Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material: Caged-electron States and Split-electron States in Endohedral Alkali C_{60}

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Table 1. Cartesian coordinates of the X@$C_{60}(I_h)$ used in the EA-EOM-CCSD calculation. Units in Angstrom.

X@$C_{60}(I_h)$	X	0.00000000	0.00000000	0.00000000
	C	2.312979	2.609047	-0.729000
	C	-2.312979	-2.609047	-0.729000
	C	-2.312979	2.609047	0.729000
	C	2.312979	-2.609047	0.729000
	C	-2.312979	-2.609047	0.729000
	C	2.312979	2.609047	0.729000
	C	2.312979	-2.609047	-0.729000
	C	-2.312979	2.609047	-0.729000
	C	3.041979	1.429500	1.179547
	C	-3.041979	-1.429500	1.179547
	C	-3.041979	1.429500	-1.179547
	C	3.041979	-1.429500	-1.179547
	C	-3.041979	-1.429500	-1.179547
	C	3.041979	1.429500	-1.179547
	C	3.041979	-1.429500	1.179547
	C	-3.041979	1.429500	1.179547
	C	3.492526	0.700500	0.000000
	C	-3.492526	-0.700500	0.000000
	C	-3.492526	0.700500	0.000000
	C	3.492526	-0.700500	0.000000
	C	2.609047	0.729000	-2.312979
	C	-2.609047	-0.729000	-2.312979
	C	-2.609047	0.729000	2.312979
	C	2.609047	-0.729000	2.312979
	C	-2.609047	-0.729000	2.312979
	C	2.609047	0.729000	2.312979
	C	2.609047	-0.729000	-2.312979
	C	-2.609047	0.729000	-2.312979
	C	1.429500	1.179547	3.041979
	C	-1.429500	-1.179547	3.041979
	C	-1.429500	1.179547	-3.041979
	C	1.429500	-1.179547	-3.041979
	C	-1.429500	-1.179547	-3.041979
	C	1.429500	1.179547	-3.041979
	C	1.429500	-1.179547	3.041979
	C	-1.429500	1.179547	3.041979
	C	0.729000	2.312979	2.609047
	C	-0.729000	-2.312979	2.609047

Table 1. (continued)

$X@C_{60}(I_h)$	C	-0.729000	2.312979	-2.609047
	C	0.729000	-2.312979	-2.609047
	C	-0.729000	-2.312979	-2.609047
	C	0.729000	2.312979	-2.609047
	C	0.729000	-2.312979	2.609047
	C	-0.729000	2.312979	2.609047
	C	1.179547	3.041979	1.429500
	C	-1.179547	-3.041979	1.429500
	C	-1.179547	3.041979	-1.429500
	C	1.179547	-3.041979	-1.429500
	C	-1.179547	-3.041979	-1.429500
	C	1.179547	3.041979	-1.429500
	C	1.179547	-3.041979	1.429500
	C	-1.179547	3.041979	1.429500
	C	0.000000	3.492526	0.700500
	C	0.000000	-3.492526	0.700500
	C	0.000000	3.492526	-0.700500
	C	0.000000	-3.492526	-0.700500
	C	-0.700500	0.000000	3.492526
	C	0.700500	0.000000	3.492526
	C	0.700500	0.000000	-3.492526
	C	-0.700500	0.000000	-3.492526

Figure S1.

