

Correction to “CO<sub>2</sub> Adsorption on Ti<sub>3</sub>O<sub>6</sub><sup>−</sup>: A Novel Carbonate Binding Motif”

Sreekanta Debnath, Xiaowei Song, Matias R. Fagiani, Marissa L. Weichman, Min Gao, Satoshi Maeda, Tetsuya Taketsugu, Wieland Schöllkopf, Andrey Lyalin,\* Daniel M. Neumark,\* and Knut R. Asmis\*

*J. Phys. Chem. C* **2019**, *123*, 13, 8439–8446. DOI: 10.1021/acs.jpcc.8b10724Cite This: <https://dx.doi.org/10.1021/acs.jpcc.0c01893>

Read Online

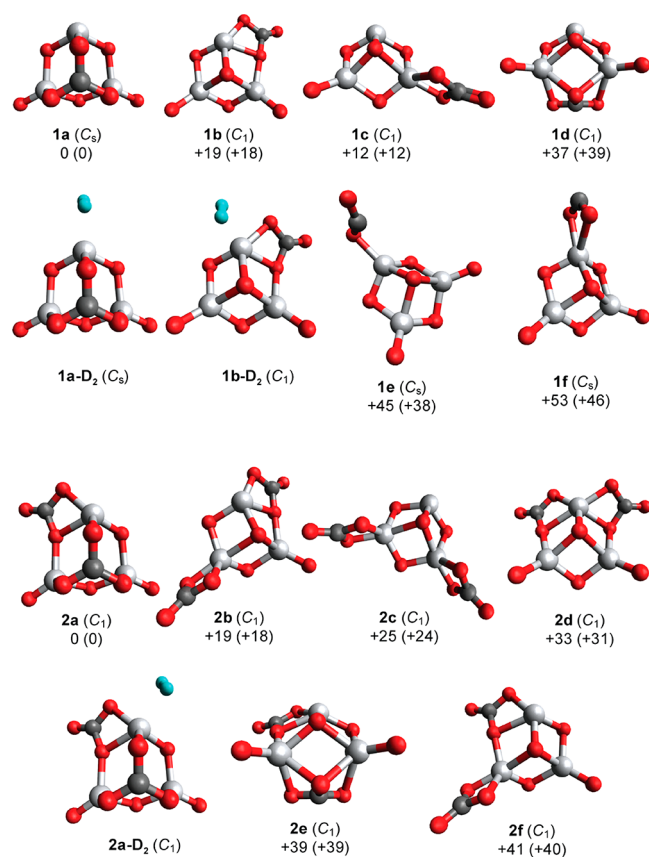
ACCESS |

Metrics &amp; More

Article Recommendations

Supporting Information

The published article contained erroneous CCSD(T) electronic energies. This concerns all CCSD(T) energies mentioned in the article, including values in Figure 3 and Table 2 as well as Figure S4 and Tables S2 and S3 of the



**Figure 3.**  $\omega$ B97X-D/aug-cc-pVTZ minimum-energy structures, symmetry (in parentheses) and relative energy  $\Delta E_{\text{DFT}}$  (in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of energetically low-lying  $[\text{Ti}_3\text{O}_6(\text{CO}_2)_{n=1,2}]^-$  isomers. The ZPE-corrected energies  $\Delta E_{0,\text{DFT}}$  are given in parentheses. The isomers are labeled with  $nx$ , where  $n$  is the number of  $\text{CO}_2$  molecules adsorbed and  $x = a, b, c, \dots$  indicates the energetic ordering. Atoms in gray represent Ti, dark gray C, red O, and blue H. The structures of  $\text{D}_2$ -tagged species for 1a, 1b, and 2a are also shown.

