SUPPORTING INFORMATION

Same but Different:
Dipole-Stabilized Shape Resonances in CuF^- and AgF^-

Thomas-C. Jagau[a], Diep B. Dao[b], Nicholas S. Holtgrewe[b], Anna I. Krylov[a], Richard Mabbs[b]

[a]Department of Chemistry, University of Southern California, Los Angeles, California 90089, USA

[b]Department of Chemistry, Washington University in St. Louis, St. Louis, Missouri 63130, USA

I. ADDITIONAL EXPERIMENTAL RESULTS

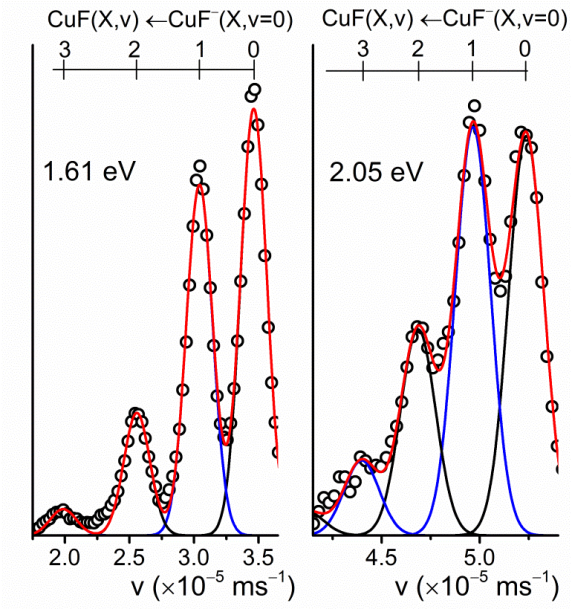

FIG. S1: Photoelectron spectra for CuF^- detachment at 1.61 eV and 2.05 eV in a selected region of the velocity domain. The series of peaks corresponds to detachment via different vibrational levels of the neutral CuF X $^1\Sigma^+$ ground state. All vibrational features in these spectra are sufficiently resolved for vibration-specific analysis. The spectra are integrated over all angles, hence the transition β values do not affect the relative intensities of the transitions.

II. ADDITIONAL THEORETICAL RESULTS

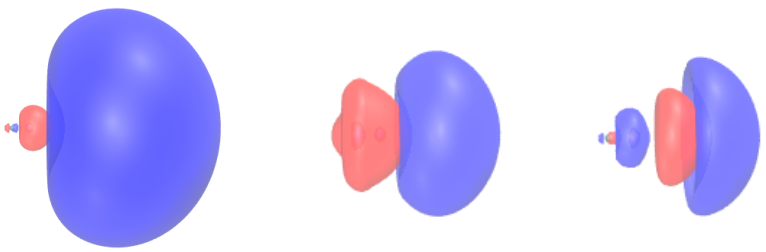

FIG. S2: : Hartree-Fock orbitals dominating the dipole bound 1 $^2\Sigma^+$ state of AgF^- obtained from CAP-free (left) and CAP-augmented (η = 0.0020 a.u., center: real part, right: imaginary part) calculations. Basis set: aug-cc-pVTZ-PP+6s6p3d, R(AgF) = 2.107894 Å, isovalue = 0.002.

TABLE S1: Absolute energies and attachment energies for the X $^2\Sigma^+$ ground state and the 1 $^2\Sigma^+$ dipole bound state of CuF^- as a function of bond distance computed by EOM-EA- CCSD/aug-cc-pVTZ+6s6p3d. Absolute energies for the X $^1\Sigma^+$ ground state of neutral CuF computed by CCSD/aug-cc-pVTZ+6s6p3d are also given.

	X $^1\Sigma^+$	X $^2\Sigma^+$		1 $^2\Sigma^+$	
R(CuF)/Å	E/a.u.	E/a.u.	ΔE/eV	E/a.u.	ΔE/eV
1.666437	-1739.162335	-1739.191743	-0.8002	-1739.162517	-0.0050
1.766437	-1739.167770	-1739.201813	-0.9264	-1739.168074	-0.0083
1.780034	-1739.167834	—	—	—	—
1.782057	-1739.167832	-1739.202609	-0.9463	-1739.168157	-0.0089
1.866437	-1739.165625	-1739.204423	-1.0557	-1739.166084	-0.0125
1.868563	-1739.165523	-1739.204424	-1.0585	—	—
1.966437	-1739.159127	-1739.202811	-1.1887	-1739.159781	-0.0178
2.066437	-1739.150242	-1739.198929	-1.3248	-1739.151140	-0.0244

Core electrons were not included in the correlation treatment. For technical reasons, g functions were removed from the basis set.