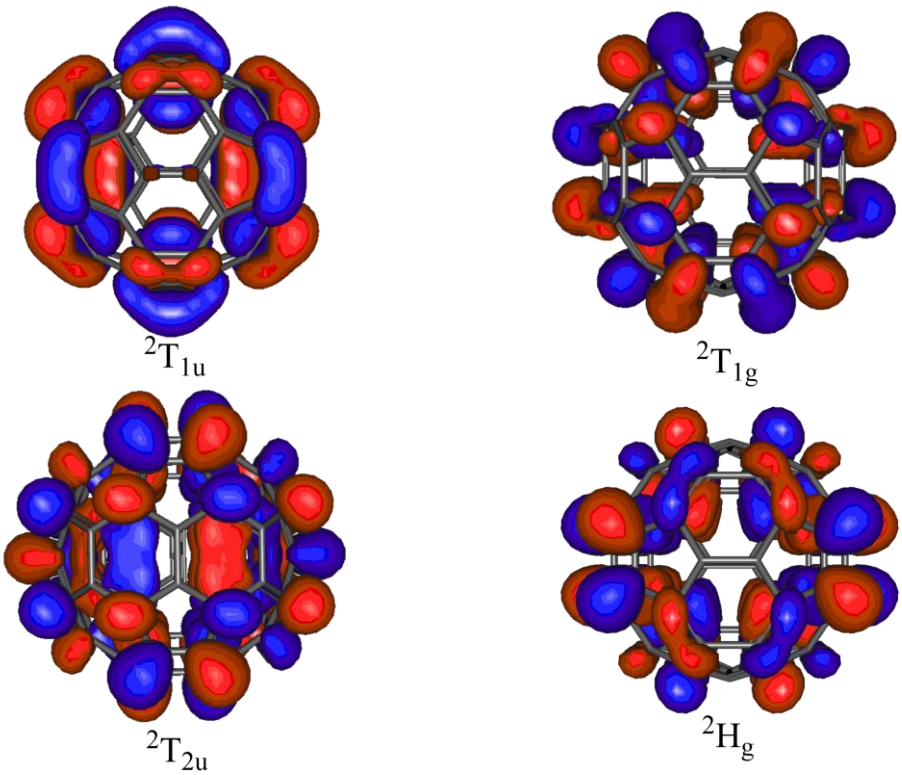

Figure S1. Image of the singly occupied natural orbitals of the valence charge-separated states of X@C_{60}. The surfaces shown enclose 80% of the electron density.

Figure S2.

