Supporting Information: IR and NIR absorption spectroscopy of C_{60}^{2+} and C_{60}^{3+} in Neon Matrixes.

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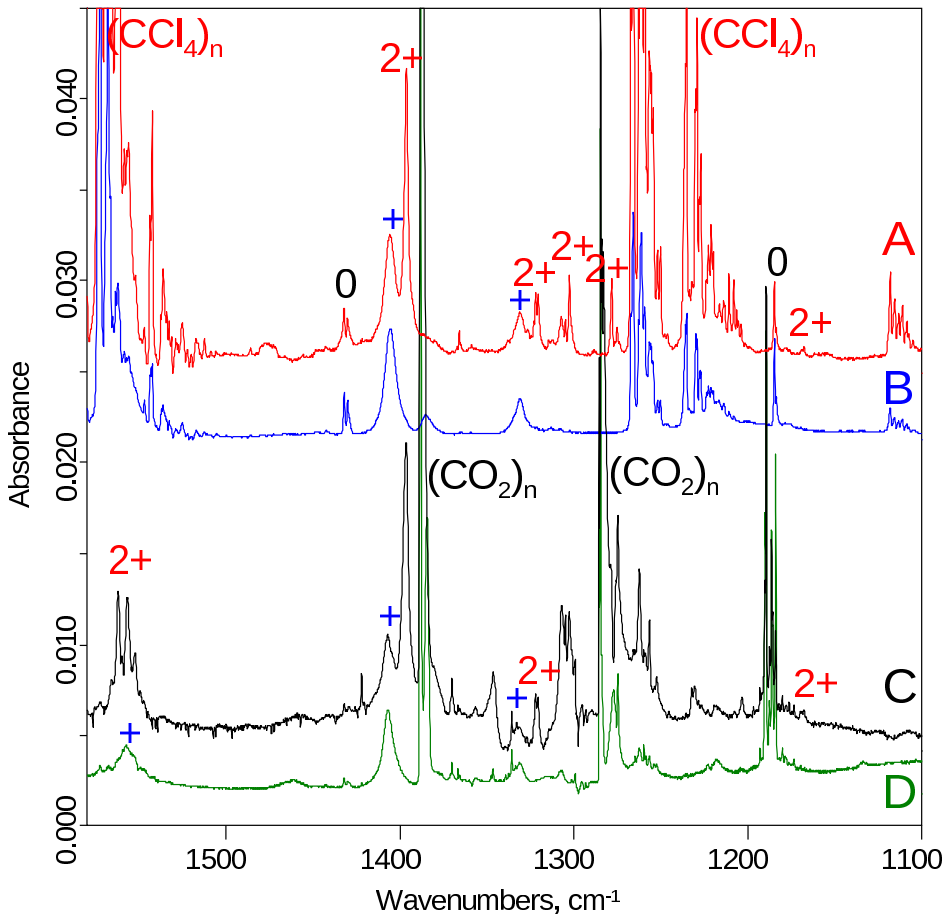

Figure 1: IR absorption spectra obtained upon depositing C_{60}^{2+} (A,C) and C_{60}^{+} (B,D) in Ne+0.15% CCl_4 (A,B) and Ne+1%CO_2 (C,D) matrixes at 5 K. Spectra A and C were scaled to have similar C_{60}^{2+} absorption strengths. Furthermore, spectrum B was scaled to A so as to have similar C_{60}^{+} absorption strengths (as was spectrum D to C). A: Ne+0.15% CCl_4 matrix containing $C_{60}^{2+/+/0}$ (red), B: Ne+0.15% CCl_4 matrix containing $C_{60}^{+/0}$ (blue), C: Ne+1%CO_2 matrix containing $C_{60}^{2+/+}$ (black), D: Ne+1%CO_2 matrix containing C_{60}^{+} (green).

