DIMERS OF ALKALINE EARTH METAL HALIDE RADICALS, $(MX)_2$ (M = Be, Mg, Ca; X = F, Cl): A THEORETICAL STUDY

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Alkaline earth metal halide radicals, MX, di-halides, MX_2, and halide radical dimers, $(MX)_2$ (M = Be, Mg, Ca and X = F, Cl), are studied using density functional theory, MP2 and CCSD(T) methods. The ground states of MX_2 are all singlet $^1\Sigma_g{}^+$ with $D_{\infty h}$ symmetry except that of CaF_2 which is $^1A_1$ with C_{2v} symmetry. The ground states of $(MX)_2$ are all singlet ^1A_g with D_{2h} symmetry except that of $(CaF)_2$ which is $^3A_1$ with C_{2v} (distorted D_{2h}) symmetry. Stabilities of the halide radical dimers have been examined versus some reactions, such as $(MX)_2 \longrightarrow 2M + 2X$, $(MX)_2 \longrightarrow M_2 + X_2$, $(MX)_2 \longrightarrow 2MX$ and $(MX)_2 \longrightarrow MX_2 + M$. Several transition states of these reactions have been established at the MP2/6-311+G* level. The calculated results for the halide radicals and di-halides are in good agreement with experimental values. The calculated results for the halide radical dimers can serve as a guide for spectroscopic studies of these species.