AB INITIO POTENTIAL ENERGY SURFACE AND EIGENVALUES OF $A^2\Delta$ STATE OF ArCH[a]

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Rotationally resolved spectra of A-X transition of ArCH/D van der Waals complex have been reported previously and 7 bands were tentatively assigned. In order to make more definite assignments high level ab initio calculations have been performed.

2-D interaction potential for CH(A)-Ar (with CH bond fixed at r_e=1.102$\mathring{A}$ for $A^2\Delta$) was calculated with MRSDCI method including Davidson and counterpoise correction. The basis set was Dunning's correlation-consistent vqz with diffuse *s* and *p* orbitals.

The potential surface exhibits two minima, linear Ar...H-C and Ar...C-H whose respective well depths are 85 cm^{-1} and 60 cm^{-1}. The potential anisotropy is dominated by dipole and quadrupole terms on CH. Bound ro-vibrational eigentates were calculated for various **J** values and compared with experimental results.

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