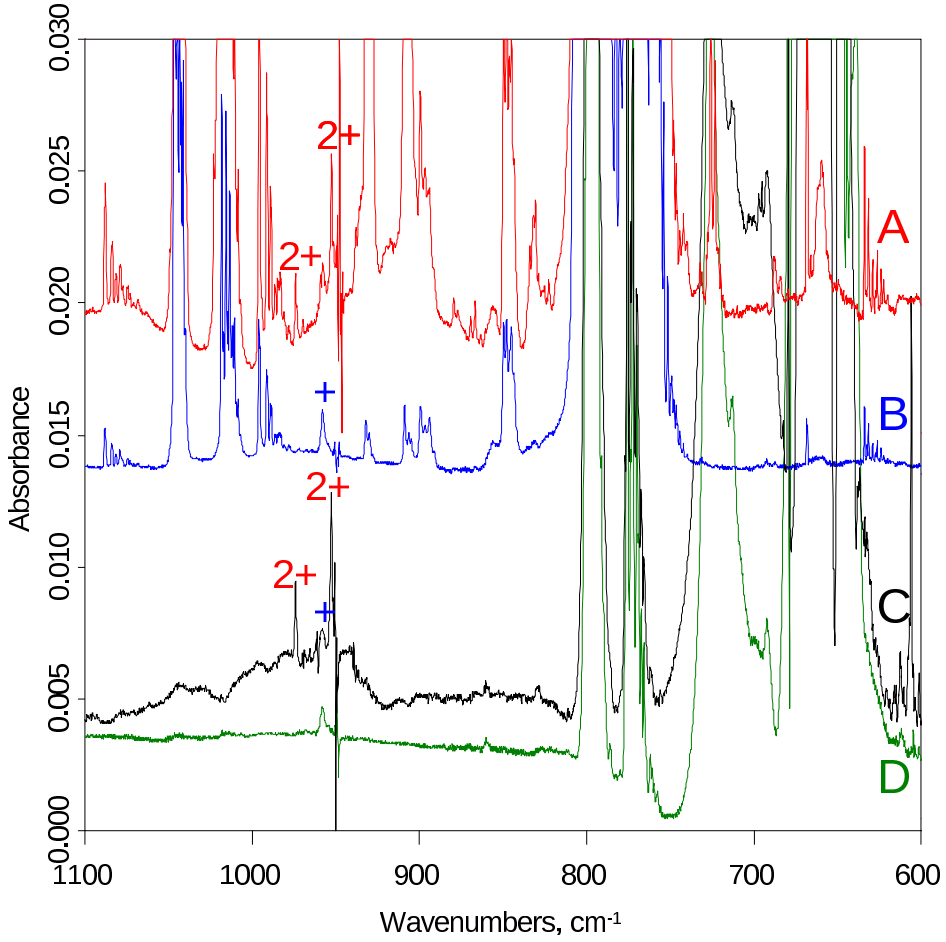

Figure 2: IR absorption spectra obtained upon depositing C_{60}^{2+} and C_{60}^{+} in Ne+0.15% CCl_4 and Ne+1%CO_2 matrixes at 5 K. Spectra A and C were scaled to have similar intensities of C_{60}^{2+} absorptions. Spectra A and B, as well as C and D were pairwise scaled to have similar intensities of C_{60}^{+} absorptions. A: $C_{60}^{2+/+}$ in Ne+0.15% CCl_4 (red), B: C_{60}^{+} in Ne+0.15% CCl_4 (blue), C: $C_{60}^{2+/+}$ in Ne+1%CO_2 (black), D: C_{60}^{+} in Ne+1%CO_2 (green).

