SECOND MOMENTS (PLANAR MOMENTS) AND THEIR APPLICATION IN SPECTROSCOPY

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Second moments, also called planar moments ($P_{ii} = \Sigma m_i x_i^2$), are the spectroscopic parameters[a] used to determine substitution structures (r_s)) by Kraitchman's method from spectra of a molecule and its isotopologs. They are also useful for discussing other molecular structural properties. Just as bond lengths and angles are considered transferable among similar molecules, second moments of many common groups are also transferable. This paper discusses applications of second moments of methylene/methyl groups, singly or multiply, isopropyl/tert-butyl groups, phenyl groups, perfluoro methylene/methyl groups, combinations of any of them, and planarity of molecules, the historically most common application of second moments. The inertial defect is $\Delta = (I_c - I_a - I_b)$ or $-2P_{cc}$. Some authors err by assuming each isotopolog provides three independent rotational constants, but in some cases they are not all independent.

[a] J. Kraitchman, *Am. J. Phys.* ***21*** *(17), 1953.*