Comparison of SO_2 and CO_2 absorption by diamines

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The presence of SO_2 gas out of standard value at the atmosphere causes damages to human health and environment. There are various methods to remove SO_2 exhaust from the flue gas. One of the latest considered methods is the absorption in which diamines are used as solvent. In the current study, quantum density functional theory computation at gas phase was applied to study the absorption characteristics of SO_2 and CO_2. First, the optimum structure and energy of all three diamine compounds, SO_2 and CO_2 were explored by the computational level of theory B3LYP/6-31G(d,p) [1]. Then, the frequency analysis of the combinations was performed to guarantee the structures are at the ground state; notice that frequency must be positive. Studying the interaction of the diamines with SO_2 and CO_2 was carried out by introducing the gases to the diamines at the initial distance of 3 Å. Finally, the compounds at the same computational level were optimized and E_{abs} was obtained through the following relation; see Table 1 for the results.

$$E_{abs} = E_{diamine\ with\ SO_2\ or\ CO_2} - \left(E_{pure\ diamine} + E_{pure\ SO_2\ or\ CO_2}\right) \quad (1)$$

Table 2: The absorption energy and the final distance of the diamine from the gas

System	Absorption energy (kJ mol^{-1})	Final distance (Å)	System	Absorption energy (kJ mol^{-1})	Final distance (Å)
N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + SO_2	-55.25	2.40	N,N'N'-(trimethyl)-N-(2-hydroxyethyl)-ethylenediamine + CO_2	-24.39	3.05
N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + SO_2	-62.55	2.39	N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine + CO_2	-23.46	3.08
N,N'-dimethylpiperazine + SO_2	-43.21	2.50	N,N'-dimethylpiperazine + CO_2	-15.35	2.86

The results show that N,N,N',N'-tetrakis (2-hydroxyethyl) ethylenediamine has the highest absorption energy for SO_2 than CO_2 in comparison with other diamines. In addition, this solvent shows the lowest distance from SO_2.

Keywords: Flue Gas, Absorption Energy, Diamine, DFT

Reference

[1] N. Hedin, L. Chen and A. Laaksonen, *Nanoscale*, 2010, 2, 1819