TABLE S2: Absolute energies and attachment energies for the X $^2\Sigma^+$ ground state and the 1 $^2\Sigma^+$ dipole bound state of CuF^- as a function of bond distance computed by EOM-EA- CCSD/aug-cc-pVTZ-PP+6s6p3d. Absolute energies for the X $^1\Sigma^+$ ground state of neutral CuF computed by CCSD/aug-cc-pVTZ-PP+6s6p3d are also given.

	X $^1\Sigma^+$	X $^2\Sigma^+$		1 $^2\Sigma^+$	
R(CuF)/Å	E/a.u.	E/a.u.	ΔE/eV	E/a.u.	ΔE/eV
1.666437	-296.712138	-296.742938	-0.8381	-296.712304	-0.0045
1.752240	-296.715399	—	—	—	—
1.753000	-296.715399	-296.750621	-0.9585	-296.715683	-0.0077
1.766437	-296.715320	-296.751232	-0.9772	-296.715616	-0.0080
1.839200	-296.712924	-296.752588	-1.0793	—	—
1.866437	-296.711337	-296.752417	-1.1178	-296.711789	-0.0123
1.966437	-296.703346	-296.749675	-1.2607	-296.704304	-0.0261
2.066437	-296.693250	-296.744903	-1.4055	-296.694160	-0.0247

See below for details of the basis set.

TABLE S3: Absolute energies and attachment energies for the X $^2\Sigma^+$ ground state and the 1 $^2\Sigma^+$ dipole bound state of AgF^- as a function of bond distance computed by EOM-EA- CCSD/aug-cc-pVTZ-PP+6s6p3d. Absolute energies for the X $^1\Sigma^+$ ground state of neutral AgF computed by CCSD/aug-cc-pVTZ-PP+6s6p3d are also given.

	X $^1\Sigma^+$	X $^2\Sigma^+$		1 $^2\Sigma^+$	
R(AgF)/Å	E/a.u.	E/a.u.	ΔE/eV	E/a.u.	ΔE/eV
1.907894	-246.447659	-246.490326	-1.1610	-246.448027	-0.0100
1.986178	-246.449623	—	—	—	—
1.988072	-246.449622	-246.496616	-1.2788	-246.450140	-0.0141
2.007894	-246.449477	-246.497543	-1.3079	-246.450033	-0.0151
2.107894	-246.446098	-246.499589	-1.4556	-246.446891	-0.0216
2.113760	-246.445787	-246.499597	-1.4642	—	—
2.207894	-246.439625	-246.498556	-1.6036	-246.440706	-0.0294
2.307894	-246.431424	-246.495785	-1.7513	-246.432851	-0.0388

See below for details of the basis set.

TABLE S4: Absolute energies, resonance positions and widths, as well as optimal CAP strengths for the 2 $^2\Sigma^+$ and the 1 $^2\Pi$ resonance state of CuF^- as a function of bond distance computed by CAP-EOM-EA-CCSD/aug-cc-pVTZ+6s6p3d.

	Zeroth-order values				First-order values			
R(CuF)/Å	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.
	2 $^2\Sigma^+$ resonance							
1.666437	-1739.127071	0.9596	1.0458	0.0004	—	—	—	—
1.746437	-1739.131585	0.9752	1.0687	0.0004	—	—	—	—
1.756437	-1739.131731	0.9770	1.0715	0.0004	—	—	—	—
1.766437	-1739.131801	0.9787	1.0742	0.0004	—	—	—	—
1.776437	-1739.131797	0.9805	1.0768	0.0004	—	—	—	—
1.786437	-1739.131724	0.9822	1.0795	0.0004	—	—	—	—
1.866437	-1739.128287	1.0160	1.1514	0.0005	—	—	—	—
1.966437	-1739.121422	1.0260	1.1639	0.0005	—	—	—	—
2.066437	-1739.112296	1.0326	1.1678	0.0005	—	—	—	—
	1 $^2\Pi$ resonance							
1.666437	-1739.130364	0.8699	0.9023	0.0007	-1739.136336	0.7075	0.5880	0.0012
1.766437	-1739.137309	0.8288	0.8597	0.0007	-1739.142746	0.6809	0.5750	0.0010
1.776437	-1739.137528	0.8245	0.8553	0.0007	-1739.142956	0.6769	0.5711	0.0100
1.786437	-1739.137678	0.8202	0.8510	0.0007	-1739.143096	0.6728	0.5672	0.0100
1.796437	-1739.137762	0.8158	0.8467	0.0007	-1739.143170	0.6687	0.5633	0.0100
1.806437	-1739.137785	0.8114	0.8423	0.0007	-1739.143183	0.6645	0.5595	0.0100
1.816437	-1739.137749	0.8070	0.8379	0.0007	-1739.143137	0.6604	0.5557	0.0100
1.866437	-1739.136802	0.7843	0.8159	0.0007	-1739.142131	0.6393	0.5368	0.0010
1.966437	-1739.132953	0.7122	0.7559	0.0006	-1739.137242	0.5955	0.5003	0.0010
2.066437	-1739.125888	0.6627	0.7094	0.0006	-1739.130042	0.5497	0.4652	0.0010

