

$K^+[K(CO)_8]^-$: an antipodal crystalline salt of alkalide $[K(C222)]^+K^-$

xiaoyong yang¹

¹Qilu University of Technology

November 16, 2020

Abstract

Here we propose an antipodal conjecture, which is based on the synthetic scheme of alkalide $[K(C222)]^+K^-$, to prepare $K^+[K(CO)_8]^-$. By introducing the concept of antipodal salts of alkalides, $K^+[K(CO)_8]^-$ is defined as antipodal salt of $[K(C222)]^+K^-$. As Group 1 elements of the Periodic Table, the alkali metal K is conventionally considered to form chemical bonding through its 4s and 4p valence orbitals. Our theoretical results show that the 3d orbitals of K element in $>[K(CO)_8]^-$ participate in chemical bonding of $>[K(CO)_8]^-$. This makes the alkali metal K shows typical transition metal chemical properties, which also provides the possibility for the synthesis of $K^+[K(CO)_8]^-$. Based on the Born-Haber thermodynamic cycle, the upper-limit stable temperature of $K^+[K(CO)_8]^-$ is estimated to be 24.426 K. Our theoretical results indicate that antipodal salts of alkalides will be a new family of compounds with good synthetic prospects.

Hosted file

manuscript -IJQC.pdf available at <https://authorea.com/users/290682/articles/493211-k-k-co-8-an-antipodal-crystalline-salt-of-alkalide-k-c222-k>