Quantifying Intrinsic Ion-driven Conformational Changes in Diphenylacetylene Supramolecular Switches with Cryogenic Ion Vibrational Spectroscopy

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Supporting Information

Supplemental Table 1. Comparison of Experimental (± 4 cm^{-1}) and Calculated (B3LYP/6-31+G(d,p)) Frequencies for NH and CO Fundamentals of the Molecular Switch Complexes Characterized in This Study (cm^{-1})

complex	NH_a	NH_b	NH_c	amide CO[a]	ester CO
1-$TMA^+(D_2)_2$					
experimental	3395	3335	3467	1701	1731
calculated[b]	3394	3342	3464	1704, 1694	1731
1-$Na^+(D_2)_2$					
experimental	3432	3443	3464	1705, 1695	1747
calculated[b]	3450	3461	3464	1715, 1707	1747
2-$Cl^-(D_2)_2$					
experimental	2744	3194[c]	3357	1725, 1711	1749
calculated[b]	2886	3244	3374	1735, 1717	1750
1-$Cl^-(D_2)_2$					
experimental	2867[c]	3196[c]	3357	1709	1753
calculated[b]	2982	3260	3376	1726, 1714	1750
1-$Br^-(D_2)_2$					
experimental	2945[c]	3208[c]	3357	1710	1752
calculated[b]	3080	3293	3377	1725, 1717	1751
1-$I^-(D_2)_2$					
experimental	3034[c]	3231[c]	3357	1712	1748
calculated[b]	3139	3321	3376	1725, 1717	1751

[a]When the two amide CO functionalities are observed as a doublet, both frequencies are given.

[b]The empirically scaled calculated frequencies are given. Energies above 2000 cm^{-1} are scaled by .957 (to match the free NH frequency to that observed in 1-$Na^+(D_2)_2$) and below 2000 cm^{-1} by .987 (to match the free CO frequency to that observed in 2-$Na^+(D_2)_2$).

[c]Occurs in a congested spectral region, approximate assignment given.