No stationary point was found in the η trajectory of the first-order corrected energy of the $^2\Sigma^+$ resonance. CAP onset was chosen as $X_0 = Y_0 = 3.53$ bohr, $Z_0 = 9.55$ bohr. Core electrons were not included in the correlation treatment. For technical reasons, g functions were removed from the basis set.

TABLE S5: Absolute energies, resonance positions and widths, as well as optimal CAP strengths for the 2 $^2\Sigma^+$ and the 1 $^2\Pi$ resonance state of CuF^- as a function of bond distance computed by CAP-EOM-EA-CCSD/aug-cc-pVTZ-PP+6s6p3d.

	Zeroth-order values				First-order values			
R(CuF)/Å	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.
	2 $^2\Sigma^+$ resonance							
1.666437	-296.678833	0.9063	1.0203	0.0004	—	—	—	—
1.716437	-296.681011	0.9125	1.0311	0.0004	—	—	—	—
1.726437	-296.681290	0.9143	1.0328	0.0004	—	—	—	—
1.736437	-296.681603	0.9171	1.0381	0.0004	—	—	—	—
1.746437	-296.681640	0.9183	1.0417	0.0004	—	—	—	—
1.756437	-296.681590	0.9198	1.0440	0.0004	—	—	—	—
1.766437	-296.681476	0.9209	1.0467	0.0004	—	—	—	—
1.866437	-296.677071	0.9324	1.0702	0.0004	—	—	—	—
1.966437	-296.668760	0.9411	1.0885	0.0004	—	—	—	—
2.066437	-296.658443	0.9471	1.1000	0.0004	—	—	—	—
	1 $^2\Pi$ resonance							
1.666437	-296.680938	0.8490	0.9025	0.0007	-296.687736	0.6640	0.5848	0.0009
1.736437	-296.686141	0.7936	0.8453	0.0007	-296.691715	0.6420	0.5603	0.0009
1.746437	-296.686359	0.7899	0.8411	0.0007	-296.691917	0.6387	0.5569	0.0009
1.756437	-296.686500	0.7862	0.8368	0.0007	-296.692041	0.6354	0.5535	0.0009
1.766437	-296.686567	0.7824	0.8325	0.0006	-296.692093	0.6321	0.5501	0.0009
1.776437	-296.686567	0.7786	0.8282	0.0006	-296.692076	0.6287	0.5467	0.0009
1.786437	-296.686502	0.7747	0.8239	0.0006	-296.691993	0.6253	0.5433	0.0009
1.796437	-296.686375	0.7708	0.8196	0.0006	-296.691849	0.6219	0.5400	0.0009
1.866437	-296.684049	0.7425	0.7891	0.0006	-296.689397	0.5970	0.5167	0.0009
1.966437	-296.677655	0.6991	0.7453	0.0006	-296.682801	0.5590	0.4841	0.0009
2.066437	-296.669285	0.6521	0.7012	0.0006	-296.674202	0.5183	0.4522	0.0009

No stationary point was found in the η trajectory of the first-order corrected energy of the $^2\Sigma^+$ resonance. CAP onset was chosen as $X_0 = Y_0 = 3.53$ bohr, $Z_0 = 9.55$ bohr. See below for details of the basis set.

TABLE S6: Absolute energies, resonance positions and widths, as well as optimal CAP strengths for the 2 $^2\Sigma^+$ and the 3 $^2\Sigma^+$ resonance states of AgF^- as a function of bond distance computed by CAP-EOM-EA-CCSD/aug-cc-pVTZ-PP+6s6p3d.

