Supporting Information

Coupling of Two Curved Polyaromatic Radical-Anions:

Stabilization of Dimer by Counterions

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Table S1. Absolute energies for all systems under consideration at PBE0/cc-pVDZ(C,H,O)//def2-TZVP(Cs) level of theory.

System	Energy, a.u.
$[(Cs^+)_2(18C6)_2\{(C_{28}H_{14})_2^{2-}\}]$	-4033.072493646
$[(Cs^+)_2(diglyme)_4\{(C_{28}H_{14})_2^{2-}\}]$	-4037.7913202669
$[(Cs^+)_2\{(C_{28}H_{14})_2^{2-}\}]$	-2188.9726627062
$(C_{28}H_{14})_2^{2-}$	-2148.5853290382
$[(Cs^+)(18C6)\{(C_{28}H_{14})^-\}]$	-2016.5281455409
$[(Cs^+)(diglyme)_2\{(C_{28}H_{14})^-\}]$	-2018.8869382208
$[(Cs^+)\{(C_{28}H_{14})^-\}]$	-1094.4754275893
$(C_{28}H_{14})^-$	-1074.3185777516
$[(Cs^+)_2(18C6)_2\{(C_{20}H_{10})_2^{2-}\}]$	-3419.1124435815
$[(Cs^+)_2(diglyme)_4\{(C_{20}H_{10})_2^{2-}\}]$	-3423.8296987797
$[(Cs^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-1575.0211338753
$(C_{20}H_{10})_2^{2-}$	-1534.6153554856
$[(Cs^+)(18C6)\{(C_{20}H_{10})^-\}]$	-1709.5485860056
$[(Cs^+)(diglyme)_2\{(C_{20}H_{10})^-\}]$	-1711.9083483116
$[(Cs^+)\{(C_{20}H_{10})^-\}]$	-787.5006656103
$(C_{20}H_{10})^-$	-767.3374308988
$[(Li^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-1550.0050909929
$[(Na^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-1859.3783520144
$[(K^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-2734.5357712758
$[(Rb^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-1583.2171957478
$[(Li^+)\{(C_{20}H_{10})^-\}]$	-774.9851710864
$[(Na^+)\{(C_{20}H_{10})^-\}]$	-929.6761665696
$[(K^+)\{(C_{20}H_{10})^-\}]$	-1367.2586915055
$[(Rb^+)\{(C_{20}H_{10})^-\}]$	-791.6005293487
$[(Li^+)_2\{(C_{28}H_{14})_2^{2-}\}]$	-2164.0884941124
$[(Na^+)_2\{(C_{28}H_{14})_2^{2-}\}]$	-2473.4625486566
$[(K^+)_2\{(C_{28}H_{14})_2^{2-}\}]$	-3348.6199771188

$[(Rb^+)_2\{(C_{28}H_{14})_2^{2-}\}]$	-2197.3018439256
$[(Li^+)\{(C_{28}H_{14})^-\}]$	-1082.0264214623
$[(Na^+)\{(C_{28}H_{14})^-\}]$	-1236.7173763050
$[(K^+)\{(C_{28}H_{14})^-\}]$	-1674.2998667380
$[(Rb^+)\{(C_{28}H_{14})^-\}]$	-1098.6418419983
$[(Li^+)_2(diglyme)_4\{(C_{20}H_{10})_2^{2-}\}]$	-3399.4003788767
$[(Li^+)(diglyme)_2\{(C_{20}H_{10})_2^-\}]$	-1699.6975212547
$[(N(CH_3)_4^+)_2\{(C_{20}H_{10})_2^{2-}\}]$	-1963.2110231826
$[(N(CH_3)_4^+)\{(C_{20}H_{10})_2^-\}]$	-981.6023621402

a)   **b)**

$[\{(P(CH_3)_4^+\}(C_{20}H_{10}^-)]$ $[\{(P(CH_3)_4^+\}(C_{28}H_{14}^-)]$
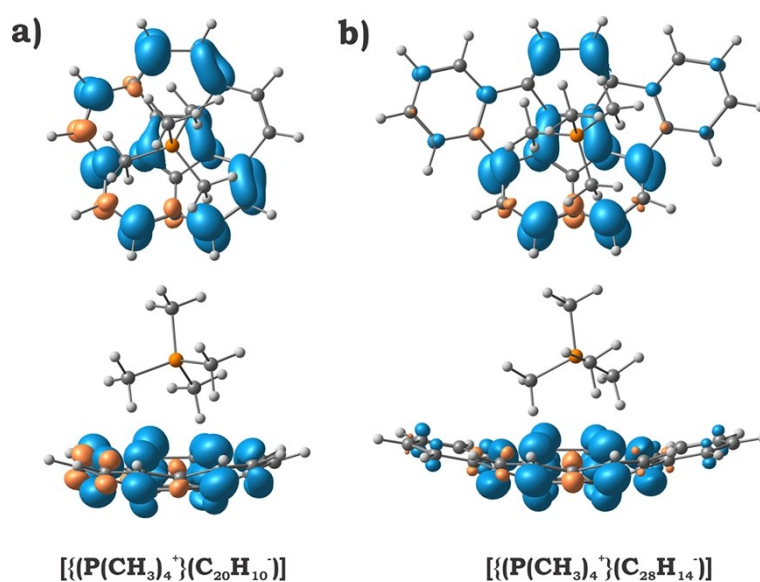
Figure S1. Spin density distribution (isosurface level 0.0035 a.u.) in corannulene-based (*a*) and dibenzo[*a,g*]corannulene-based (*b*) solvent-separated ion pairs $[\{(P(CH_3)_4^+\}(PAH^-)]$ (PBE0/cc-pVTZ(C,H,O,P)).