Symmetry breaking in a nutshell.

The *odyssey* of a pseudo problem in molecular physics.

The $\tilde{X}\,^2\Sigma_u^+$ BNB case revisited.

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The $\tilde{X}\,^2\Sigma_u^+$ BNB state considered to be of symmetry broken (SB) character has been studied by high level multi reference variational and full configuration interaction methods. We discuss in great detail the roots of the so called SB problem and we offer an in depth analysis of the unsuspected reasons behind the double minimum topology found in practically all previous theoretical investigations. We argue that the true reason of failure to recover a $D_{\infty h}$ equilibrium geometry lies on the lack of permutational symmetry of the wavefunctions employed and is by no means a real effect.[1]

[1] Apostolos Kalemos, submitted for publication to J. Chem. Phys.