ELECTRONIC STATE OF CoH: A PROBLEM RELATED TO THE SIZE-INCONSISTENCY OF THE MR-SDCI METHOD AND THE MIXING OF $^3\Phi$ AND $^3\Pi$

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The ground state of CoH has been determined experimentally as the $^3\Phi$ by the far-infrared magnetic resonance study,[a] and theoretically by *ab initio* methods.[b] However, MR-SDCI and MR-SDCI + Q *ab initio* molecular orbital calculations predicted that the lowest electronic state is $^5\Phi$. The size-consistent MR-ACPF method correctly predicted that $^3\Phi$ should be the ground state. As is previously reported by Tanaka *et al.*[c] on FeH, the controversial results in MR-SDCI may arise through truncation error inherent in the size-inconsistent MR-SDCI method.

Another difficulty is that we cannot clearly separate the Φ and Π states when CoH is treated under C_{2v} symmetry, not under its real symmetry of $C_{\infty v}$. The best results we obtained at the moment are: r_e = 1.528 Å, B_e = 7.291 cm^{-1}, and ω_e = 2005 cm^{-1} at the level of the MR-ACPF + relativistic correction using the Roos ANO (Co) and Dunning aug-cc-pVQZ (H) basis sets.

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[b] D.P. Chong, S.R. Langhoff, C.W. Bauschlicher, Jr., S.P. Walch, and H. Partridge, *J. Chem. Phys.*, 85, 2850-2860 (1986); M. Freindorf, C. M. Marian, and B. A. Hess, *J. Chem. Phys.*, **99**, 1215-1223 (1993).

[c] K. Tanaka, M. Sekiya, and M. Yoshimine, *J. Chem. Phys.*, **115**, 4558-4564 (2001).