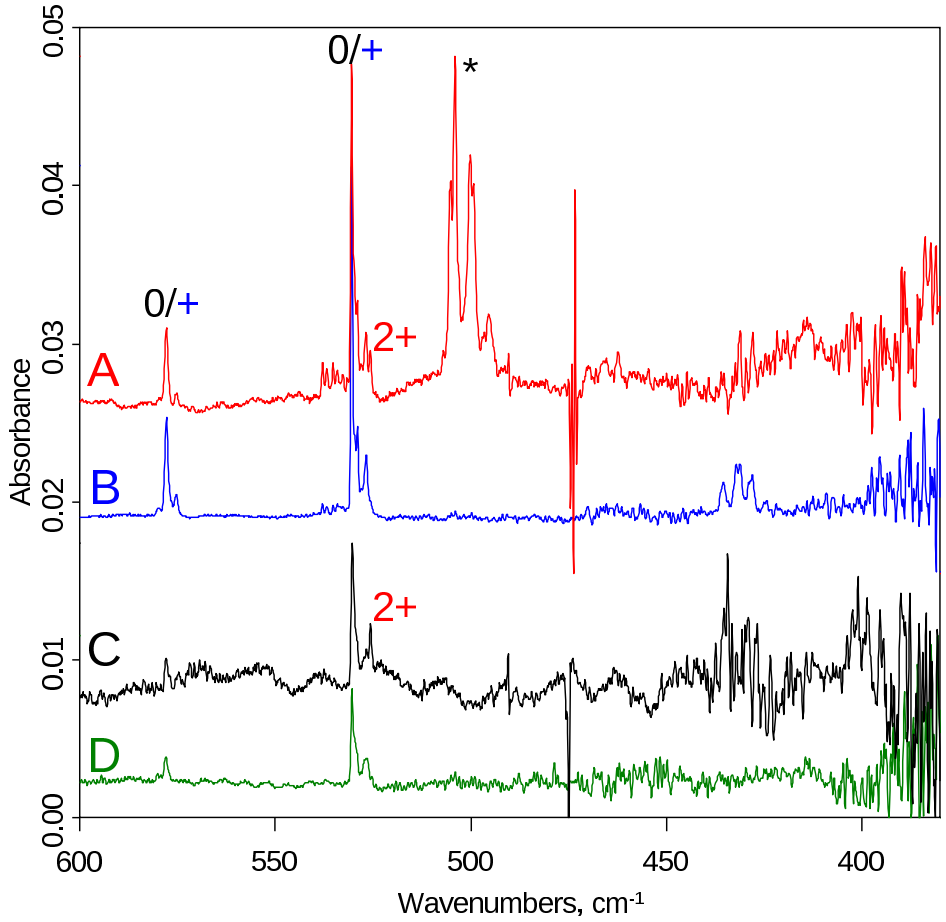

Figure 3: IR absorption spectra of C_{60}^{2+} (A,C) and C_{60}^{+} (B,D) deposited in Ne+0.15% CCl_4 (A,B) and Ne+1%CO_2 (C,D) matrixes at 5 K. Spectra A and C were scaled to have similar intensities of C_{60}^{2+} absorptions. Spectra A and B, as well as C and D were pairwise scaled to have similar intensities of C_{60}^{+} absorptions. The feature labeled by an asterisk was assigned to $Cl_2CCl\cdot\cdot Cl$ [Lugez, C. L.; Jacox, M. E.; Johnson, R. D. J. Chem. Phys. 1998, 109, 7147–7156], however its appearance only in matrixes containing C_{60}^{2+} suggests that it is due to $(CCl_4)_nCCl_3^+$ or $(CCl_4)_nCCl_4^+$. A: $C_{60}^{2+/+}$ in Ne+0.15% CCl_4 (red), B: C_{60}^{+} in Ne+0.15% CCl_4 (blue), C: $C_{60}^{2+/+}$ in Ne+1%CO_2 (black), D: C_{60}^{+} in Ne+1%CO_2 (green).

