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CORRECTION

Correction to: Determination of trace metal concentration in compost, DAP, and TSP fertilizers by neutron activation analysis (NAA) and insights from density functional theory calculations

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Correction to: Environ Monit Assess (December 2017) 189:618 https://doi.org/10.1007/s10661-017-6328-1

The original version of this article unfortunately contained an error in the body text and in Tables 4 and 6.

The corrected version of the sentences and Tables are given below.

The online version of the original article can be found at https://doi.org/10.1007/s10661-017-6328-1.

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Results and discussion

Page 9, under Interaction and binding of Cr, Sb, and As with DAP section, second paragraph, lines 3–6 should be rewritten as: As predicted, the binding energy, enthalpy, and the Gibbs free energy of CrO3-DAP is −87.46, − 88.06, and −37.17 kcal/mol;

Page 10, under Interaction and binding of Cr, Sb, and As with DAP section, last paragraph, lines 16–18 should be rewritten as: Compared to DAP, the HOMO and LUMO energies of the CrO_3-DAP, Sb_2O_3-DAP, and AsO_3-DAP complexes are significantly changed.

Page 10, under Interaction and binding of Cr, Sb, and As with DAP section, last paragraph, lines 24–25 should be rewritten as: And the HOMO and LUMO energies of the AsO_3-DAP complex are −9.53 and −4.07 eV respectively with a HOMO–LUMO gap of 5.46 eV.

Page 9, Title of Table 4 is corrected below.

Table 4 Selected bond distances (Å) and angles (°) of all complexes calculated at the B3LYP/SDD level of theory.

Page 10, The amended and corrected Table 6 is given in the next page.

Table 6 Energies (eV) of HOMO, LUMO orbitals, and HOMO–LUMO gaps are calculated at the B3LYP/SDD level of theory for all complexes

Molecular orbitals	CrO_3	Sb_2O_3	AsO_3	DAP	CrO_3-DAP	Sb_2O_3-DAP	AsO_3-DAP
LUMO + 2	−1.15	−0.84	−0.76	0.07	−0.41	1.97	−0.90
LUMO + 1	−1.27	−3.55	−4.35	−0.01	−0.72	−0.51	−1.72
LUMO	−1.27	−3.55	−5.46	−1.49	−1.82	−0.62	−4.07
HOMO	−8.95	−7.47	−10.26	−9.42	−9.48	−7.10	−9.53
HOMO-1	−10.09	−7.47	−10.35	−9.52	−9.55	−7.32	−9.62
HOMO-2	−10.09	−8.52	−11.06	−9.94	−9.85	−7.41	−10.00
Gap	7.68	3.92	4.80	7.93	7.66	6.48	5.46