Electronic Supplementary Material (ESI) for RSC Advances.

Remarkable Mixture of Germanium with Phosphorus and Arsenic Atoms Making Stable Pentagonal Hetero-Prisms $[M@Ge_5E_5]^+$, E = P, As and M = Fe, Ru, Os

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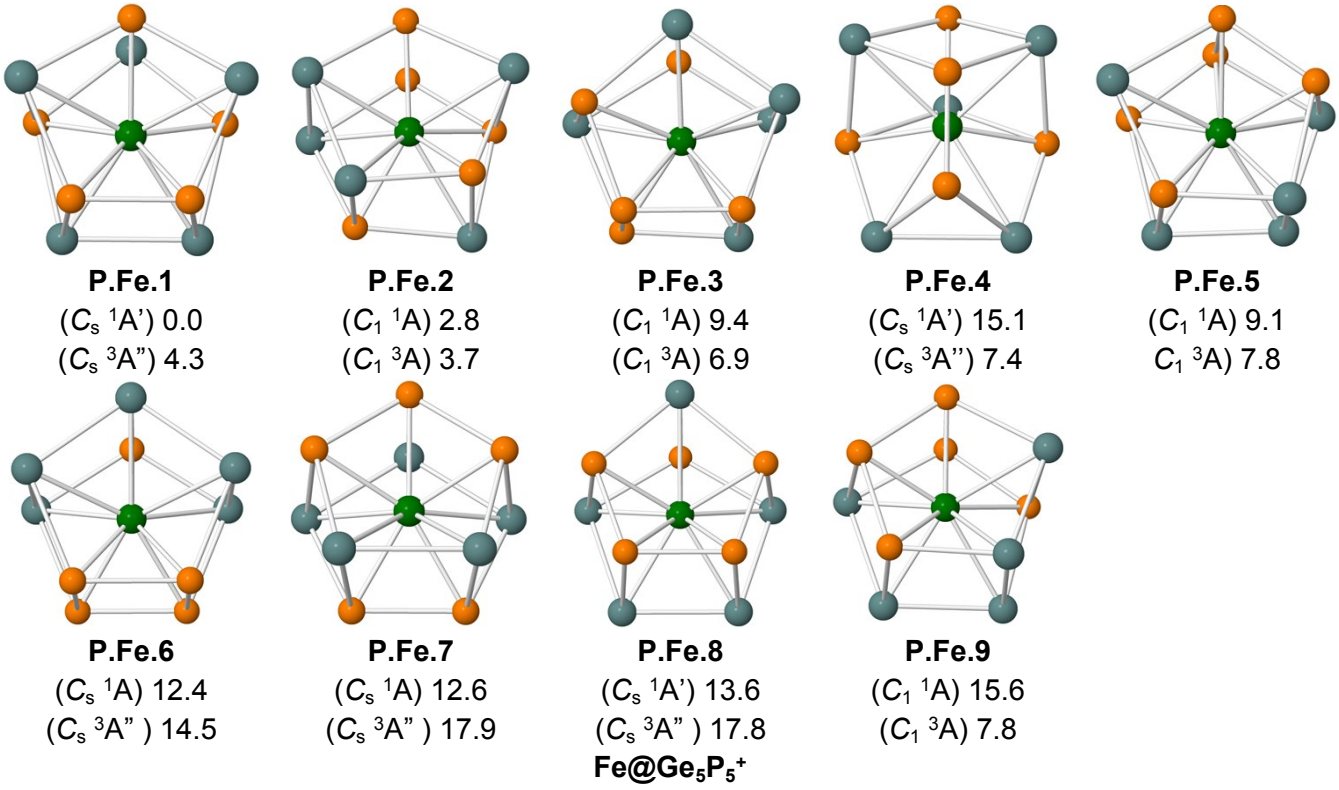


Figure S1. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $FeGe_5P_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge, P and aug-cc-pVTZ basis for Fe.

