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CORRECTION

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Correction: Chemical space: limits, evolution and modelling of an object bigger than our universal library

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Correction for 'Chemical space: limits, evolution and modelling of an object bigger than our universal library' by Guillermo Restrepo *et al.*, *Digital Discovery*, 2022, **1**, 568–585, https://doi.org/10.1039/D2DD00030J.

The originally published version of this article included errors, the corrections for which are summarised below.

The first paragraph of Section 2.1 should read:

"It has been estimated that the number of particles in the universe is about 10^{80},[28–30]** which amounts to 7×10^{76} atoms.†† A first approach to estimating the possible number of substances is determining the theoretical number of collections of atoms held together by chemical bonds. The number of such possible atomic ensembles is given by $\mathscr{C} = \sum_{k=1}^{10^{76}} \binom{k + 10^{76} - 1}{k}$, where $\binom{k + 10^{76} - 1}{k}$ is the number of ways of selecting k atoms from a collection of 10^{76} atoms, such that order is not important and repetitions are allowed.[32] So, here we are counting mono-, di, tri-, …, n-atomic ensembles up to the ultimate largest compound made of all 10^{76} atoms in the universe.‡‡ As usual in chemistry, we do not require the simultaneous "existence" of those substances, but the mere theoretical possibility of their existence and, importantly, of recording it.§§"

Footnote ‡‡ should read:

"This material upper bound requires further adjustments to touch physical and, above all, chemical reality. It requires taking some few atoms out of the 10^{76} to account for the synthesiser of the largest compound, which may be either a human or a robot. Besides the constraints discussed in note ‖, energetic conditions constitute the key factors determining whether an atomic ensemble is chemically feasible or not. This requires determining the suitable conditions of pressure and temperature holding together the given atoms by electrostatic interactions. Although the chemical space has been traditionally regarded at ambient conditions (see Section 4), there is uncharted land at extreme conditions.[33]"

In footnote ‖, the sentence beginning "An account of the 19th-century…" should read:

"An account of the 19th-century evolution of similarities among chemical elements is found in ref. 27."

In the PDF version of footnote ‡‡‡‡‡, two expressions have been typeset incorrectly. The relevant sentences should read:

"The number of disjoint parts of subsets for sets of size k is given by $\binom{n}{k}(2^{n-k} - 1)$. Finally, the total number of disjoint pairs of subsets for any size $k \leq n$ is given by $\sum_{k=1}^{n} \binom{n}{k}(2^{n-k} - 1)$."

In the caption for Fig. 3 and the first sentence of Section 5.1, the expression for s_t should read $s_t = 51.85e^{0.04324(t-1800)}$.

In Section 5.1, the expression for S_t should read $S_t = 1310.29e^{0.04305(t-1800)}$, and the equality should read $10^{200} = e^{0.04305(t-1800)}$.

In footnote ¶¶¶¶¶¶, the sentence beginning "In the directed hypergraph…" should read:

"In the directed hypergraph model, the density of the chemical network by year t (d_t), consisting of s_t substances and r_t reactions, is given by r_t/s_t, where r_t corresponds to the amount of directed hyperedges."

In the first paragraph of Section 6, the expression for $\mathscr{C}$ should read $\mathscr{C} = \sum_{k=1}^{10^{76}} \binom{k + 10^{76} - 1}{k}$.

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In Section 6, the sentence beginning "The charm of chemistry…" should read:
"The charm of chemistry is finding the function $f(t)$ mapping $\mathbb{C}$ to $\mathbb{I}(t)$."
The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.