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Dative versus electron-sharing bonding in the isoelectronic argon compounds ArR^+ (R = CH_3, NH_2, OH, F)

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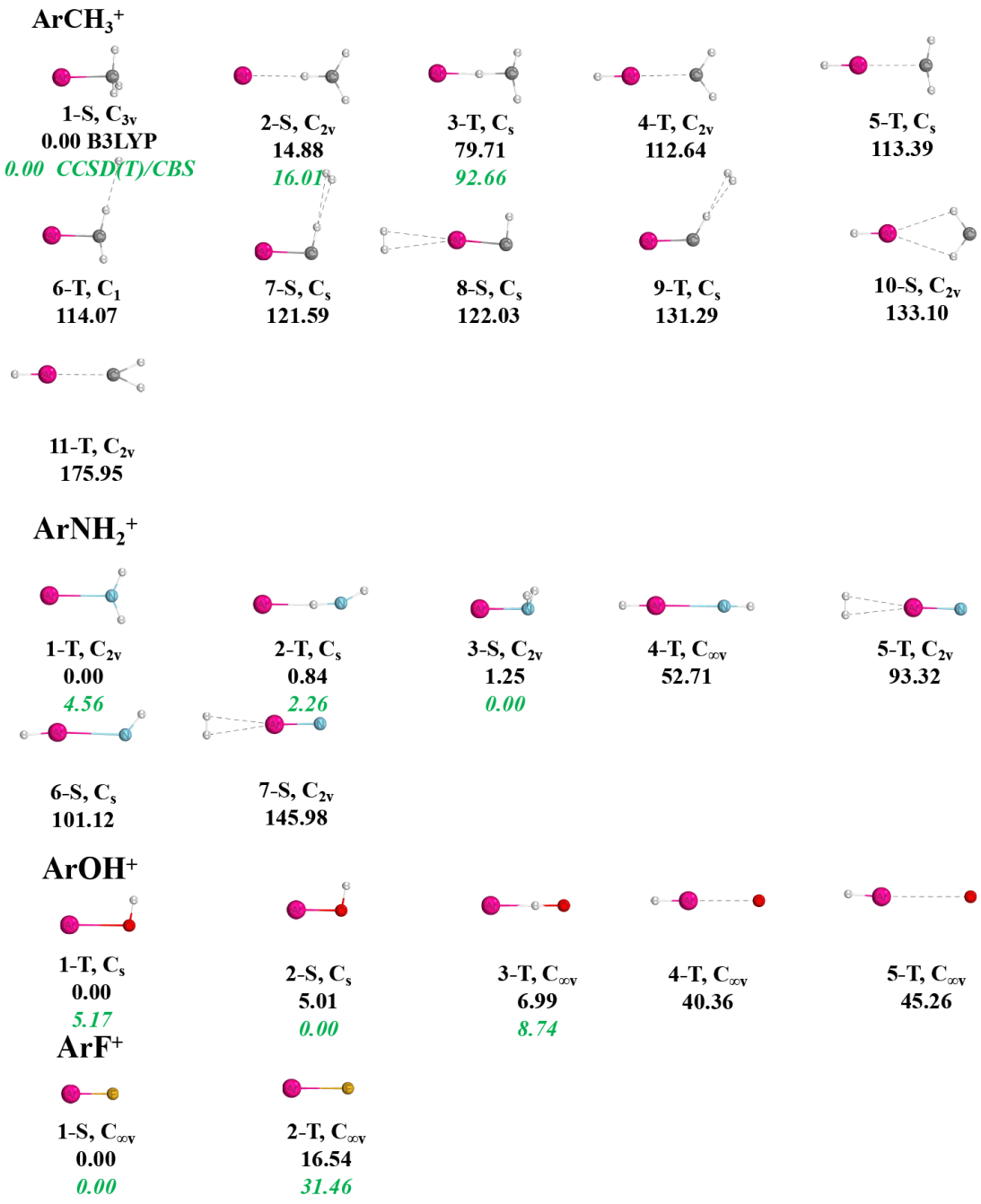

Figure S1. Optimized low-lying geometries of ArR^+ cations (R = CH_3, NH_2, OH, F) at the B3LYP-D3(BJ)/aug-cc-pVTZ level. The symmetries and relative energies (in kcal·mol^{-1}) relative to the ground-state anion are indicated. The numbers in *italic* are the relative energies calculated at CCSD(T)/CBS//B3LYP-D3(BJ)/aug-cc-pVTZ level. The letters **S** and **T** behind the serial number stand for the singlet and triplet electronic states, respectively.

