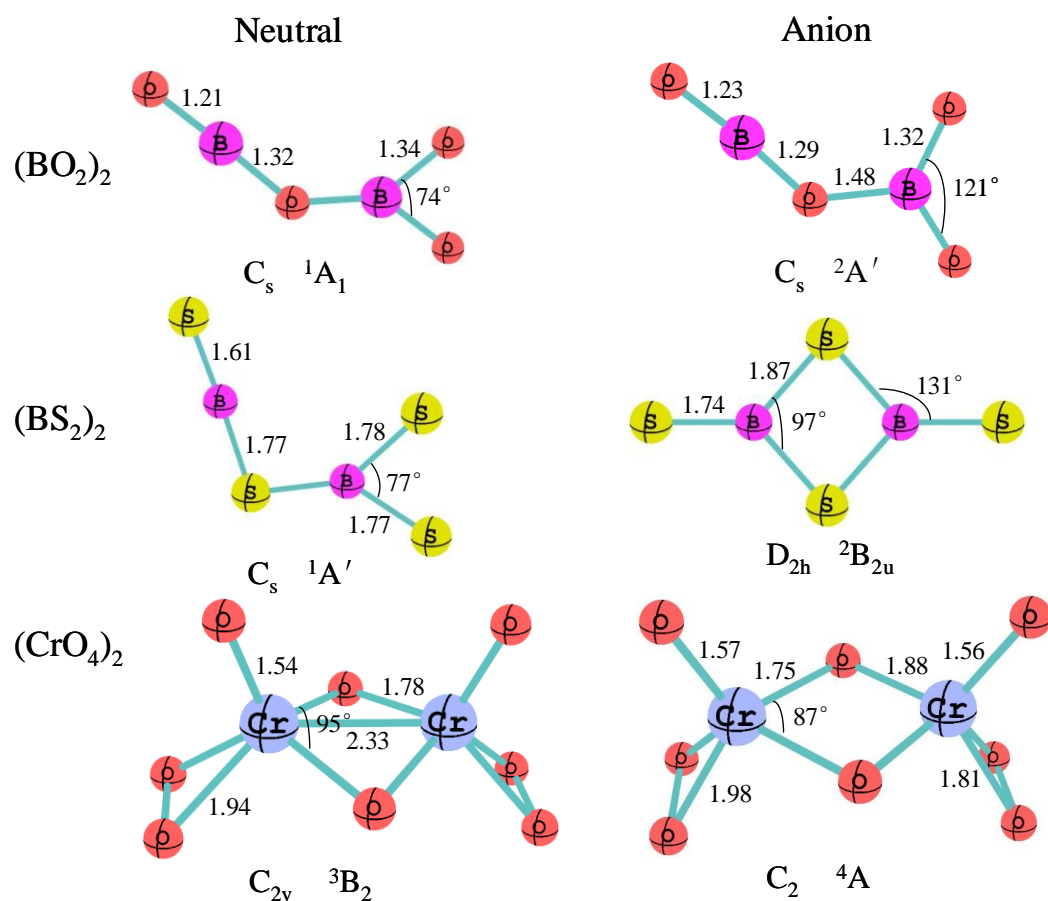


Theoretical search for potential candidates as building block of hyperhalogens: BS_2 and CrO_4 molecules

Supplementary Information

Li-Ping Ding,^a Xiao-Yu Kuang,^{a,*} Peng Shao,^a Ming-Min Zhong^a, Ya-Ru Zhao^b

Fig. S1 The low-lying isomer structures of neutral and anionic $(\text{BO}_2)_2$, $(\text{BS}_2)_2$ and $(\text{CrO}_4)_2$ clusters at B3LYP/6-311+G(3df) level. All the bond lengths are given in Å.



^a Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China

^b Department of Physics and Information Technology, Baoji University of Arts and Sciences, Baoji 721016, China.

*Correspondence to: Kuang Xiao-Yu, Institute of Atomic and Molecular Physics, Sichuan University, Chengdu 610065, China. Tel./fax: +86 28 85405515.

E-mail address: scu_kuang@163.com (X-Y Kuang).

Fig. S2 The low-lying isomer structures of neutral and anionic Au(BO₂)₂ clusters along with their geometrical parameters. All the bond lengths are given in Å.