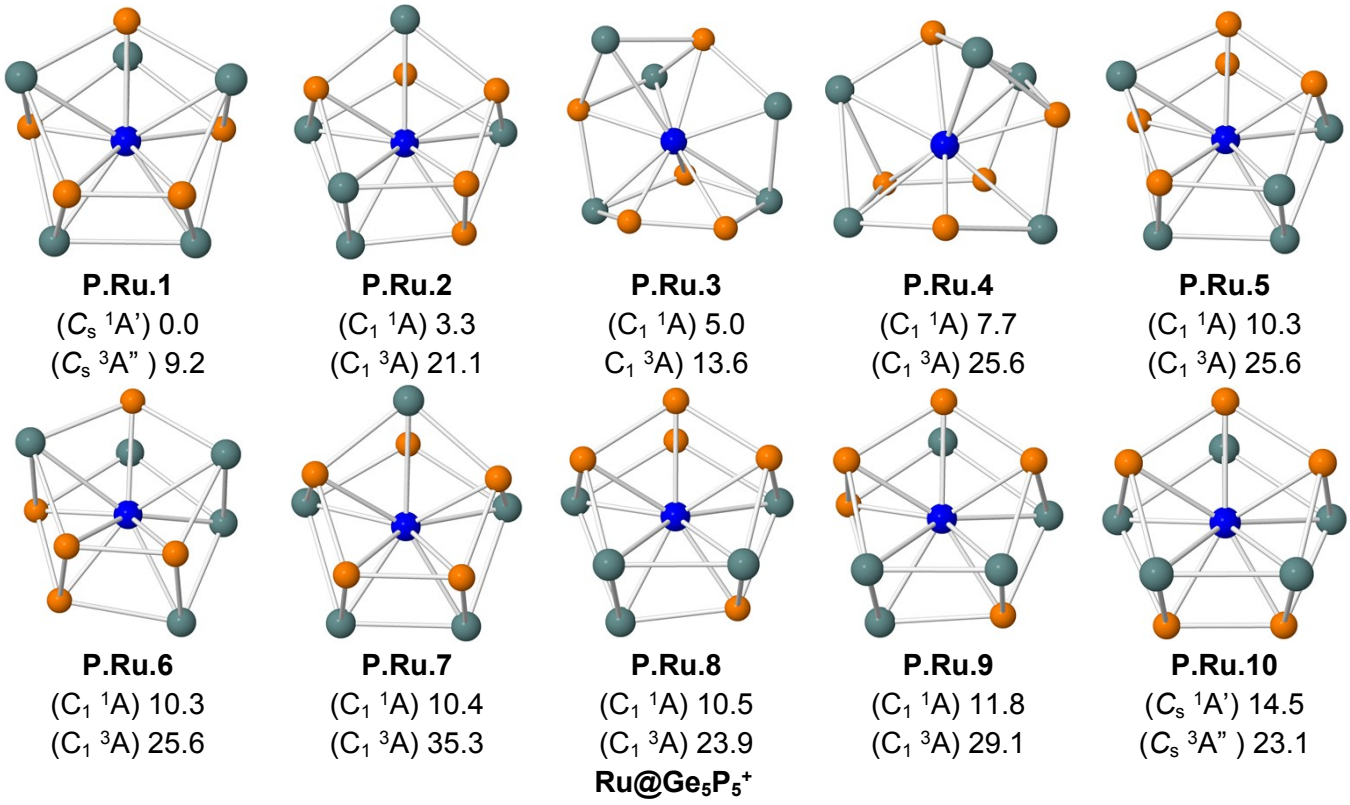


Figure S2. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $RuGe_5P_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,P and aug-cc-pVTZ-PP basis set for Ru.

