# Atomvolumen, Packungsdichte und chemische Bindung in festem Iod unter Druck

Atomic Volume, Packing Density and Chemical Bonding in Solid Iodine under Pressure

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The volume changes of solid iodine under pressure are discussed with respect to the packing density of the atoms and to valence. The packing density of solid iodine which is 0.805 under ambient pressure increases to 0.976 in monoatomic iodine-II, 0.993 in iodine-III, and 1 in fcc iodine-IV. Simultaneously, the valence increases from 1 in the free molecule to 1.78 in the crystal structure under ambient pressure, 2.72 – 2.81 in iodine-II, 2.86 – 2.96 in iodine-III, and 3 in fcc iodine-IV. The valence then remains constant up to about 180 GPa and rises moderately to 3.15 at the highest investigated pressure of 276 GPa. Parameters for calculating bond numbers, valences and atomic volumes of densely packed halogens, hydrogen, oxygen, and nitrogen are given.

*Key words:* Iodine, High Pressure, Atomic Volume, Packing Density, Chemical Bonding