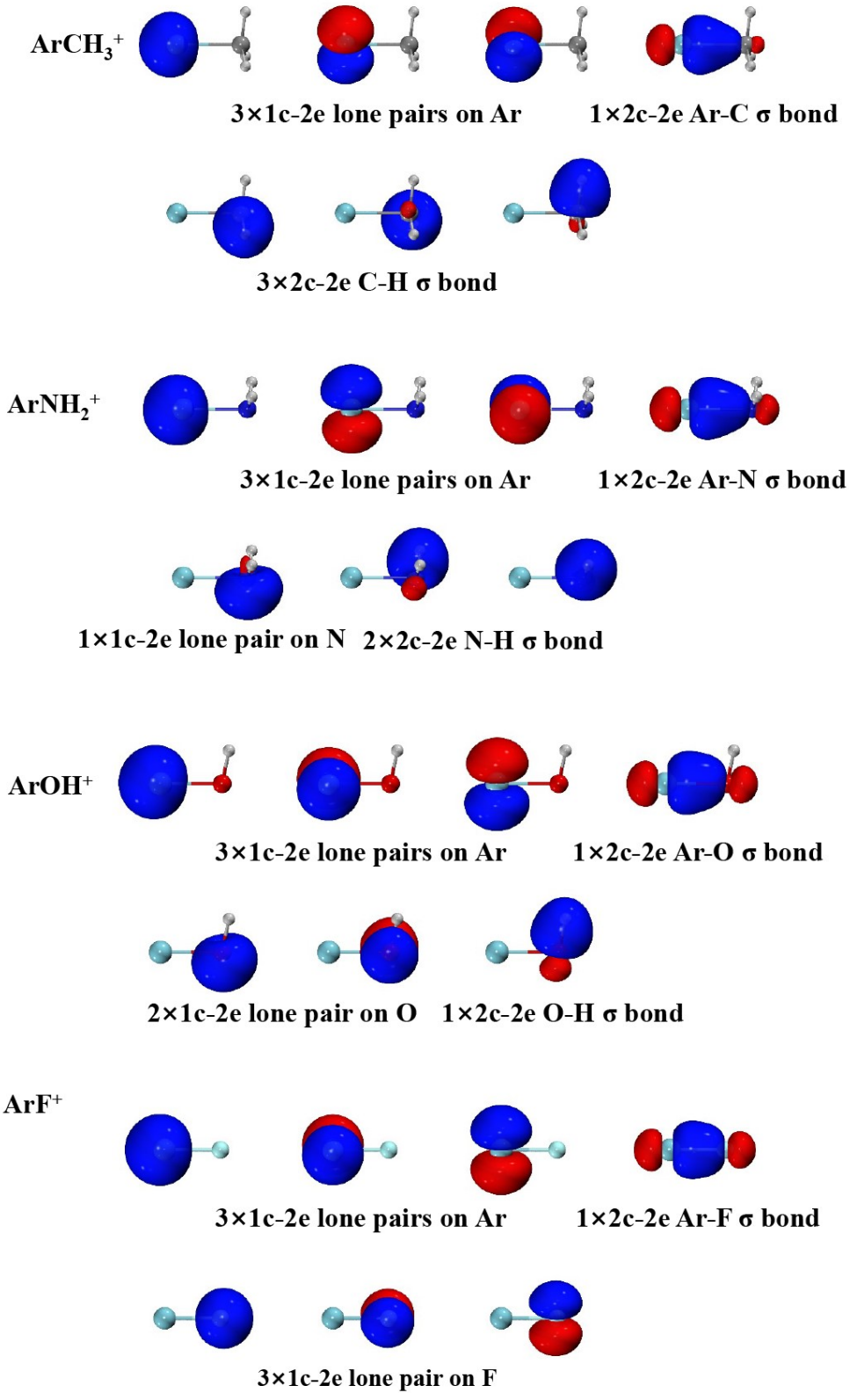

Figure S2. The NLMO analysis for the lowest singlet ArR^+ cations (R = CH_3, NH_2, OH, F) at the B3LYP-D3(BJ)/aug-cc-pVTZ level. (isosurface = 0.08 a.u.)

The cartesian coordinates of the lowest singlet ArR^+ (R = F, OH, NH_2, CH_3) complexes at the B3LYP-D3(BJ)/aug–cc–pVTZ level of theory.

$ArCH_3^+$

Ar	0.000000000000	0.000000000000	0.702254000000
C	0.000000000000	0.000000000000	-1.354393000000
H	0.000000000000	1.072941000000	-1.504737000000
H	0.929194000000	-0.536471000000	-1.504737000000
H	-0.929194000000	-0.536471000000	-1.504737000000

$ArNH_2^+$

Ar	-0.044788000000	-0.646804000000	0.000000000000
N	-0.044788000000	1.264386000000	0.000000000000
H	0.559849000000	1.395884000000	0.829016000000
H	0.559849000000	1.395884000000	-0.829016000000

$ArOH^+$

Ar	0.036063000000	-0.589928000000	0.000000000000
O	0.036063000000	1.158332000000	0.000000000000
H	-0.937647000000	1.352049000000	0.000000000000

ArF^+

Ar	0.000000000000	0.000000000000	0.544661000000
F	0.000000000000	0.000000000000	-1.089322000000