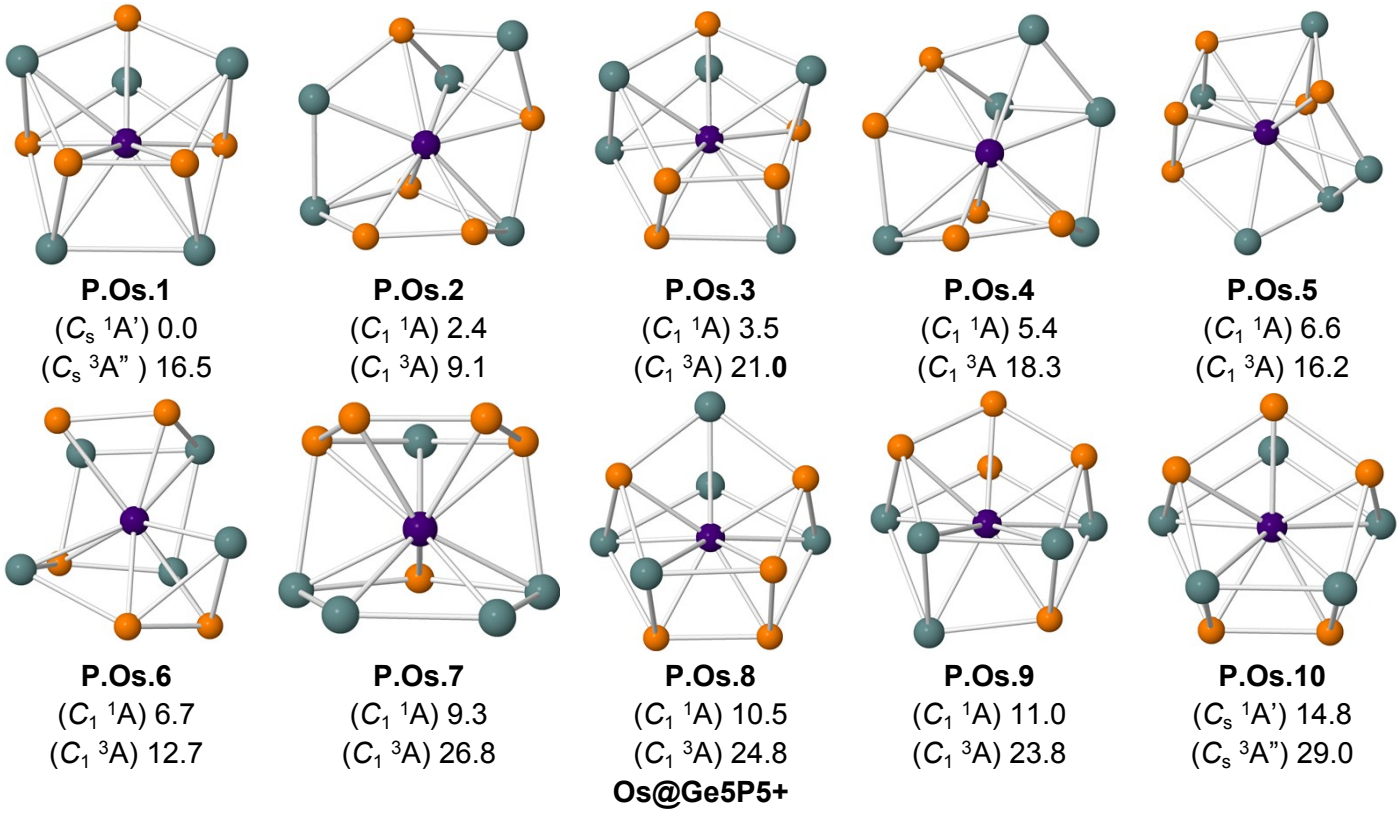
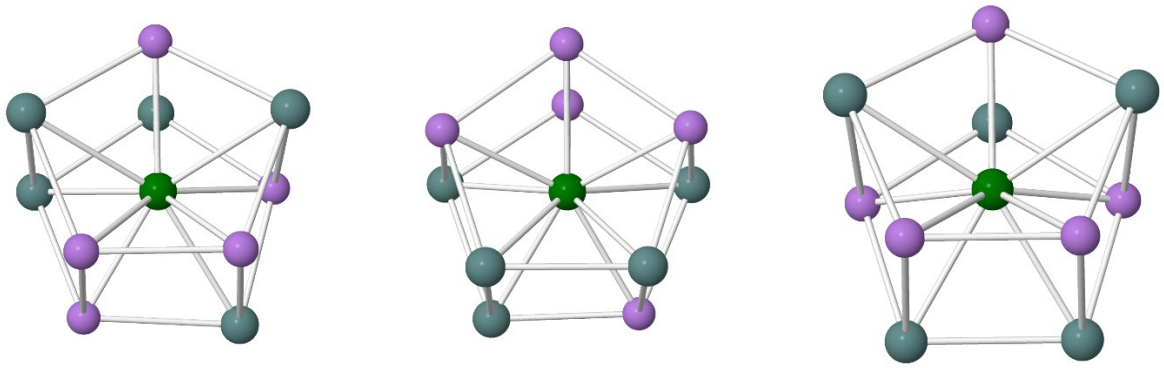


Figure S3. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $OsGe_5P_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,P and aug-cc-pVTZ-PP basis set for Os.