	Zeroth-order values				First-order values			
R(AgF)/Å	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.
	2 $^2\Sigma^+$ resonance							
1.907894	-246.390409	1.5577	1.2838	0.0022	-246.397703	1.3594	1.1494	0.0020
1.947894	-246.392915	1.5313	1.2650	0.0018	-246.399830	1.3433	1.2148	0.0018
1.957894	-246.393034	1.5336	1.2662	0.0018	-246.399869	1.3477	1.2117	0.0018
1.967894	-246.393090	1.5358	1.2673	0.0018	-246.399840	1.3522	1.2087	0.0018
1.977894	-246.393088	1.5378	1.2684	0.0018	-246.399753	1.3566	1.2052	0.0018
1.987894	-246.393029	1.5399	1.2694	0.0018	-246.399607	1.3610	1.2015	0.0018
1.997894	-246.392916	1.5418	1.2703	0.0018	-246.399407	1.3653	1.1976	0.0018
2.007894	-246.392753	1.5436	1.2713	0.0018	-246.399151	1.3696	1.1934	0.0018
2.107894	-246.389498	1.5401	1.2688	0.0016	-246.394314	1.4091	1.1375	0.0018
2.207894	-246.382765	1.5472	1.2603	0.0016	-246.386731	1.4393	1.0588	0.0018
2.307894	-246.374929	1.5373	1.2315	0.0014	-246.377928	1.4557	0.9667	0.0018
	3 $^2\Sigma^+$ resonance							
1.907894	-246.365588	2.2331	1.5842	0.0022	-246.361695	2.3392	0.9256	0.0026
1.987894	-246.368675	2.2025	1.5532	0.0022	-246.365702	2.2836	0.8895	0.0026
1.997894	-246.368759	2.1991	1.5494	0.0022	-246.365893	2.2772	0.8856	0.0026
2.007894	-246.368788	2.1957	1.5456	0.0022	-246.366033	2.2708	0.8820	0.0026
2.017894	-246.368762	2.1924	1.5419	0.0022	-246.366114	2.2646	0.8785	0.0026
2.027894	-246.368683	2.1893	1.5382	0.0022	-246.366141	2.2586	0.8752	0.0026
2.107894	-246.365953	2.1807	1.4871	0.0020	-246.365210	2.2011	0.7285	0.0028
2.207894	-246.360341	2.1573	1.4588	0.0020	-246.360437	2.1548	0.7367	0.0028
2.307894	-246.352611	2.1445	1.4430	0.0020	-246.353819	2.1117	0.6672	0.0030

CAP onset was chosen as $X_0 = Y_0 = 4.10$ bohr, $Z_0 = 11.41$ bohr. See below for details of the basis set.

TABLE S7: Absolute energies, resonance positions and widths, as well as optimal CAP strengths for the 1 $^2\Pi$ resonance states of AgF^- as a function of bond distance computed by CAP-EOM-EA-CCSD/aug-cc-pVTZ-PP+6s6p3d.

	Zeroth-order values				First-order values			
R(AgF)/Å	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.
1.907894	-246.351887	2.6058	1.6856	0.0034	-246.352320	2.5943	0.7958	0.0046
2.007894	-246.355094	2.5683	1.6563	0.0032	-246.356820	2.5215	0.6983	0.0050
2.017894	-246.355134	2.5632	1.6552	0.0032	-246.356893	2.5156	0.6955	0.0500
2.027894	-246.355125	2.5581	1.6541	0.0032	-246.356918	2.5096	0.6928	0.0500
2.037894	-246.355070	2.5530	1.6531	0.0032	-246.356896	2.5036	0.6901	0.0500
2.107894	-246.353577	2.5174	1.6466	0.0032	-246.355646	2.4613	0.6743	0.0050
2.207894	-246.348664	2.4750	1.6227	0.0030	-246.350912	2.4140	0.7114	0.0048
2.307894	-246.342363	2.4233	1.6154	0.0030	-246.344897	2.3545	0.6991	0.0048

CAP onset was chosen as $X_0 = Y_0 = 4.10$ bohr, $Z_0 = 11.41$ bohr. See below for details of the basis set.

TABLE S8: Absolute energies, resonance positions and widths as well as optimal CAP strengths for the resonance states of CuF^- ($2\ ^2\Sigma^+$, $1\ ^2\Pi$) and AgF^- ($2\ ^2\Sigma^+$, $3\ ^2\Sigma^+$, $1\ ^2\Pi$) computed by CAP-EOM-EA-CCSD and different basis sets including additional diffuse functions. Absolute energies and attachment energies for the bound anionic states ($X\ ^2\Sigma^+$, $1\ ^2\Sigma^+$) as well as absolute energies for the neutral ground states ($X\ ^1\Sigma^+$) are also given.

