Comments and Errata to the Article "Mean Amplitudes of Vibration in Molecules with Internal Rotation: Halogenated Ethanes"  
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In the first article of the series on molecules with internal rotation 1 the following approximate formula was developed for the framework mean-square amplitude.

\[ \langle \Delta q^2 \rangle_{\text{frm}} = (\alpha + \beta \cos \theta + \gamma \cos 2\theta) \rho^2 \]  

(1)

one of the conclusions which have been reached.  
The coefficients \( \alpha(\theta, T) \), \( \beta(\theta, T) \) and \( \gamma(\theta, T) \) approach \( \theta \)-independent values when \( T \to \infty \).

This theorem was derived from the known properties of classical limits of mean-square amplitudes. In the present application to halogenated ethanes the above theorem has been verified numerically in the following way. The formula (1) with constant (\( \theta \)-independent) coefficients was found to reproduce the rigorously calculated framework mean amplitudes with numerical exactness (within 5 to 6 significant figures) at 298°K, as was already stated in the previous paper.  

At absolute zero on the other hand some deviations were detectable within the accuracy of the numerical computations. We have reached the conclusion that the approximation of constant \( \alpha \), \( \beta \), and \( \gamma \) is perfectly sound for halogenated ethanes at room temperature, and even valid with a high degree of accuracy at absolute zero.

Table 1. \( \alpha \), \( \beta \), and \( \gamma \) coefficients of eqn. (1) in Å² units.

<table>
<thead>
<tr>
<th></th>
<th>( T = 0 )</th>
<th>298°K</th>
<th>( T = 0 )</th>
<th>298°K</th>
<th>( T = 0 )</th>
<th>298°K</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )</td>
<td>0.03882</td>
<td>0.05978</td>
<td>0.00030</td>
<td>0.01194</td>
<td>-0.00029</td>
<td>-0.00037</td>
</tr>
<tr>
<td>( \beta )</td>
<td>0.05261</td>
<td>0.12823</td>
<td>-0.00316</td>
<td>0.02454</td>
<td>-0.00436</td>
<td>-0.02131</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>0.04126</td>
<td>0.15023</td>
<td>-0.00386</td>
<td>0.03136</td>
<td>-0.00321</td>
<td>-0.02620</td>
</tr>
</tbody>
</table>

The mentioned article 1 should be consulted for explanation of the adopted symbols. In the application to halogenated ethanes unfortunately the coefficients of \( \alpha \) and \( \gamma \) were given incorrectly. The reported coefficients 1 in fact apply to the form

\[ \langle \Delta q^2 \rangle_{\text{frm}} = (\alpha' + \beta \cos \theta + \gamma' \cos 2\theta) \rho^2 \]  

(2)

In Table 1 we give the correct coefficients, which are consistent with eqn. (1). They are given both at absolute zero and 298°K, and have been computed by means of an adjustment to the rigorous values at \( \theta = 0°, 90°, \) and 180°.

Some further studies have been made 2 on the nature of the inherent approximation of eqn. (1), including a consideration of the apparent constancy of the \( \alpha \), \( \beta \), and \( \gamma \) coefficients. The following statement is


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