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Atom-diatom intermolecular forces and three body dispersion coefficients for doublet Li_3 JASON N. BYRD, JOHN A. MONTGOMERY, H. HARVEY MICHELS, ROBIN COTE, University of Connecticut Storrs — We calculate *ab initio* the ground state interaction potential surface for the lithium doublet trimer for both long range and near equilibrium geometries. A variety of methods are used to calculate the interaction energy, including complete active space SCF, full valence configuration interaction and coupled cluster theories as appropriate. Interpolation between *ab initio* points is accomplished with a dual-level interpolant moving least squares fitting algorithm using a scaled gaussian weight function. The global potential energy surface is found to have a large three-body interaction contribution. The atom-diatom dispersion coefficients ($C_n^\lambda(r,\theta)$) for long range interactions ($R \gg r$) are found by fitting to the *ab initio* surface.

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