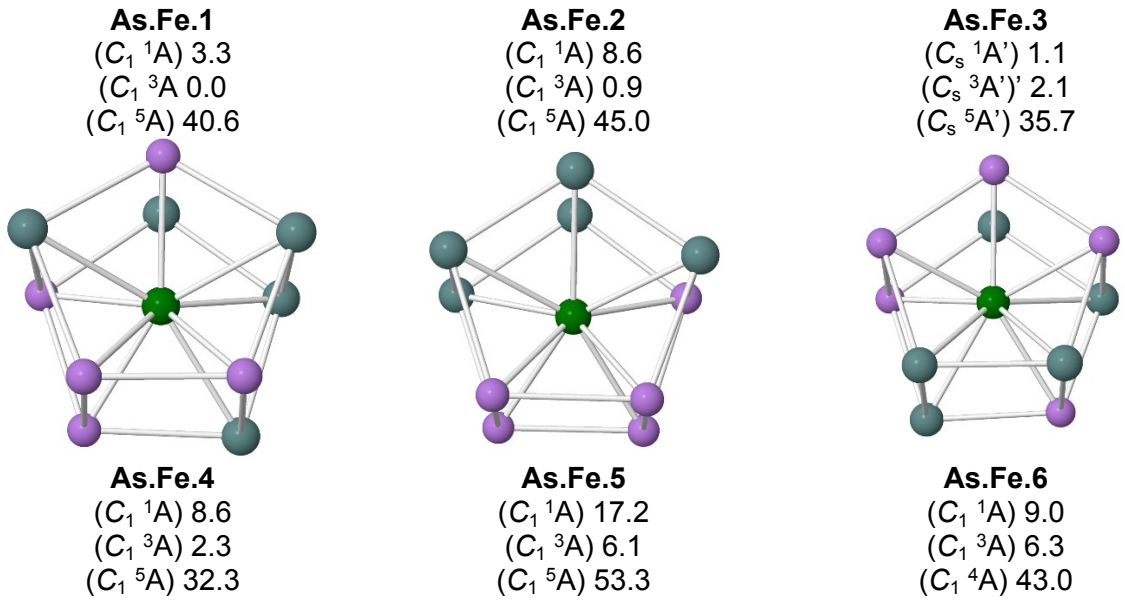
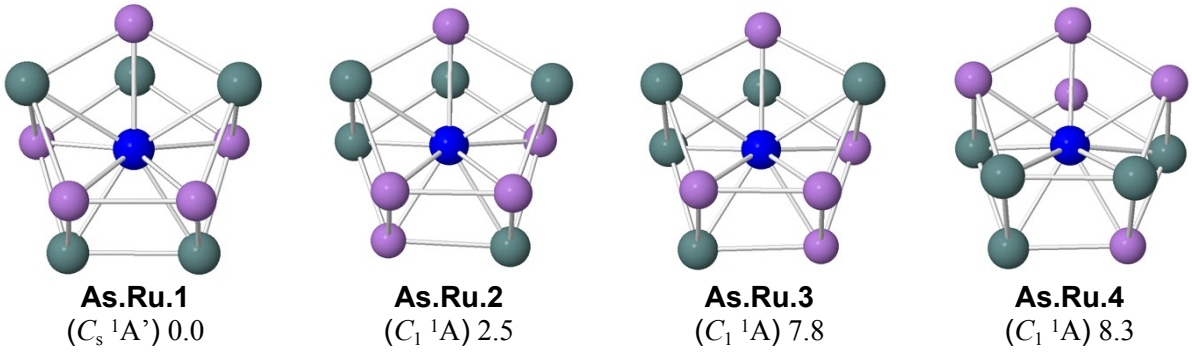


Figure S4. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $FeGe_5As_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,As and aug-cc-pVTZ basis set for Fe.