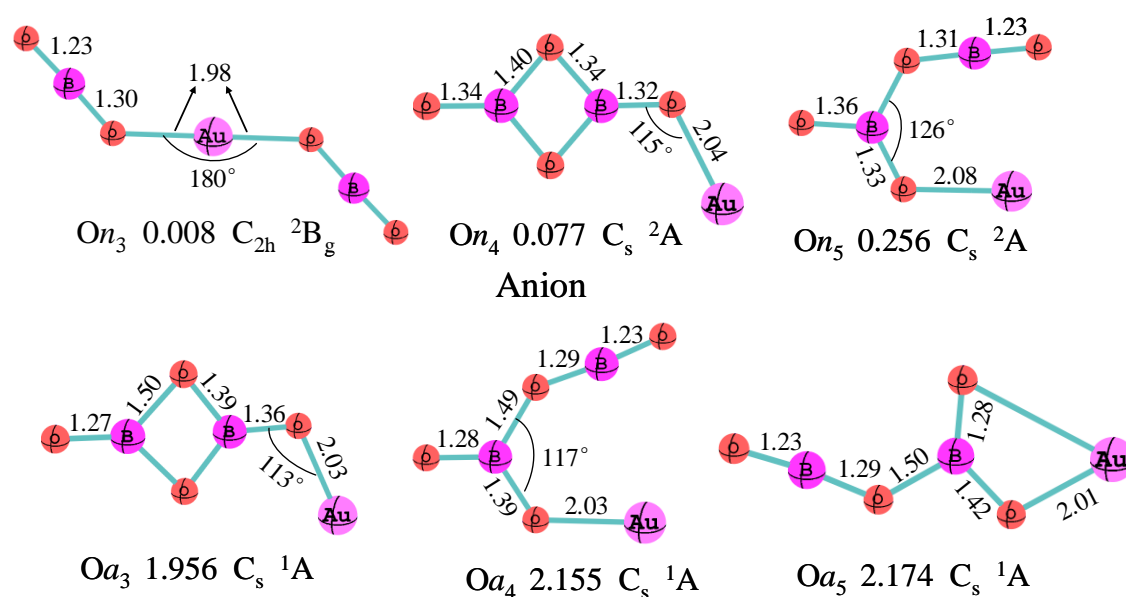


Fig. S3 The low-lying isomer structures of neutral and anionic Au(BS₂)₂ clusters along with their geometrical parameters. All the bond lengths are given in Å.

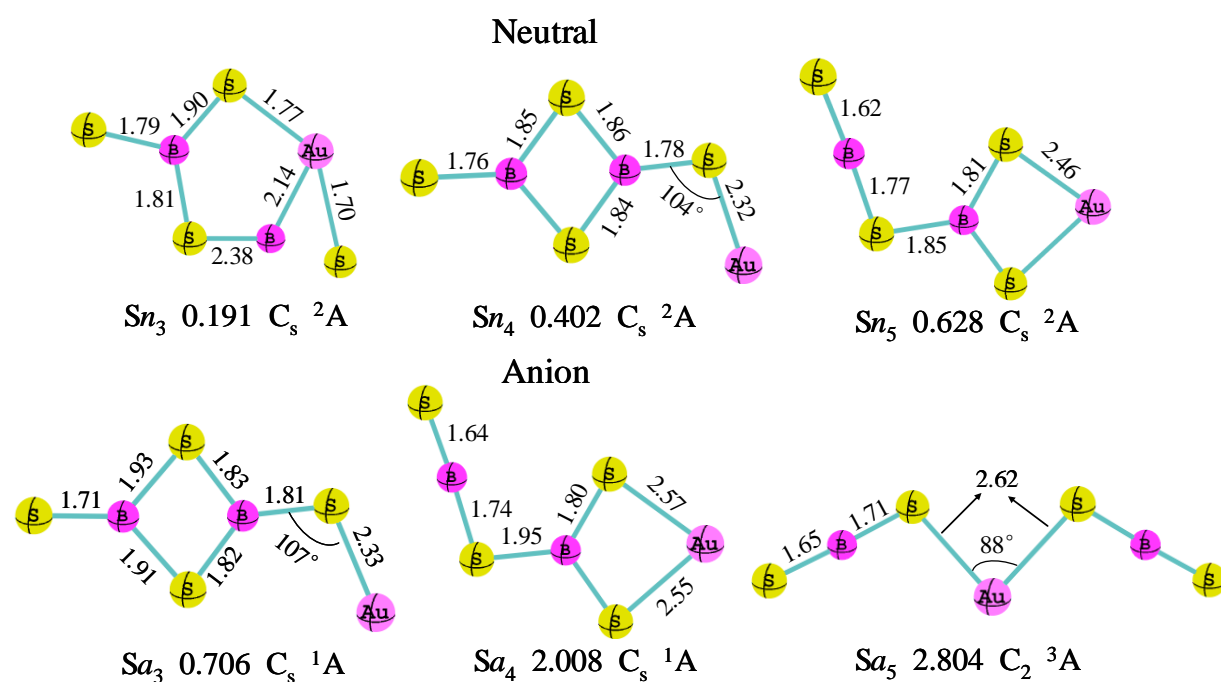


Fig. S4 The low-lying isomer structures of neutral and anionic $\text{Au}(\text{CrO}_4)_2$ clusters along with their geometrical parameters. All the bond lengths are given in Å.

