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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November 20, 2020

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 \times 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 \rightarrow IV with three redox sites 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 \times 10^{-4} < F_x < -30 \times 10^{-4} au and 30 \times 10^{-4} < F_x < 111 \times 10^{-4} au; 2) CS singlet state in range of F_x \leq 111 \times 10^{-4} and F_x \geq -120 \times 10^{-4} au; 3) OS singlet state in ranges of -30 \times 10^{-4} < F_x < -5 \times 10^{-4} au and 5 \times 10^{-4} < F_x < 30 \times 10^{-4} au.

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(a) Diagram of molecular structures with labels for cage 1, cage 2, and cage 3, along with angles and distances labeled.

(b) Sequence of structures labeled I, II, III, and IV with connections indicated by arrows.

(a) HOMO, HOMOα, HOMOβ

(b) SOMO1, SOMO2

(c) Spin density