

Mid-infrared spectroscopy of 1-cyanonaphthalene cation for astrochemical consideration

Supplementary Information

Julianna Palotás,¹ Francis C. Daly,¹ Thomas E. Douglas-Walker,¹ and Ewen K. Campbell^{1, a)}
*School of Chemistry, University of Edinburgh, Joseph Black Building, Kings Buildings, David Brewster Road,
Edinburgh EH9 3FJ, UK*

VIBRATIONAL SPECTRUM OF 1-CNN⁺

Supplementary Table 1: Theoretical vibrational spectrum for 1-CNN⁺ calculated with B3LYP/6-311+G(d,p). These harmonic vibrational frequencies are not scaled.

Frequency cm ⁻¹	IR Intensity km mol ⁻¹
96.4811	2.302
134.4237	4.0451
160.1473	2.085
195.1337	0.0175
352.4561	0.3915
353.765	0.7042
412.979	15.1987
426.7545	1.6737
436.7784	1.3859
482.6889	0.9804
520.0865	0.7291
528.762	4.0026
600.0496	1.2156
642.0438	0.1187
688.6932	5.1583
735.536	3.4059
772.3591	53.5917
805.5288	0.0728
814.4496	39.5099
865.3156	3.0543
905.2601	0.8754
967.4357	0.0195
998.0272	0.5573
1022.2571	0.1819
1026.8969	0.0081
1030.817	25.233
1062.7431	0.7272
1094.8426	1.6975
1132.0589	5.6244
1194.9307	35.2163
1205.413	4.3861
1241.1139	47.5891
1253.8201	146.8056
1300.7081	13.919
1374.1414	56.3955
1403.741	3.5901
1435.3095	34.9246