Electronic	Zeroth-order values				First-order values			
State	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.	Re(E)/a.u.	E_R/eV	Γ/eV	η_{opt}/a.u.
	CuF/aug-cc-pVTZ+6s6p6d							
$X\ ^1\Sigma^+$	-1739.165667	—	0.0000	0.0000	—	—	—	—
$X\ ^2\Sigma^+$	-1739.204467	-1.0558	0.0000	0.0000	—	—	—	—
$1\ ^2\Sigma^+$	-1739.166133	-0.0127	0.0000	0.0000	—	—	—	—
$2\ ^2\Sigma^+$	-1739.130304	0.9623	1.1102	0.0004	—	—	—	—
$1\ ^2\Pi$	-1739.136368	0.7972	0.8838	0.0008	-1739.142166	0.6395	0.6517	0.0014
	CuF/aug-cc-pVTZ+9s9p9d							
$X\ ^1\Sigma^+$	-1739.165669	—	0.0000	0.0000	—	—	—	—
$X\ ^2\Sigma^+$	-1739.204468	-1.0558	0.0000	0.0000	—	—	—	—
$1\ ^2\Sigma^+$	-1739.166142	-0.0129	0.0000	0.0000	—	—	—	—
$2\ ^2\Sigma^+$	-1739.129970	0.9714	1.1372	0.0004	—	—	—	—
$1\ ^2\Pi$	-1739.136320	0.7985	0.8841	0.0008	-1739.141981	0.6446	0.6519	0.0014
	AgF/aug-cc-pVTZ-PP+6s6p6d							
$X\ ^1\Sigma^+$	-246.446267	—	0.0000	0.0000	—	—	—	—
$X\ ^2\Sigma^+$	-246.499763	-1.4557	0.0000	0.0000	—	—	—	—
$1\ ^2\Sigma^+$	-246.447066	-0.0217	0.0000	0.0000	—	—	—	—
$2\ ^2\Sigma^+$	-246.386602	1.6235	1.1827	0.0016	-246.388940	1.5599	0.9675	0.0020
$3\ ^2\Sigma^+$	-246.366380	2.1737	1.2664	0.0020	-246.362677	2.2746	0.7809	0.0028
$1\ ^2\Pi$	-246.351023	2.5915	1.7792	0.0036	-246.347681	2.6827	1.7886	0.0034

All calculations were carried out at bond distances R(CuF) = 1.866437 Å and R(AgF) = 2.107894 Å. For CAP onset, see tables S4–S7. No stationary point was found in the η trajectory of the first-order corrected energy of the $^2\Sigma^+$ resonance of CuF^-.

TABLE S9: Zero-point vibrational energies for the relevant electronic states of CuF and AgF in eV. Calculated within the harmonic approximation at the CCSD level for the neutral ground state, at the EOM-EA-CCSD level for the bound anionic states, and at the CAP-EOM-EA-CCSD level for resonance states. Basis set: aug-cc-pVTZ-PP+6s6p3d.

Electronic State	CuF/CuF$^-$	AgF/AgF$^-$
X $^1\Sigma^+$	0.0384	0.0317
X $^2\Sigma^+$	0.0297	0.0227
1 $^2\Sigma^+$	0.0408	0.0319
2 $^2\Sigma^+$	0.0411	0.0344
3 $^2\Sigma^+$	—	0.0306
1 $^2\Pi$	0.0365	0.0288

Modified aug-cc-pVTZ-PP Basis Set for CuF

The basis set for copper was generated from the aug-cc-pVTZ-PP basis (Peterson, K. A.; Puzzarini, C. *Theor. Chem. Acc.* **2005**, *114*, 283–296) by adding 6 *s*, 6 *p*, and 3 *d* diffuse functions. The basis set for fluorine was generated from the aug-cc-pVTZ basis (Dunning, T. H. *J. Chem. Phys.* **1989**, *90*, 1007–1023 and Kendall, R. A.; Dunning, T. H.; Harrison, R. J. *J. Chem. Phys.* **1992**, *96*, 6796–6806) by adding 6 *p* and 3 *d* diffuse functions. For technical reasons, no diffuse *s* functions were added to the basis set for fluorine and *g* functions were removed from all basis sets.

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Cu     0
S   9   1.00
   1946.3500000              0.0001730
    277.9450000              0.0009580
     60.0108000             -0.0139320
     37.5138000              0.0666720
     10.9688000             -0.4144860
      2.3353600              0.7319850
      0.9775800              0.4735590
      0.1858870              0.0288600
      0.0948510             -0.0143780
S   9   1.00
   1946.3500000             -0.0000430
    277.9450000             -0.0001730
     60.0108000              0.0021820
     37.5138000             -0.0132150
     10.9688000              0.0954600
      2.3353600             -0.2048920
      0.9775800             -0.2429550
      0.1858870              0.2128160
      0.0948510              0.5320730
S   9   1.00
   1946.3500000             -0.0000850
    277.9450000             -0.0004180
     60.0108000              0.0051250
     37.5138000             -0.0280790
     10.9688000              0.2066260
      2.3353600             -0.6763950
      0.9775800              0.0068900
      0.1858870              1.6771590
      0.0948510             -0.4592680
S   9   1.00
   1946.3500000             -0.0003310
    277.9450000              0.0007840
     60.0108000             -0.0199370
     37.5138000             -0.0064730
     10.9688000              0.4304630
      2.3353600             -2.3103570
      0.9775800              2.2981990
      0.1858870              0.3918090
      0.0948510             -2.2238270
S   1   1.00
      0.0403630              1.0000000
S   1   1.00
      0.0172000              1.0000000
P   8   1.00
    395.0250000              0.0002060
     64.7808000              0.0038720
     17.8335000             -0.0831640
      4.3595800              0.3467890
      2.0181600              0.4867620
      0.9023120              0.2722850
      0.3122900              0.0339860
      0.1156800             -0.0036900
P   8   1.00
    395.0250000             -0.0000510
     64.7808000             -0.0007000
     17.8335000              0.0170850
      4.3595800             -0.0814680
      2.0181600             -0.1198010
      0.9023120             -0.0599620
      0.3122900              0.2354600
      0.1156800              0.5603760
```

