Correction: Terahertz spectroscopy of the helium endofullerene He@C₆₀

Tanzeeha Jafari, George Razvan Bacanu, Anna Shugai, Urmas Nagel, Mark Walkey, Gabriela Hoffman, Malcolm H. Levitt, Richard J. Whitby and Toomas Rõõm*


Eqn (12) in the published version of this manuscript contained some errors. The equation should have read as:

\[
\langle l_f \mid T_k \mid l_i \rangle = (-1)^k \sqrt{\frac{(2l_f + 1)(2k + 1)(2l_i + 1)}{4\pi}} \left( \begin{array}{ccc}
0 & 0 & 0 \\
l_f & k & l_i \\
\end{array} \right)
\]

In addition, the published version of this manuscript contains missing information in some of the sentences. The corrected sentences are listed as follows:

1. Introduction:
   Page 9944, left column, 1st paragraph – ‘The incarceration of large noble gas atoms results in the structural and electronic distortion of C₆₀ which has been examined by IR and Raman, NMR, X-ray and electronic spectroscopy.’
   Page 9944, left column, 2nd paragraph – ‘It was spotted by mass spectrometry when the “He atom was incorporated in C₆₀ as the highly accelerated C₆₀⁺ ions struck with helium gas” and later found in fullerenes produced by arc discharge in the He gas.’

2. Theory:
   Page 9944, left column, 1st paragraph – ‘Also, we ignore the effect of the translational motion of C₆₀ in the crystal lattice and its molecular vibrations.’
   Page 9944, right column, 1st paragraph – ‘Factor \((\eta^2 + 2)/3\) is the enhancement of radiation electric field at the molecule embedded in dielectric and \(\eta\) is the index of refraction (for C₆₀ \(\eta = 2\), ref. 48).’

3. Discussion:
   Page 9947, left column, 1st paragraph – ‘Although the anharmonic contributions to the H₂ potential have been determined experimentally, a more detailed comparison with He is not meaningful as firstly, H₂ has translation–rotation coupling terms in the potential and secondly, it misses the V₆ term in the potential fit.’
   Page 9947, right column, Fig. 3 caption – ‘The anharmonic terms in the potential, V₁ and V₆, split the energy levels with different \(l\) and each energy level has the unique \(l\) value within the spherical symmetry, on the right.’
   Page 9947, right column, 1st paragraph – ‘In general, the interaction of neutral A with C₆₀ can be separated into repulsive interaction and electrostatic interaction expanded in induction and dispersion terms. Since He has no electric dipole nor quadrupole moment the induction terms are zero.’
   Page 9947, right column, 2nd paragraph – ‘To further validate the potential parameters of He@C₆₀ obtained from the fit of single high temperature spectra we compare the temperature dependence of line intensities of measured and calculated spectra, Fig. 4.’
   Page 9948, left column, 1st paragraph – ‘The dipole moment of He is induced by the displacement from the C₆₀ cage center.’

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.