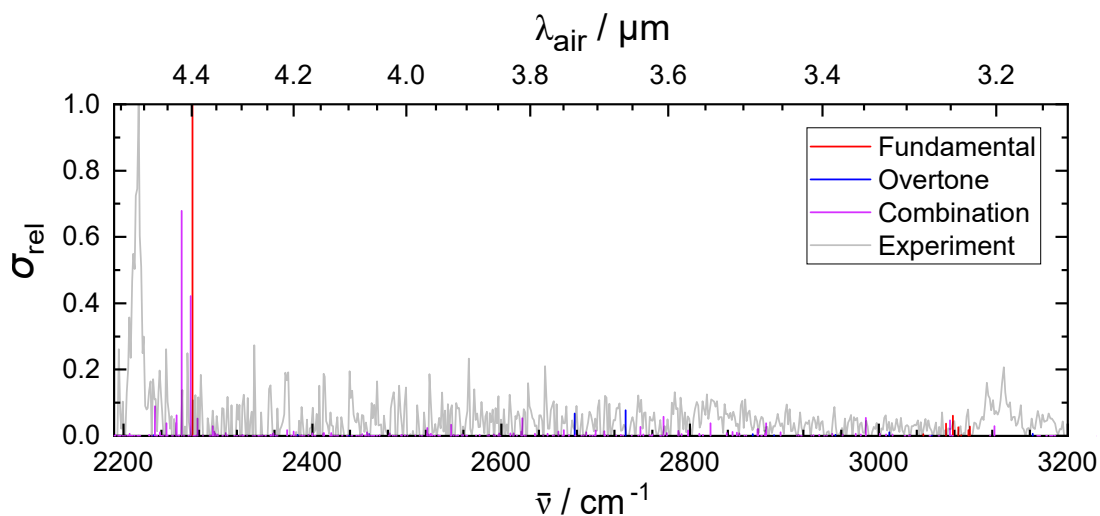
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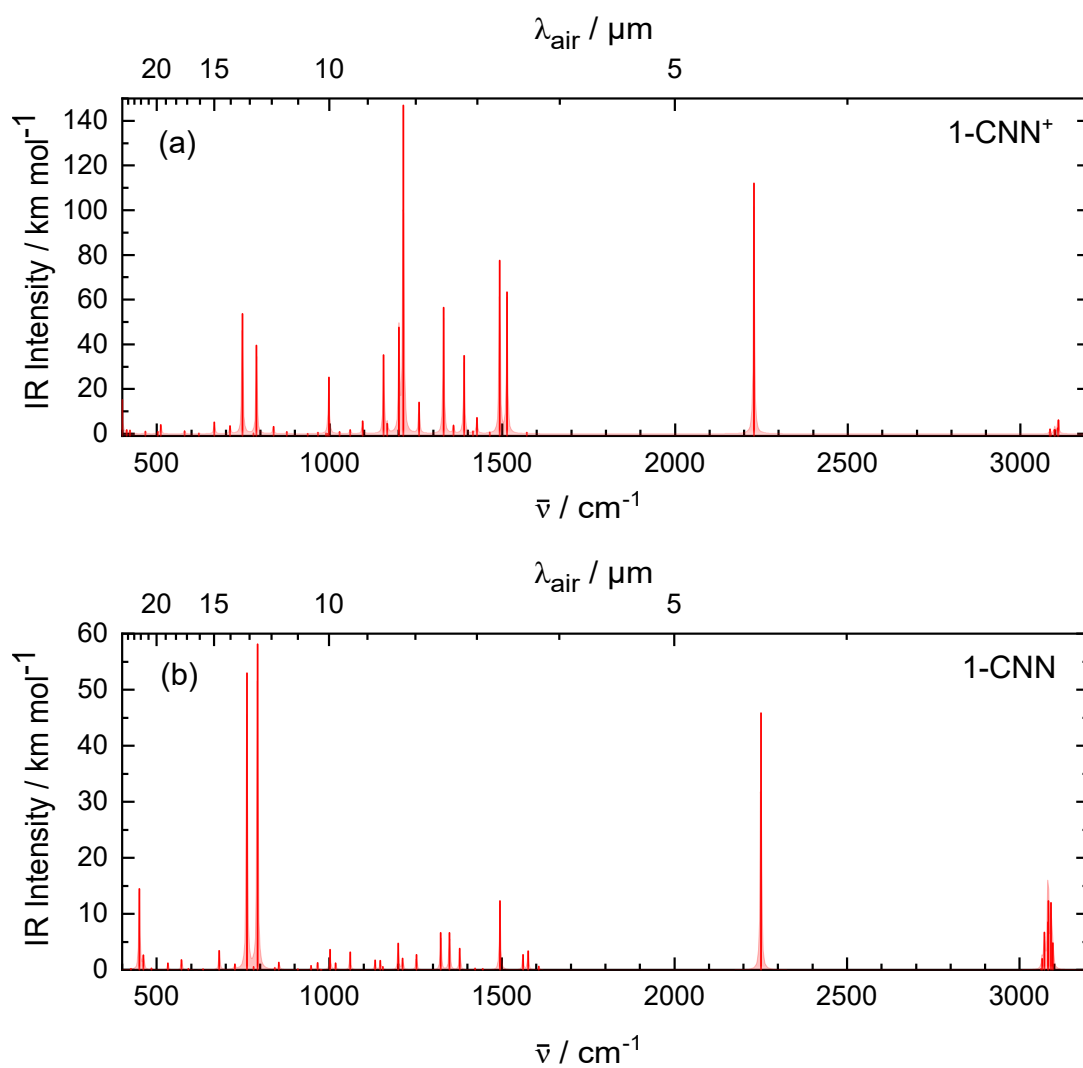
^{a)} Corresponding author: e.k.campbell@ed.ac.uk