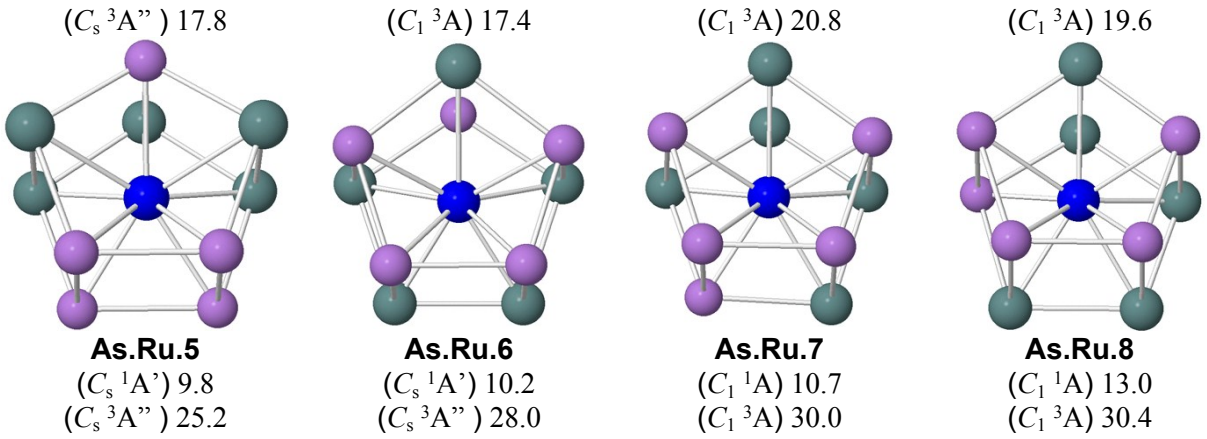
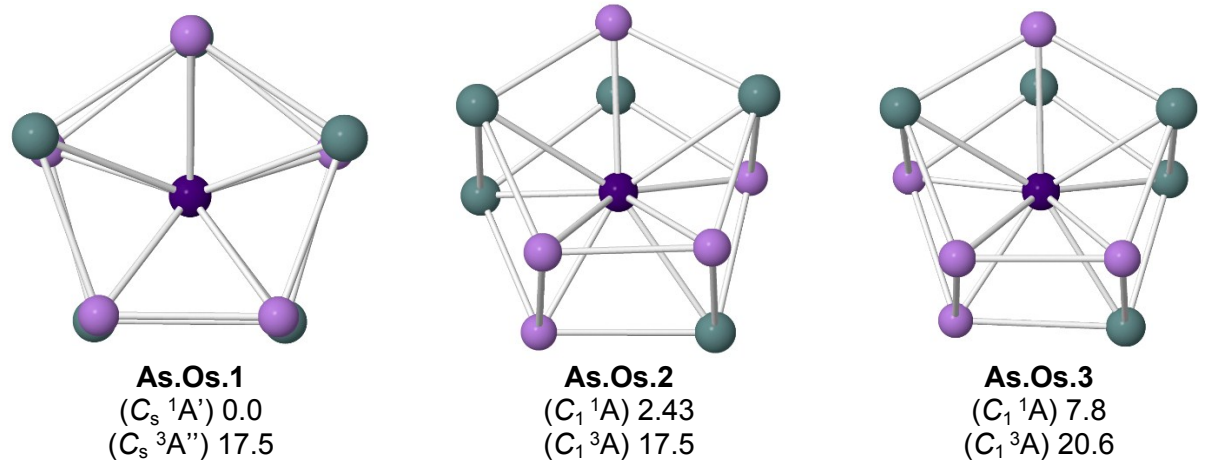
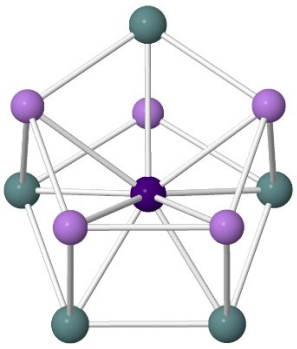


Figure S5. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $RuGe_5As_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis set for Ge,As and aug-cc-pVTZ-PP basis set for Ru.





