Erratum: Structure of amorphous selenium studied by neutron diffraction

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i.e., the $u \to 0$ approximation. It can be readily shown that with these rate constants the Master equation has an analytic solution. The population of the J level at time t, $N_J(t)$ is then of the form $N_J(t) = N_J(\infty) + [N_J(0) - N_J(\infty)] \exp(-\alpha t) = N_J(\infty)[1 - \exp(-\alpha t)] + N_J(0) \exp(-\alpha t)$. If $N_J(\infty) < N_J(0)$, $N_J(t)$ decays exponentially to its equilibrium value; if $N_J(\infty) > N_J(0)$, $N_J(t)$ rises exponentially to its equilibrium value; while if $N_J(\infty) = N_J(0)$, $N_J(t)$ stays constant. These features are evident in Fig. 1 and in the numerical simulations carried out by other workers.[1-3] Had we employed the $u \to 0$ approximation, the only changes in Fig. 1 would be an exact exponential relaxation of the moments and the absence of the weak "overshoot" in $N_J(t)$ for $J = 6$ (and 7). For lower values of u (or for a less skewed initial distribution than that employed in Fig. 1) the results would be even better. The only realistic exception[21] is H_2.

The intermediate region, $u \sim 1$, is under active study. The preliminary evidence is that the maximal entropy procedure[10] which is valid at both extremes will cover this region as well.

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Erratum: Structure of amorphous selenium studied by neutron diffraction [J. Chem. Phys. 62, 1556 (1975)]

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Since the publication of this article it has been brought to the authors' attention that the method developed to extrapolate the structure factor, measured by neutron diffraction, is very similar to the procedure described previously by J. H. Konnert and J. Karle in Acta Cryst. A 29, 702 (1973). We regret not having made reference to their work in the original manuscript.

Further, if we had known about this work, we should probably not, in the abstract of our paper, have referred to our method as "new."