Supplementary Table 1 – *Continued from previous page*

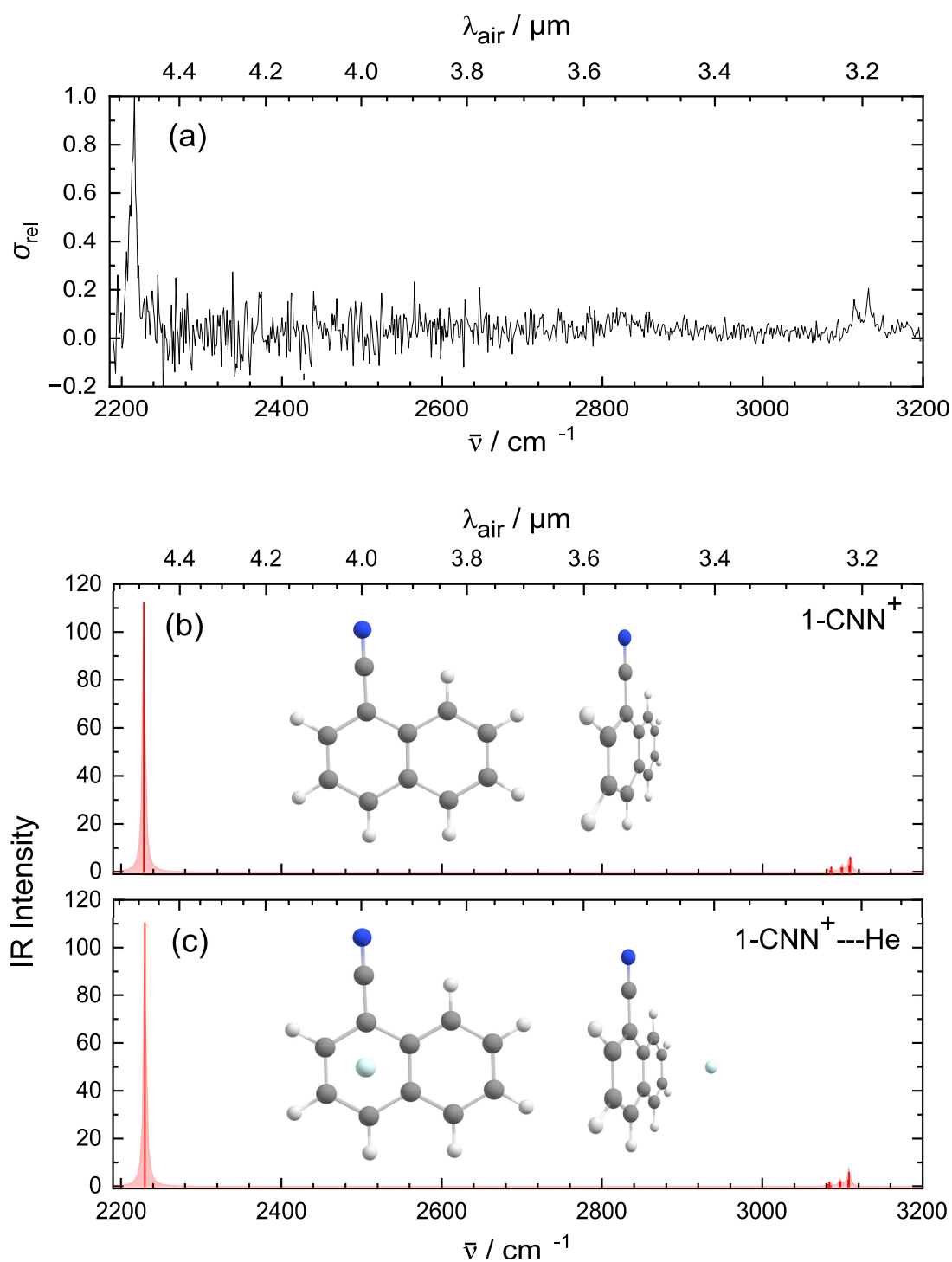
Frequency cm^{-1}	IR Intensity km mol^{-1}
1461.7486	0.975
1473.6637	7.1372
1512.1793	0.4328
1541.9639	77.435
1563.7494	63.3084
1623.463	0.529
2302.151	112.0524
3186.2976	0.3993
3188.0749	1.8831
3189.8613	0.0807
3200.9298	1.6922
3202.1043	1.66
3211.0373	2.5264
3212.5844	6.0202

ANHARMONIC CALCULATION

Supplementary Figure 1. Anharmonic vibrational spectrum of 1-CNN⁺ calculated with B3LYP/6-311+G(d,p) overlaid with the experimental spectrum. The anharmonic intensities are normalised to the CN fundamental.

COMPARISON OF 1-CNN AND 1-CNN⁺

Supplementary Figure 2. Theoretical vibrational spectra of a) 1-CNN⁺ and b) 1-CNN. The spectra were calculated at the DFT level with B3LYP/6-311+G(d,p). The vibrational frequencies are scaled by 0.9679.

EXPERIMENT AND THEORY FOR 1-CNN⁺-HE

Supplementary Figure 3. (a) Photofragmentation spectrum of 1-CNN⁺-He. Harmonic frequency calculations using B3LYP/6-311+G(d,p) on 1-CNN⁺-He_n with $n = 0$ (b) and $n = 1$ (c). The vibrational temperature was set to 4 K. The vibrational frequencies were convoluted with a Lorentzian function with a FWHM of 4 cm^{-1} . All calculations used the 0.9679 scaling factor. The stick spectra have units of km mol^{-1} .