```
P   8   1.00
    395.0250000             -0.0001220
     64.7808000             -0.0012420
     17.8335000              0.0352160
      4.3595800             -0.1894850
      2.0181600             -0.2432280
      0.9023120              0.0252340
      0.3122900              0.5801290
      0.1156800              0.4825400
P   8   1.00
    395.0250000             -0.0003940
     64.7808000             -0.0013450
     17.8335000              0.0791750
      4.3595800             -0.5949390
      2.0181600             -0.4104190
      0.9023120              1.0418980
      0.3122900              0.3430100
      0.1156800             -0.8397400
P   1   1.00
      0.0417450              1.0000000
P   1   1.00
      0.0151000              1.0000000
D   7   1.00
    134.0680000              0.0029660
     42.2407000              0.0273300
     16.5467000              0.1001680
      7.0122700              0.2319250
      3.0244600              0.3392610
      1.2646100              0.3452250
      0.4962380              0.2466370
D   7   1.00
    134.0680000             -0.0036790
     42.2407000             -0.0338610
     16.5467000             -0.1283960
      7.0122700             -0.3011240
      3.0244600             -0.3197480
      1.2646100              0.0845510
      0.4962380              0.5018780
D   7   1.00
    134.0680000              0.0045260
     42.2407000              0.0423250
     16.5467000              0.1662100
      7.0122700              0.4031220
      3.0244600              0.0713050
      1.2646100             -0.7108880
      0.4962380             -0.1463320
D   1   1.00
      0.1731340              1.0000000
D   1   1.00
      0.0604000              1.0000000
F   1   1.00
      5.1411000              1.0000000
F   1   1.00
      1.2848000              1.0000000
F   1   1.00
      0.4587000              1.0000000
S   1   1.00
      0.0086000              1.0000000
S   1   1.00
      0.0043000              1.0000000
S   1   1.00
      0.0021500              1.0000000
S   1   1.00
      0.0010750              1.0000000
S   1   1.00
      0.0005375              1.0000000
S   1   1.00
      0.0002688              1.0000000
P   1   1.00
      0.0075500              1.0000000
P   1   1.00
      0.0037750              1.0000000
P   1   1.00
      0.0018875              1.0000000
P   1   1.00
      0.0009438              1.0000000
P   1   1.00
      0.0004719              1.0000000
P   1   1.00
      0.0002359              1.0000000
D   1   1.00
      0.0302000              1.0000000
D   1   1.00
      0.0151000              1.0000000
D   1   1.00
      0.0075500              1.0000000
****
F     0
S   8   1.00
  19500.0000000              0.0005070
   2923.0000000              0.0039230
    664.5000000              0.0202000
    187.5000000              0.0790100
     60.6200000              0.2304390
     21.4200000              0.4328720
      7.9500000              0.3499640
      0.8815000             -0.0078920
S   8   1.00
  19500.0000000             -0.0001170
   2923.0000000             -0.0009120
    664.5000000             -0.0047170
    187.5000000             -0.0190860
     60.6200000             -0.0596550
     21.4200000             -0.1400100
      7.9500000             -0.1767820
      0.8815000              0.6050430
S   1   1.00
      2.2570000              1.0000000
S   1   1.00
      0.3041000              1.0000000
S   1   1.00
      0.0915800              1.0000000
```

