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Interaction of nitrogen dioxide with free base phthalocyanine

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Abstract

Quantum chemical *ab initio* method was used to investigate interactions between NO_2 and H_2Pc. Four possible sites for NO_2 adsorption were considered. Full geometry optimisation together with frequency calculation was performed for the isolated molecules and the NO_2–H_2Pc complexes with the use of 6-31*g*(*d*, *p*) and minimal basis sets, respectively. Two stable and two transition states were found. The H_2Pc molecular structure was found to be largely affected under the influence of NO_2. It was found that for a certain chemisorption site H_2Pc molecule might disintegrate and its building blocks could react with NO_2 forming other species.

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