

A DIATOMIC MOLECULE WITH EXTREMELY LARGE AMPLITUDE MOTION IN ITS VIBRATIONAL STATES THAT HAVE LENGTHS OF AT LEAST 12,000 ÅNGSTRÖMS.

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The state-of-the-art empirical potential, *and* the state-of-the-art *ab initio* potential for the $b(1^3\Pi_{2u})$ state of ${}^{7,7}\text{Li}_2$ agree with each other that the $(v = 100, J = 0)$ ro-vibrational state has an outer classical turning point larger than the diameter of most bacteria and many animal cells. The 2015 empirical potential^a based on a significant amount of spectroscopic data, predicts the $(v = 100, J = 0)$ level to be bound by only $0.000\,000\,000\,004\text{ cm}^{-1}$ ($< 0.2\text{ Hz}$). The outer turning point of the vibrational wavefunction is about $671\,000\text{ Å}$ or 0.07 mm . Here, the two Li atoms are bound to each other, despite being nearly as far apart as the lines on a macroscopic ruler. The 2014 *ab initio* calculation based on a powerful Fock space MRCC method^b and with the long-range tail anchored by C_3^{Li}/r^3 with the ultra-high precision 2015 value of C_3^{Li} , has this same level bound by $0.000\,000\,000\,1\text{ cm}^{-1}$ ($< 3\text{ Hz}$), with an outer turning point of $> 0.01\text{ mm}$. While this discovery occurred during a study of Li_2 , the $b(1^3\Pi_{2u})$ states of heavier alkali diatomics are expected to have even larger amplitude vibrational states. While it might be tempting to call these very large molecules “Rydberg molecules”, it is important to remember that this term is already used to describe highly excited *electronic* states whose energy levels follow a formula similar to that for the famous Rydberg series. The highly delocalized *vibrational* states are a truly unfamiliar phenomenon.

^aDattani (2015) <http://arxiv.org/abs/1508.07184v1>

^bMusial & Kucharski (2014) *Journal of Chemical Theory and Computation*, **10**, 1200.