GeAs.Os.5
(C_1 ^{1}A) 9.7
(C_1 ^{3}A) 25.0

Figure S6. Shapes, and relative energies (in kcal/mol) of the lower-lying isomer of $OsGe_5As_5^+$ cluster. The geometry optimizations and energy calculations were performed using B3P86 functional with 6-311+G(d) basis setfor Ge,As and aug-cc-pVTZ basis set for Os.

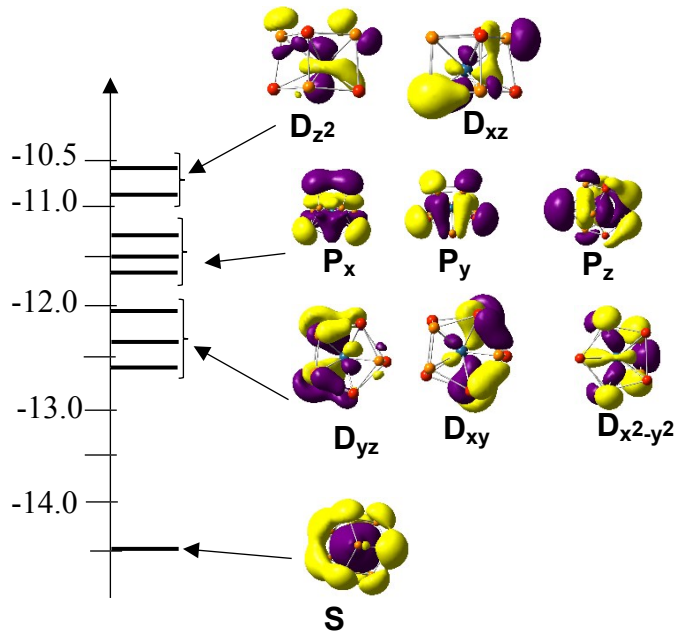


Figure S7. The MO diagram containing 18 electrons of $RuGe_5P_5^+$ structure.

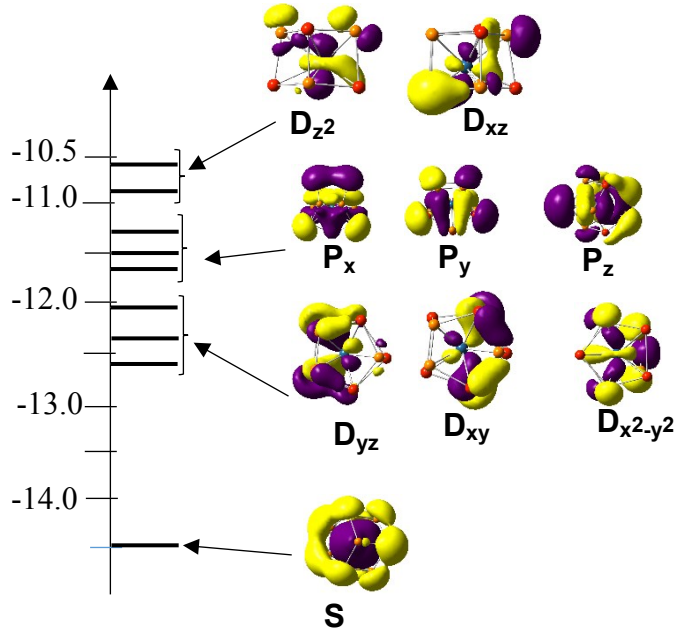


Figure S8. The MO diagram containing 18 electrons of $OsGe_5P_5^+$ structure.