```
P   3   1.00
     43.8800000              0.0166650
      9.9260000              0.1044720
      2.9300000              0.3172600
P   1   1.00
      0.9132000              1.0000000
P   1   1.00
      0.2672000              1.0000000
P   1   1.00
      0.0736100              1.0000000
P   1   1.00
      0.0368050              1.0000000
P   1   1.00
      0.0184025              1.0000000
P   1   1.00
      0.0092013              1.0000000
P   1   1.00
      0.0046006              1.0000000
P   1   1.00
      0.0023003              1.0000000
P   1   1.00
      0.0011502              1.0000000
D   1   1.00
      3.1070000              1.0000000
D   1   1.00
      0.8550000              1.0000000
D   1   1.00
      0.2920000              1.0000000
D   1   1.00
      0.1460000              1.0000000
D   1   1.00
      0.0730000              1.0000000
D   1   1.00
      0.0365000              1.0000000
F   1   1.00
      1.9170000              1.0000000
F   1   1.00
      0.7240000              1.0000000
```

Modified aug-cc-pVTZ-PP Basis Set for AgF

The basis set for silver was generated from the aug-cc-pVTZ-PP basis (Peterson, K. A.; Puzzarini, C. *Theor. Chem. Acc.* **2005**, *114*, 283–296) by adding 6 *s*, 6 *p*, and 3 *d* diffuse functions. The basis set for fluorine was generated from the aug-cc-pVTZ basis (Dunning, T. H. *J. Chem. Phys.* **1989**, *90*, 1007–1023 and Kendall, R. A.; Dunning, T. H.; Harrison, R. J. *J. Chem. Phys.* **1992**, *96*, 6796–6806) by adding 6 *p* and 3 *d* diffuse functions. For technical reasons, no diffuse *s* functions were added to the basis set for fluorine and *g* functions were removed from all basis sets.

```
Ag     0
S   9   1.00
    222.6450000              0.0007000
     20.1725000             -0.0798090
     12.7197000              0.4589790
      8.0021100             -0.5218260
      5.0205300             -0.4075440
      1.5208500              0.8414580
      0.6949200              0.4956480
      0.1729330              0.0276600
      0.0818970             -0.0086430
S   9   1.00
    222.6450000             -0.0002080
     20.1725000              0.0228050
     12.7197000             -0.1373250
      8.0021100              0.1730850
      5.0205300              0.1057550
      1.5208500             -0.3140630
      0.6949200             -0.2985340
      0.1729330              0.2313240
      0.0818970              0.5969110
```

```
S   9   1.00
    222.6450000             -0.0002500
     20.1725000              0.0210250
     12.7197000             -0.1682510
      8.0021100              0.1442000
      5.0205300              0.4139110
      1.5208500             -1.1739400
      0.6949200              0.1871810
      0.1729330              1.7116850
      0.0818970             -0.5350550
S   9   1.00
    222.6450000             -0.0007140
     20.1725000              0.0726550
     12.7197000             -0.4696600
      8.0021100              0.5845510
      5.0205300              0.5663560
      1.5208500             -3.2222430
      0.6949200              3.1502630
      0.1729330             -0.1517250
      0.0818970             -1.9921310
S   1   1.00
      0.0351900              1.0000000
S   1   1.00
      0.0151000              1.0000000
S   1   1.00
      0.0075500              1.0000000
S   1   1.00
      0.0037750              1.0000000
S   1   1.00
      0.0018875              1.0000000
S   1   1.00
      0.0009438              1.0000000
S   1   1.00
      0.0004719              1.0000000
S   1   1.00
      0.0002359              1.0000000
P   8   1.00
     22.0490000             -0.0058860
     13.8356000              0.0763570
      7.6299400             -0.2661720
      2.1037200              0.4622010
      1.0626200              0.4894950
      0.5193830              0.2000890
      0.2051990              0.0193450
      0.0829790             -0.0007170
P   8   1.00
     22.0490000              0.0005940
     13.8356000             -0.0170800
      7.6299400              0.0679410
      2.1037200             -0.1427200
      1.0626200             -0.1683930
      0.5193830             -0.0329600
      0.2051990              0.3267400
      0.0829790              0.5580540
P   8   1.00
     22.0490000              0.0022350
     13.8356000             -0.0383630
      7.6299400              0.1454190
      2.1037200             -0.3278470
      1.0626200             -0.3817440
      0.5193830              0.2524550
      0.2051990              0.6915130
      0.0829790              0.2763110
P   8   1.00
     22.0490000              0.0087290
     13.8356000             -0.0828090
      7.6299400              0.2865900
      2.1037200             -0.8760860
      1.0626200             -0.3443670
      0.5193830              1.5334530
      0.2051990             -0.2330540
      0.0829790             -0.7471730
P   1   1.00
      0.0331440              1.0000000
P   1   1.00
      0.0132000              1.0000000
P   1   1.00
      0.0066000              1.0000000
P   1   1.00
      0.0033000              1.0000000
P   1   1.00
      0.0016500              1.0000000
P   1   1.00
      0.0008250              1.0000000
P   1   1.00
      0.0004125              1.0000000
P   1   1.00
      0.0002063              1.0000000
D   7   1.00
     73.2665000              0.0004510
     18.7729000              0.0059840
     10.9237000             -0.0189680
      3.0019700              0.1923860
      1.4717700              0.3721720
      0.6847640              0.3721880
      0.3003970              0.2300660
D   7   1.00
     73.2665000             -0.0006060
     18.7729000             -0.0075860
     10.9237000              0.0246380
      3.0019700             -0.3135690
      1.4717700             -0.5000300
      0.6847640              0.1211390
      0.3003970              0.5946850
```

