Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary information to

Photoelectron spectroscopy of boron-containing reactive intermediates using synchrotron radiation: BH_2, BH, and BF

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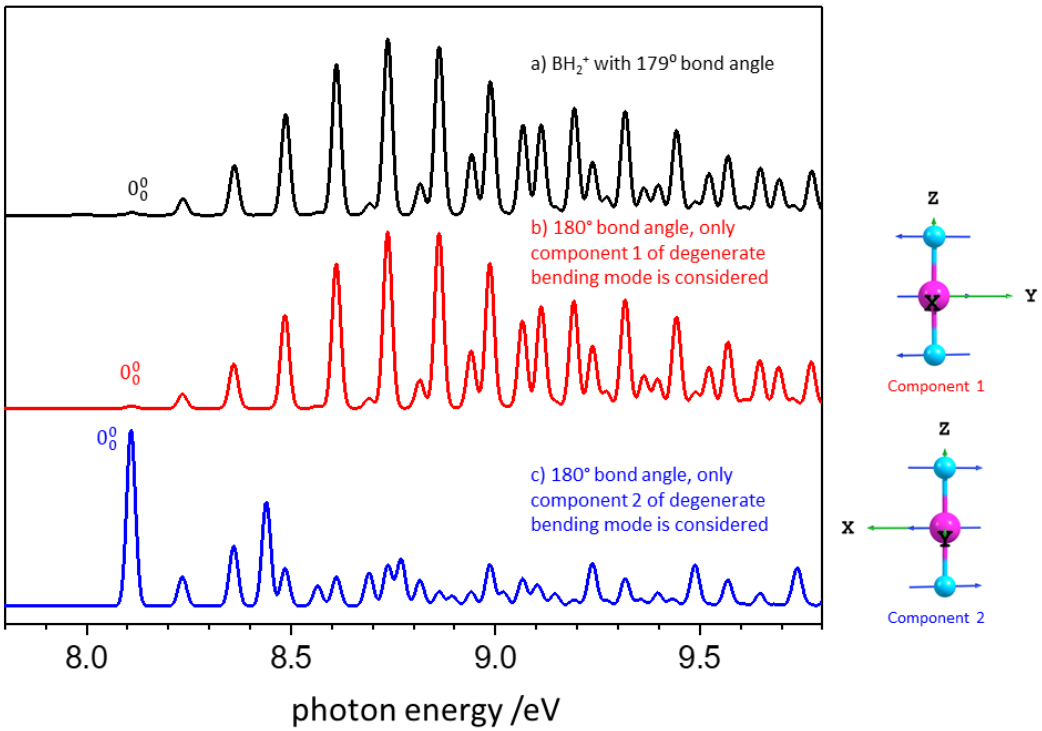

Figure S1: Comparison of different simulations of the slow photoelectron spectrum (SPES) of $^{11}BH_2$, using PGOPHER.[1] Trace a) assumes a cationic geometry with 179^0 bond angle. Trace b) and c) correspond to the linear cation, considering only the component of the bending vibration indicated on the right-hand side of the Figure. The z-axis is chosen as the principal axis. It is evident that simulations a) and b) are consistent with the experimental spectrum, while the simulation given in trace c) is inconsistent.

1. C. M. Western, *JQSRT*, 2017, **186**, 221-242.