**Table 2.**  $\omega$ B97XD/aug-cc-pVTZ and CCSD(T)/def2-TZVP Relative Electronic Energies,  $\Delta E_{\text{DFT}}$  and  $\Delta E_{\text{CCSD(T)}}$ , as Well as ZPE-Corrected Energies  $\Delta E_0$  (All Energies in  $\text{kJ}\cdot\text{mol}^{-1}$ ) of the Lowest-Energy Minimum-Energy Isomers of  $[\text{Ti}_3\text{O}_6(\text{CO}_2)_{n=1,2}]^-$  at the Corresponding  $\omega$ B97XD/aug-cc-pVTZ Minimum-Energy Geometry<sup>a</sup>

$n$	isomer	$\Delta E_{\text{DFT}}^a$	$\Delta E_{0,\text{DFT}}^b$	$\Delta E_{\text{CCSD(T)}}^a$	$\Delta E_{0,\text{CCSD(T)/DFT}}^b$
1	1a	0.0	0.0	0.0	0.0
	1b	19.1	18.0	17.6	16.4
	1c	12.0	11.9	5.3	5.2
	1d	37.4	39.2	18.2	20.1
	1e	45.1	38.2	17.5	10.7
	1f	53.4	46.2	16.3	9.1
2	2a	0.0	0.0	0.0	0.0
	2b	18.5	17.8	8.0	7.2
	2c	24.5	24.2	7.8	7.5
	2d	32.5	30.6	22.8	20.8
	2e	39.2	38.8	12.6	12.3
	2f	41.4	40.1	27.0	25.8

<sup>a</sup>Absolute energies:  $-3189.03837$  au (1a, DFT),  $-3186.14665$  au (1a, CCSD(T)),  $-3377.67800$  au (2a, DFT),  $-3374.51650$  au (2a, CCSD(T)). <sup>b</sup>ZPE determined from  $\omega$ B97XD/aug-cc-pVTZ harmonic vibrational frequencies.

**Supporting Information.** In addition, the calculated spectra of 1e and 1f were incorrectly labeled in Figure S2. Corrected Table 2 and Figure 3 are presented here, and the corrected Supporting Information figures and tables are deposited. These corrections do not affect the main conclusions drawn in the paper.

Page 8442, second paragraph (left column): “Note that the physisorbed complexes (1e, 1f) are predicted to lie even higher in energy when the CCSD(T) energies are considered (see Table 2).”

**Corrected:** “Note that the physisorbed complexes (**1e**, **1f**) are predicted to lie lower in energy when the CCSD(T) energies are considered (see Table 2).”

Page 8442, second paragraph (left column): “However, when the CCSD(T) energies are considered, structures **1a** and **1b** are nearly isoenergetic, with **1b** predicted only +0.3 kJ/mol higher in energy. Moreover, when the harmonic vibrational ZPEs from DFT are combined with the CCSD(T) electronic energies, the energetic ordering is reversed and **1b** is indeed slightly favored by 0.8 kJ/mol.”

**Corrected:** “However, when the CCSD(T) energies are considered, the energy difference between structures **1a** and **1b** is reduced from 18 kJ/mol ( $\Delta E_{0,\text{DFT}}$ ) to 16 kJ/mol ( $\Delta E_{0,\text{CCSD(T)}}$ ).”

Page 8442, first paragraph (right column): “We determined the optimized geometry of the neutral analogue of **1a** and find that it lies 20 kJ/mol above the **1d** analogue using DFT (see Table S1). However, when the CCSD(T) energies are considered, the order is reversed; the **1a** analogue is predicted 11 kJ/mol below the **1d** analogue and thus is likely the ground state structure of neutral  $[\text{Ti}_3\text{O}_6(\text{CO}_2)]$ .”

**Corrected:** “We determined the optimized geometry of the neutral analogue of **1a** and find that it lies 20 kJ/mol above the **1d** analogue using DFT (see Table S2). When the CCSD(T) energies are considered, the order is confirmed; the **1a** analogue is predicted 32 kJ/mol above the **1d** analogue.”

## ■ ASSOCIATED CONTENT

### si Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpcc.0c01893>.

Corrected Figures S2 and S4 and Tables S2 and S3 (PDF)

## ■ ACKNOWLEDGMENTS

We thank Prof. David A. Dixon (University of Alabama) for drawing our attention to this issue.