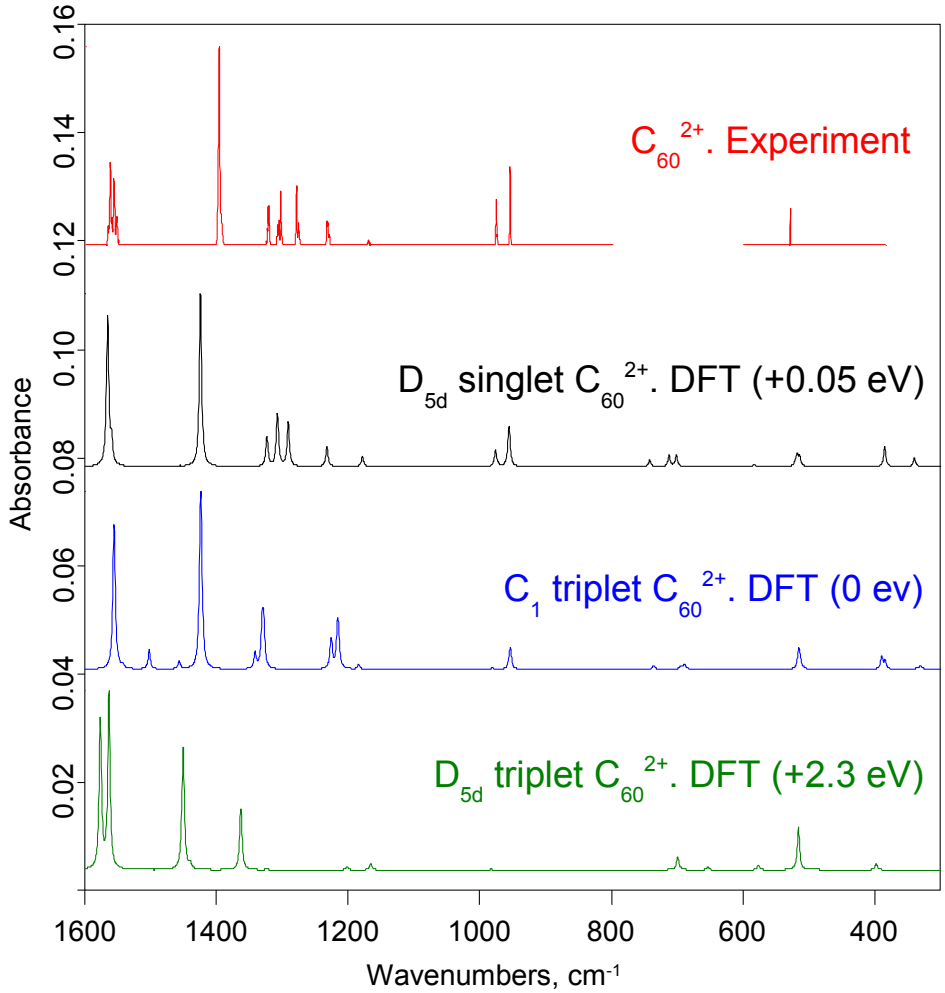

Figure 4: RI-DFT BP86/def2-SV(P) calculated spectra of C_{60}^{2+} in different ground state symmetries and multiplicities in comparison to the extracted experimental IR absorption spectrum (in Ne matrix). Calculated absorption lines were broadened by Lorentz functions having fwhm of 4 cm^{-1} to best match experimental data, frequencies are unscaled. Calculated relative energies of the ground state are in brackets.

