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Corrigendum to

"Thermodynamics of reactions of ClHg and BrHg radicals with atmospherically abundant free radicals" published in Atmos. Chem. Phys. 12, 10271–10279, 2012

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We have identified three errors in the above-referenced manuscript.

1. At the bottom of p. 10 276, the reference to Eq. (5) should be to Eq. (4).

2. The values listed in Table 5 are actually $1/K_{eq}$, where K_{eq} is the equilibrium constant for the reaction listed. The corrected Table 5, on the right-hand side, is consistent with Eq. (1a) and Eq. (1b) of the original paper.

3. We mischaracterized the compounds described by Balabanov and Peterson (2003, cited as 2003b in the original paper). Balabanov and Peterson (2003) listed compounds as HgBrO and HgClO, following a convention of stoichiometric formulae in which atoms are listed from least to most electronegative. We misread these *stoichiometric* formulae as *structural* formulae for HgBrO and HgClO (a mercury atom bound to the halogen atom of a BrO or ClO radical). In fact, Balabanov and Peterson (2003) were describing divalent Hg(II) compounds with structural formulae BrHgO and ClHgO (a mercury atom bound directly to both an oxygen atom and a halogen atom). Note these same divalent Hg(II) compounds are described by stoichiometric formulae in another paper by Balabanov and Peterson (2004). In fact, no previous paper describes molecules with the structural formula HgBrO or HgClO.

To determine if BrO or ClO could bind to Hg(0), we characterized compounds with structural formulae HgBrO and HgClO using the same approach as described in our original paper. The computed Hg–XO bond lengths were ∼3.6 Å and ∼3.8 Å for X = Br and Cl, respectively, which are more characteristic of van der Waals complexes than covalent bonds. The bond energies at CCSD(T)/aVTZ were negative, indicating extremely weak bonding. Balabanov and Peterson (2013) also obtained results suggestive of van der Waals molecules. Field studies (Obrist et al., 2011; Tas et al., 2011) and experiments (Raofie and Ariya, 2004; Spicer et al., 2005) had suggested that BrO can initiate Hg(0) oxidation. By contrast,

Table 5. Recommended equilibrium constant, $K_{eq}(T)$, for Br + Hg → BrHg as a function of temperature for two standard states.

$T(K)$	K_{eq} (standard state)	
	(1 molecule cm^{-3})	(1 bar)
200	8.03×10^{-7}	2.91×10^{13}
210	1.25×10^{-7}	4.30×10^{12}
220	2.30×10^{-8}	7.57×10^{11}
230	4.91×10^{-9}	1.55×10^{11}
240	1.19×10^{-9}	3.60×10^{10}
250	3.25×10^{-10}	9.41×10^{9}
260	9.78×10^{-11}	2.73×10^{9}
270	3.22×10^{-11}	8.64×10^{8}
280	1.15×10^{-11}	2.97×10^{8}
290	4.40×10^{-12}	1.10×10^{8}
298	2.14×10^{-12}	5.21×10^{7}
300	1.80×10^{-12}	4.35×10^{7}
310	7.80×10^{-13}	1.82×10^{7}
320	3.56×10^{-13}	8.06×10^{6}

the present work suggests that BrO cannot initiate gas-phase oxidation of Hg(0).

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