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Interactions of hydroxyl radicals with ice: A molecular dynamics study

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Molecular dynamics (MD) simulations were used to investigate the behaviour of hydroxyl radicals at air-water and air-ice interfaces. Parameters such as orientation at the surface and duration of interactions with the surface varied in expected ways as a function of temperature. This is in contrast to compounds such as aromatic species which have been shown experimentally and theoretically to interact very differently with ice and water surfaces at identical temperatures. The results were used to predict uptake coefficients including mass accommodation and reactive uptake. The predicted reactive uptake coefficients were higher on ice surfaces than on liquid water surfaces at the same temperature. This suggests that recombination of OH to form hydrogen peroxide might be much more rapid on ice; this could be an important sink for OH in snow and ice, and could help to explain recent experimental results which indicate that OH is unreactive toward some organic species at air-ice interfaces.

Please list some keywords

ice, water, quasi-liquid layer, hydroxyl radicals (OH), hydrogen peroxide (H2O2), uptake coefficient

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