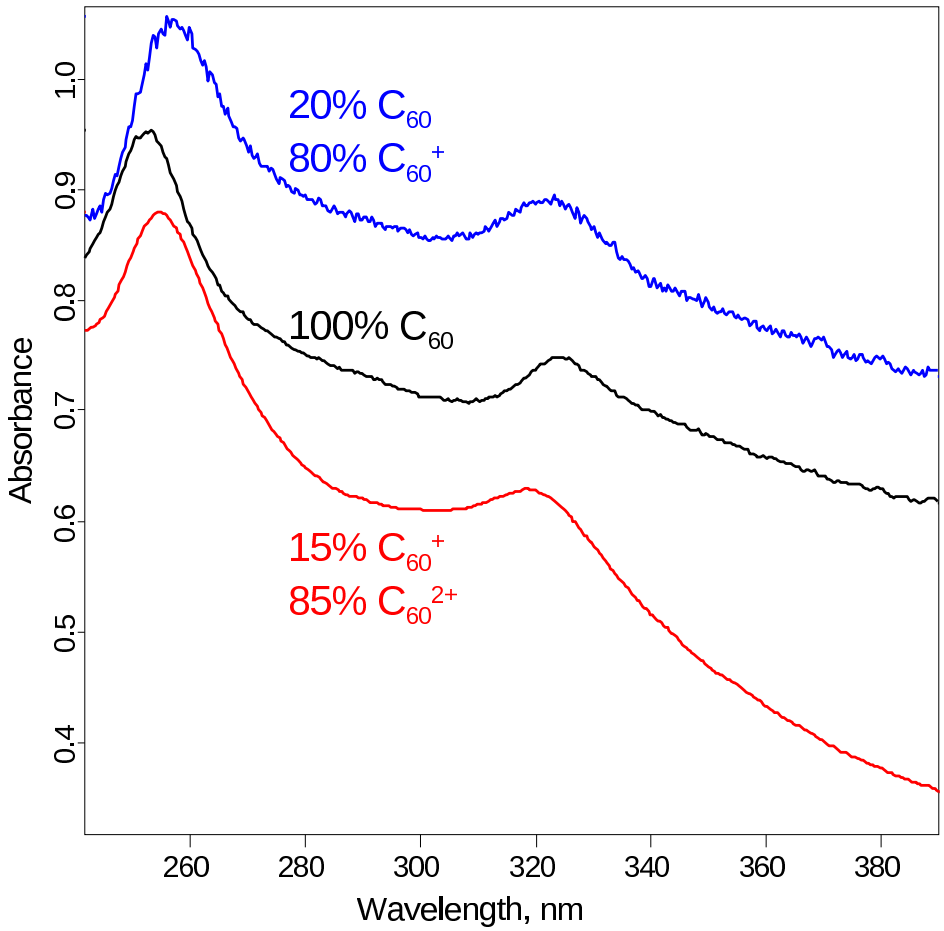

Figure 5: UV absorption spectra of C_{60}^{+}, C_{60}^{2+}, C_{60} in Ne+1%CO_2 matrixes at 5 K in various ratios as indicated. The amount of $C_{60}^{+}/C_{60}^{2+}/C_{60}$ was estimated from corresponding IR spectra. C_{60}^{-} is present in negligible amounts, if at all.

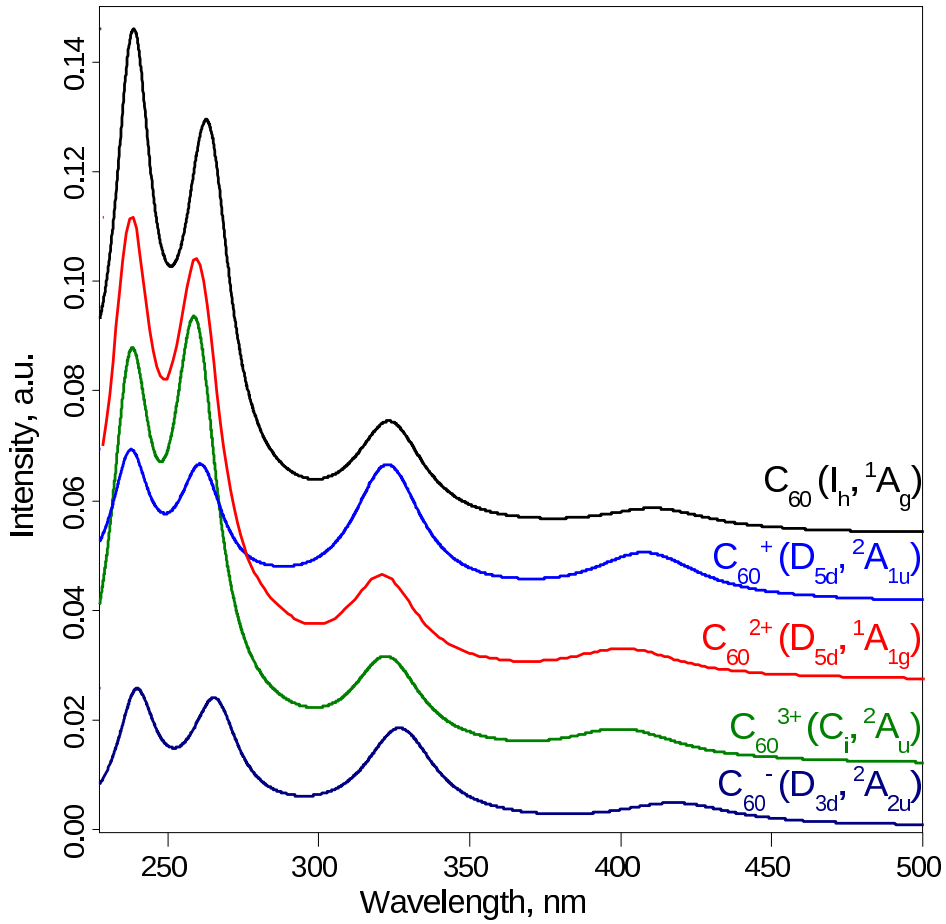

Figure 6: TDDFT calculated spectra of ionized and neutral C_{60}. The molecular symmetry groups and corresponding ground states are indicated in brackets. To fit the experimental Ne matrix data, calculated absorptions were broadened by Lorentz functions with fwhm of 3000 cm^{-1}. Frequencies were scaled by 0.88.