Corrigendum: A solid–solid phase transition in carbon dioxide at high pressures and intermediate temperatures

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In Table 1 of this article, the values of lattice constants a and b of CO₂-III calculated by second-order Møller-Plesset perturbation theory ('4.33' and '4.63' in the rightmost column) were inadvertently swapped. The correct version of Table 1 appears below.

Table 1 | Structural parameters of CO₂-I and III.

Parameter*	Expt. [†]	Calc. [‡]	Calc. [§]
a (I)/Å	4.939 ± 0.010	4.92	4.91
a (III)/Å	4.330 ± 0.015	4.17	4.63
b (III)/Å	4.657 ± 0.005	4.65	4.33
c (III)/Å	5.963 ± 0.009	6.02	5.80
φ (III)/degree	52	51.9	54.8

* a (I) is the lattice constant of CO₂-I (Pa3). a (III), b (III) and c (III) are the lattice constants of CO₂-III (Cmca). φ (III) is the tilt angle (see Fig. 1) of CO₂-III.

[†]X-ray diffraction study at 11.8 GPa (ref. 20).

[‡]Empirical-force-field calculations at 12 GPa (ref. 31).

[§]Second-order Møller-Plesset perturbation calculations at 11.8 GPa (this work).