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, MX₂, 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 MX₂ are all singlet ¹Σ⁺ with D₄h symmetry except that of CaF₂ which is ¹A₁ with C₂ᵥ symmetry. The ground states of (MX)₂ are all singlet ¹A_g with D₂h symmetry except that of (CaF)₂ which is ⁹A₁ with C₂ᵥ (distorted D₂h) symmetry. Stabilities of the halide radical dimers have been examined versus some reactions, such as (MX)₂ → 2M + 2X, (MX)₂ → MX₂ + X₂, (MX)₂ → 2MX and (MX)₂ → MX₂ + 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.