Conversions of Localized Excess Electrons and Spin States under External Electric Field: Inter-Cage Electron-transfer Isomer $(C_{20}F_{20})_3$&K_2

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Abstract

By doping two potassium atoms among three $C_{20}F_{20}$ cages, peanut-shaped single molecular solvated dielectron $(C_{20}F_{20})_3$&K_2 was theoretically presented. The triplet structures with two excess electrons individually inside left and middle cages (isomers **I** or **II**) are thermodynamically more stable than both open-shell (OS) and close-shell (CS) singlet ones with lone pair of excess electrons inside middle cage. Applying an oriented external electric field (OEEF) of -20 × 10^{-4} au (-0.1018 V/Å) or a larger one can result in both left-to-right transfers of the two excess electrons, and then releasing the OEEF can form new kind of inter-cage electron-transfer isomers (**III** or **IV**). Each triplet **I** ~ **IV** with three redox sits may be new members of mixed-valent compounds, namely, Robin-Day Class II. For electrified **I** of $(C_{20}F_{20})_3$&K_2 , the following spin states are ground state: 1) triplet state in field ranges of -120 × 10^{-4} < F_x < -30 × 10^{-4} au and 30 × 10^{-4} < F^{-4} < 111 × 10^{-4} au; 2) CS singlet state in range of F_x [?] 111 x 10^{-4} and [?] -120 x 10^{-4} au; 3) OS singlet state in ranges of -30 x 10^{-4} [?] F_x [?] -5 x 10^{-4} au and 5 x 10^{-4} [?] F_x [?] 30 x 10^{-4} au.

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