A DPF ANALYSIS YIELDS QUANTUM MECHANICALLY ACCURATE ANALYTIC POTENTIAL ENERGY FUNCTIONS FOR THE $A\,^1\Sigma^+$ and $X\,^1\Sigma^+$ STATES OF NaH

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Alkali hydride diatomic molecules have long been the object of spectroscopic studies.[a] However, their small reduced mass makes them species for which the conventional semiclassical-based methods of analysis tend to have the largest errors. To date, the only quantum-mechanically accurate direct-potential-fit (DPF) analysis for one of these molecules was the one for LiH reported by Coxon and Dickinson.[b] The present paper extends this level of analysis to NaH, and reports a DPF analysis of all available spectroscopic data for the $A\,^1\Sigma^+ - X\,^1\Sigma^+$ system of NaH which yields analytic potential energy functions for these two states that account for those data (on average) to within the experimental uncertainties.

[a] W.C. Stwalley, W.T. Zemke and S.C. Yang, J. Phys. Chem. Ref. Data **20**, 153-187 (1991).
[b] J.A. Coxon and C.S. Dickinson, *J. Chem. Phys.* **121**, 8378 (2004).