```
D   7   1.00
     73.2665000             0.0004890
     18.7729000             0.0155170
     10.9237000            -0.0470560
      3.0019700             0.6569190
      1.4717700             0.2238260
      0.6847640            -1.1068170
      0.3003970             0.1657200
D   1   1.00
      0.1201550             1.0000000
D   1   1.00
      0.0481000             1.0000000
D   1   1.00
      0.0240500             1.0000000
D   1   1.00
      0.0120250             1.0000000
D   1   1.00
      0.0060125             1.0000000
F   1   1.00
      2.5431000             1.0000000
F   1   1.00
      0.7381000             1.0000000
F   1   1.00
      0.2889000             1.0000000
****
F     0
S   8   1.00
  19500.0000000             0.0005070
   2923.0000000             0.0039230
    664.5000000             0.0202000
    187.5000000             0.0790100
     60.6200000             0.2304390
     21.4200000             0.4328720
      7.9500000             0.3499640
      0.8815000            -0.0078920
S   8   1.00
  19500.0000000            -0.0001170
   2923.0000000            -0.0009120
    664.5000000            -0.0047170
    187.5000000            -0.0190860
     60.6200000            -0.0596550
     21.4200000            -0.1400100
      7.9500000            -0.1767820
      0.8815000             0.6050430
S   1   1.00
      2.2570000             1.0000000
S   1   1.00
      0.3041000             1.0000000
S   1   1.00
      9.8120000             1.0000000
S   1   1.00
     25.9430000            1.0000000
S   1   1.00
      0.0915800             1.0000000
P   3   1.00
     43.8800000            0.0166650
      9.9260000             0.1044720
      2.9300000             0.3172600
P   1   1.00
      0.9132000             1.0000000
P   1   1.00
      0.2672000             1.0000000
P   1   1.00
     18.7560000            1.0000000
P   1   1.00
     71.3480000            1.0000000
P   1   1.00
      0.0736100             1.0000000
P   1   1.00
      0.0368050             1.0000000
P   1   1.00
      0.0184025             1.0000000
P   1   1.00
      0.0092013             1.0000000
P   1   1.00
      0.0046006             1.0000000
P   1   1.00
      0.0023003             1.0000000
P   1   1.00
      0.0011502             1.0000000
D   1   1.00
      3.1070000             1.0000000
D   1   1.00
      0.8550000             1.0000000
D   1   1.00
     19.1080000            1.0000000
D   1   1.00
      0.2920000             1.0000000
D   1   1.00
      0.1460000             1.0000000
D   1   1.00
      0.0730000             1.0000000
D   1   1.00
      0.0365000             1.0000000
F   1   1.00
      1.9170000             1.0000000
F   1   1.00
      0.7240000             1.0000000
```

Effective Core Potentials for Cu and Ag

Taken from Figgen, D.; Rauhut, G.; Dolg, M.; Stoll, H. *Chem. Phys.* **2005**, *311*, 227–244.

```
CU     0
CU-ECP     4     10
g-ul potential
  1
2      1.0000000              0.0000000
s-ul potential
  2
2     30.1105430            355.7505120
2     13.0763100             70.9309060
p-ul potential
  4
2     32.6926140             77.9699310
2     32.7703390            155.9274480
2     13.7510670             18.0211320
2     13.3221660             36.0943720
d-ul potential
  4
2     38.9965110            -12.3434100
2     39.5397880            -18.2733620
2     12.2875110             -0.9847050
2     11.4593000             -1.3187470
f-ul potential
  2
2      6.1901020             -0.2272640
2      8.1187800             -0.4687730
```

```
AG     0
AG-ECP     4     28
g-ul potential
  1
2      1.0000000              0.0000000
s-ul potential
  2
2     12.5677140            255.0547710
2      6.9976620             36.9833930
p-ul potential
  4
2     11.3164960             60.7157050
2     10.9580630            121.4438890
2      7.1114000             10.1718660
2      6.7733190             20.4865640
d-ul potential
  4
2      8.9284370             29.5049380
2     11.1025670             44.0187360
2      5.5432120              5.3683330
2      3.9288350              7.4083750
f-ul potential
  2
2     11.0129130            -12.6234030
2     11.0198980            -16.7643270
```