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High Precision Calculations of the Lennard-Jones Lattice Constants for Five Lattices MATTHEW STEIN, Southern Methodist University — The total potential energy of a crystal as described by the Lennard-Jones (L-J) potential depends in part upon the calculation of lattice constants. Knowing these constants to high precision is useful for prediction of the lattice type and simulation of crystals such as rare-gas solids or germanium detectors, but reaching higher precision is computationally costly and challenging. Presented here is the extension of the precision of the lattice constants, L_p, up to 32 decimal digits, and in some cases corrections from previous publication. The L_p terms are given for $4 \leq p \leq 30$ in the simple cubic, face-centered cubic, body-centered cubic, hexagonal-close-pack, and diamond lattices. This precision was obtained through the use of careful parallelization technique, exploitation of the symmetries of each lattice, and the "onionization" of the simulated crystal. The results of this computation, along with the tools and algorithm strategies to make this computation possible, are explained in detail graphically.

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