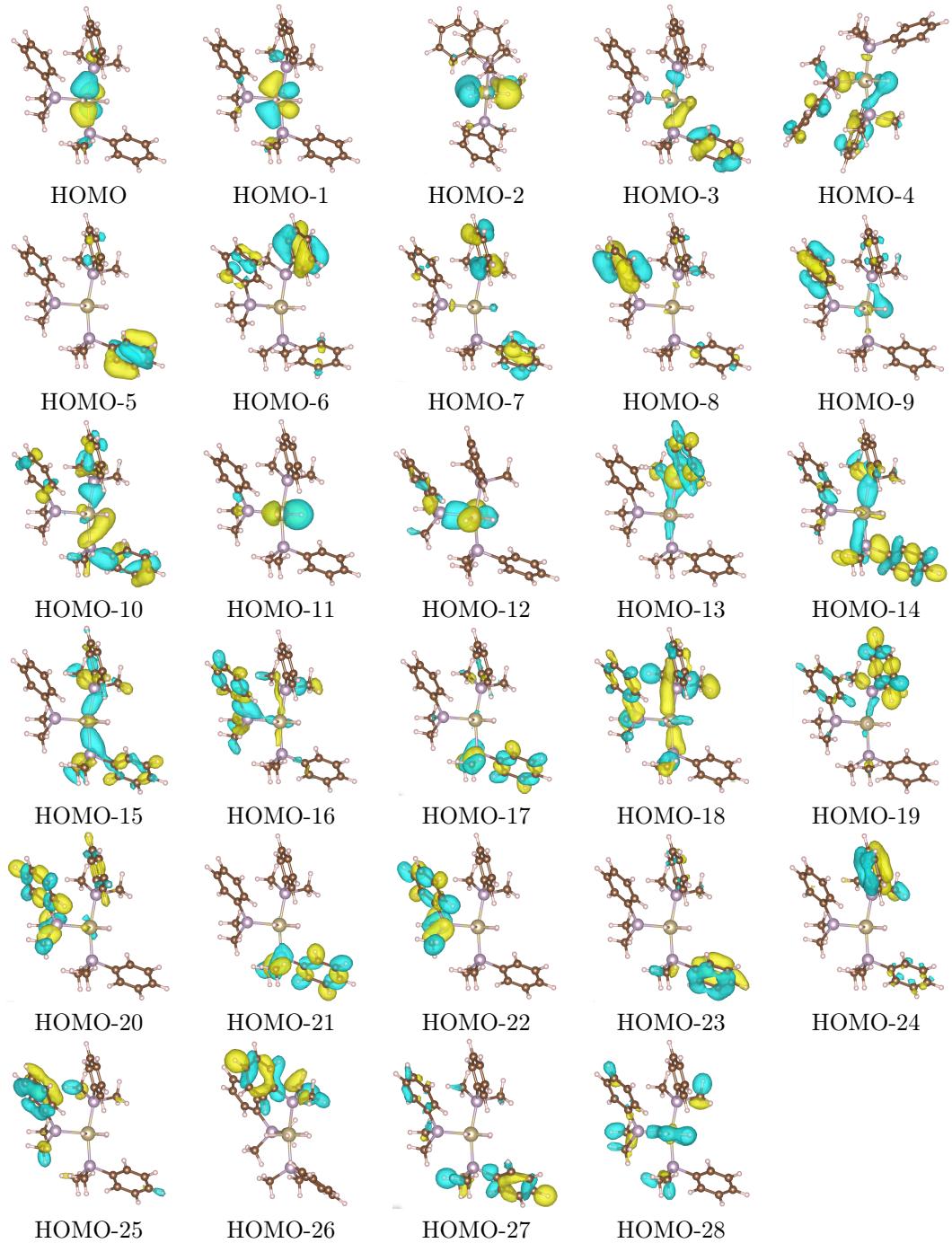


Figure 7: First MOs of $(\text{IrH}_5\text{Zn})^-$ complex hydride.

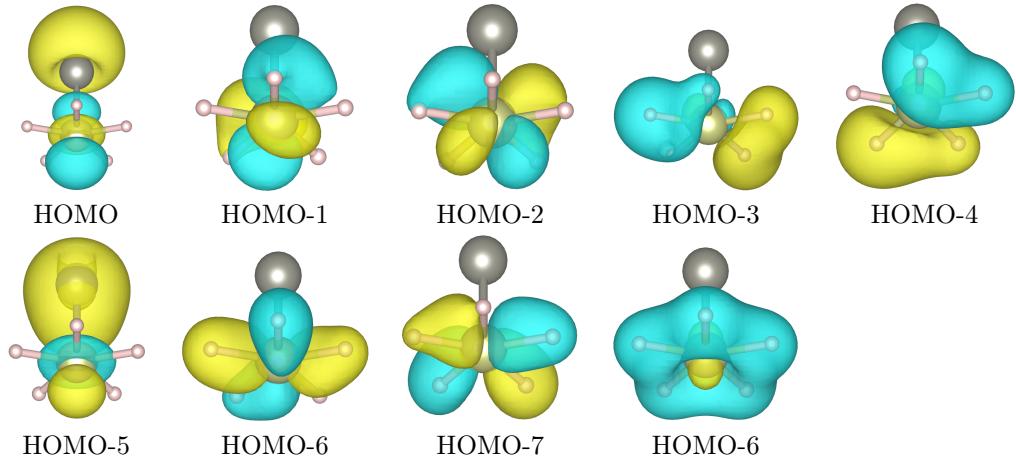


Figure 8: $(\text{TMH}_5\text{Zn})^{0,-1}$ structures not shown in the manuscript. Pt, Ru, Zn, and H are represented with blue, turquoise, violet and white spheres respectively.

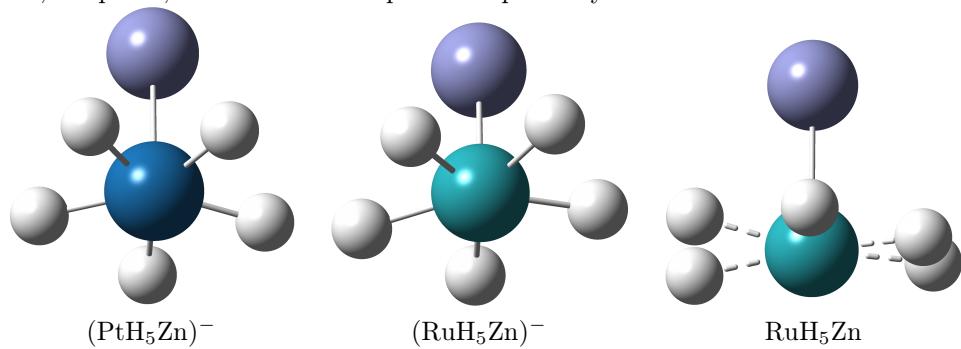


Figure 9: First MOs of $(\text{OsH}_5\text{Zn})^-$ complex hydride.

