Hydrogen bond acceptor ability of selenium is not too weak compared to sulfur and oxygen

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Quest for new hydrogen bond donor and acceptor centers is an active research area. Along the chalcogen series, O and S are the most investigated hydrogen bond motifs with almost equal strength[1]. The next element along the series is Se which is having an electronegativity of 2.55 in the Pauling scale and is almost comparable to that of S (2.58). Se is present in Selenocysteine which is the 21st amino acid. Although the potential of Se as a hydrogen bond motif is established very recently. Hence, there is a scarce of experimental evidence for the selenium centered hydrogen bonding[2-4].
In the current study, the hydrogen bond acceptor property of Se has been investigated using Matrix Isolation Infrared spectroscopy. The experiments have been performed with three different hydrogen bond donor molecules, H_2O, CH_3OH, and C_2H_5OH with $(CH_3)_2Se$ as the hydrogen bond acceptor molecule to study O-H···Se interaction. All the experiments have been performed at 8 K. The formation of the complexes is monitored by changes in the infrared spectral patterns in the mixture compared to the monomer spectra. The nature of the intermolecular complexes formed has been characterised using quantum chemical calculations. Comparing the theoretical and experimental results, it is concluded that the complexes formed under the cold condition are stabilised by O-H···Se hydrogen bonding interaction. Different conformers of the complexes with marginally different stabilization energies have also been identified under the matrix isolation condition. The nature of the selenium centered hydrogen bonding interaction has been determined using different theoretical techniques. Finally, the strength of the selenium-centered hydrogen bonding has been compared with two of the analogous chalcogens, i.e., O and S. It is found that Se forms a hydrogen bond of almost equal strength to that of O and S. Almost equivalent red-shift in the O-H stretching frequency of the hydrogen bond donor is observed by comparing similar systems that have been studied previously. In addition to this, a short discussion will be presented on N-H···Se hydrogen bonding interaction studied experimentally between NH_3, $(CH_3)_2NH$ as hydrogen bond donor and $(CH_3)_2Se$ as acceptor. A similar comparison with O, S and Se centers as hydrogen bond acceptors will be presented.

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