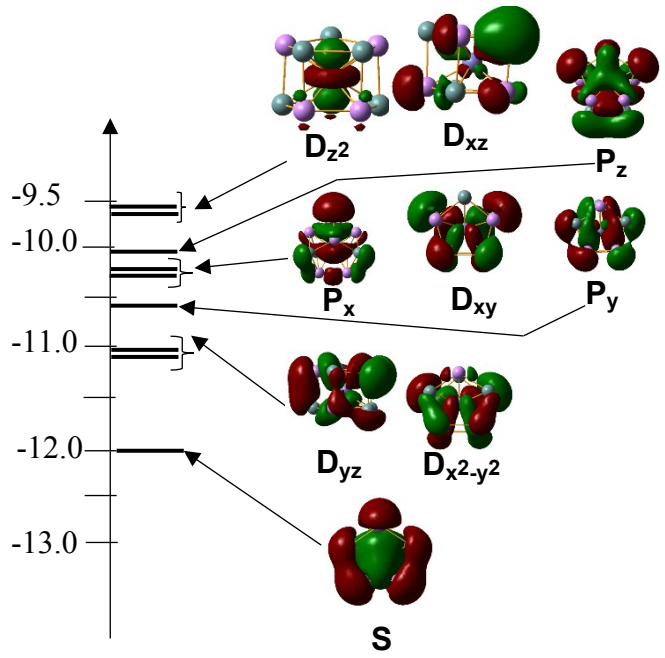


Figure S9. The MO diagram containing 18 electrons of $FeGe_5As_5^+$ structure.

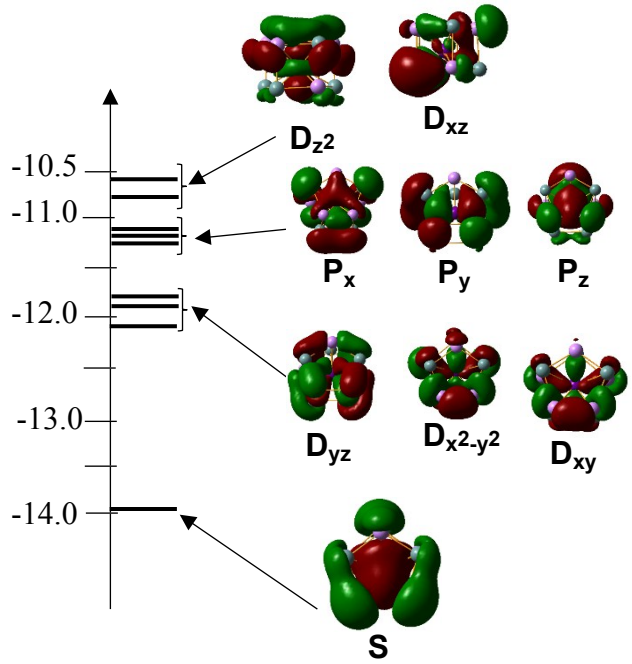


Figure S10. The MO diagram containing 18 electrons of $RuGe_5As_5^+$ structure.

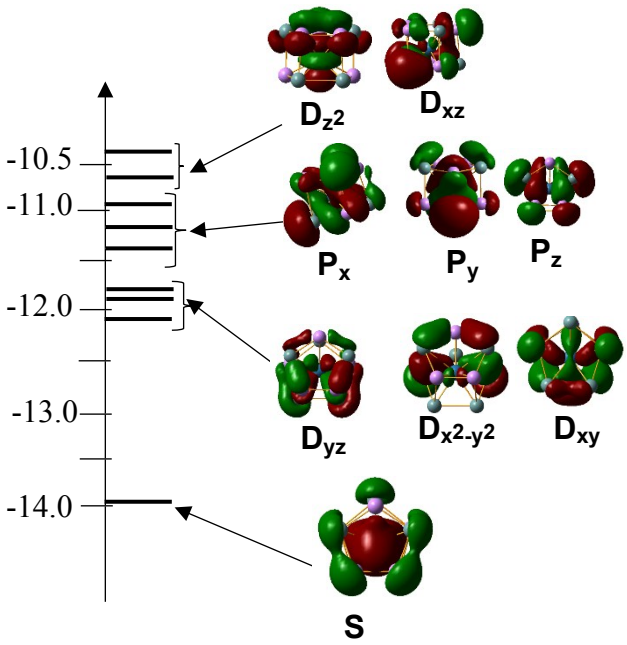


Figure S11. The MO diagram containing 18 electrons of $OsGe_5As_5^+$ structure.