

FULL PAPERS

强离子键体系电子相关能简捷计算方案的应用

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摘要 本文给出了KF和(KF)₂体系电子对相关能的计算结果, 探讨了1s_K²、1s_F²及K、

F组份内核相关效应分别在K、K⁺、KF和F、F⁻、KF体系中的传递性,

计算了K与F组份对KF分子体系相关能的贡献值。通过对强离子键体系电子相关能简捷计算方案在KF和(KF)₂

体系的计算结果, 说明该简捷计算方案不仅可以达到化学计算精度的要求而且需要很少的计算工作量。

关键词 [对内对间电子相关, 相关能贡献, 简捷计算方案](#)

分类号

Applications of Simple Estimation Scheme of Electron Correlation Energy to Strong Ionic Compounds

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Abstract The calculation results of electron correlation energies of KF and (KF)₂ were reported. The transferability of 1s_K², 1s_F² and the inner core correlation effects of K and F in both K, K⁺, KF and F, F⁻, KF systems were investigated respectively. The correlation energy contributions of K and F component to KF system were calculated. By applying the simple estimation scheme to the calculation of the correlation energy of the strong ionic compound KF and (KF)₂, it was shown that such a powerful scheme could not only reach the chemical accuracy but also need little computational work.

Key words [intrapair](#) [interpair electron correlation](#) [correlation energy contribution](#) [the simple estimation scheme](#)

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