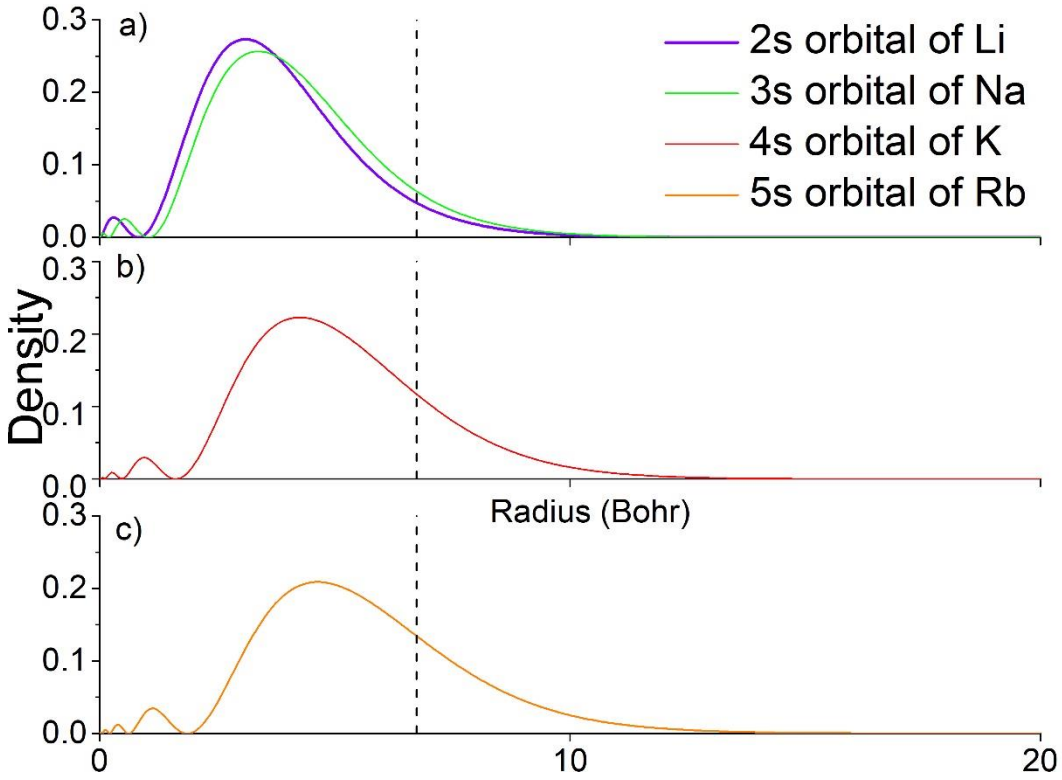

Figure S2. Radial distributions of the electron density of the singly occupied natural orbital of isolated alkali atoms. (a) 2s orbital of Li and 3s orbital of Na. (b) 4s orbital of K. (c) 5s orbital of Rb. The vertical dashed line indicates the radius of the carbon cage.

Figure S3.

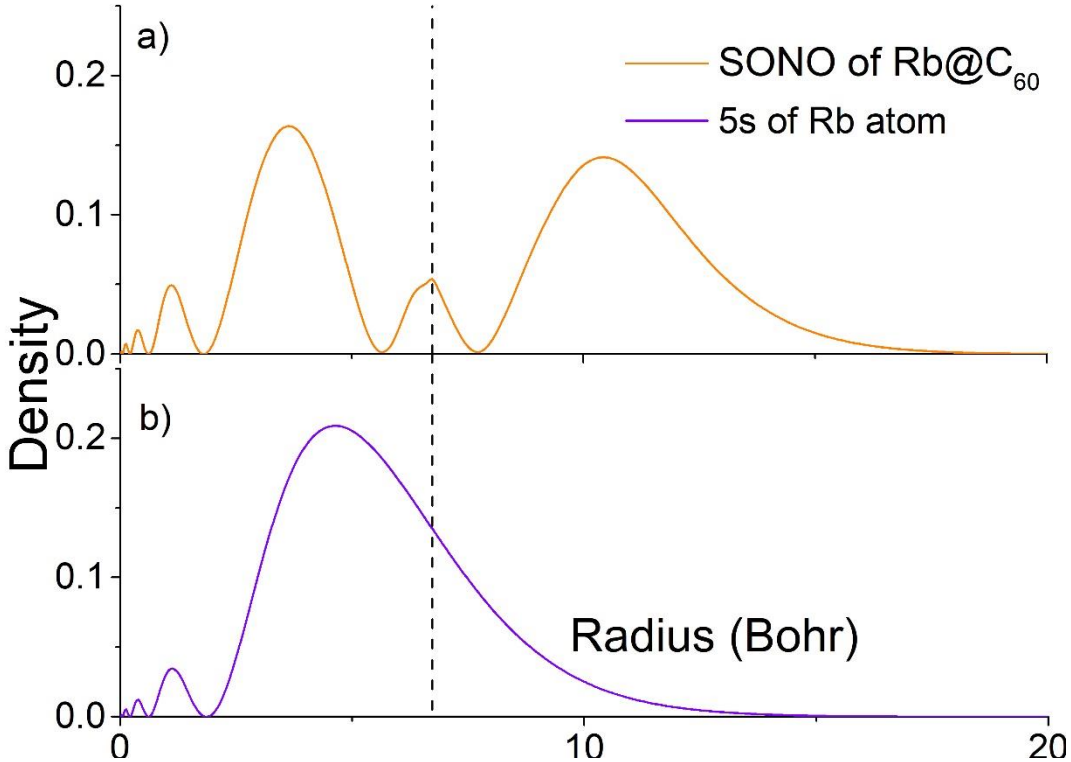

Figure S3. Radial distributions of the electron density of the singly occupied natural orbital of (a) split-electron state of $Rb@C_{60}$, (b) 5s orbital of isolated Rb with four nodes. The vertical dashed line indicates the radius of the carbon cage.