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Title:	Structure and stability of spiro-cyclic water clusters
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Atoms-in-molecules Atoms-in-molecules analysis Basis sets Cyclic clusters
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Publisher:	Indian Academy of Sciences
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Abstract:	The structure and stability of spiro-cyclic water clusters containing up to 32 water molecules have been investigated at different levels of theory. Although there exist minima lower in energy than these spiro-cyclic clusters, calculations at the Hartree-Fock level, density functional theory using B3LYP parametrization and second order Møller-Plesset perturbation theory using 6-31G* and 6-311++G** basis sets show that they are stable in their own right. Vibrational frequency calculations and atoms-in- molecules analysis of the electron density map confirm the robustness of these hydrogen bonded clusters.
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