

At the recent CCP5 meeting at Royal Holloway College I presented some M. D. results of the plastic crystalline phase of  $SF_6$  which gave a temperature, as calculated from linear velocities, systematically different from that as calculated from angular velocities. The suggestion that this is evidence that the elementary excitations in the system involve a coupling between the translational and rotational motion was not well received, but as there was no clear argument as to why this would not be so I wish to raise the matter in these pages so that people can ponder the matter at length. Equipartition takes place between the elementary excitations of the system, and if there is translational-rotational coupling therein then the use of (say) linear velocities alone to find the temperature is not valid. The system can be expressed in terms of any set of generalised coordinates, and the temperature obtained from the squares of these generalised velocities is independent of the coordinate system as long as the total number of generalised velocities is included. However one cannot take an arbitrary subset and hope to get the right temperature, and the set of linear velocities is such an arbitrary subset.