Disassociation of Molybdenum Chlorides

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The energies of the disassociation reactions of molybdenum chloride compounds were calculated using six different Density Functional Theory (DFT) methods. The molybdenum chloride compounds were modeled using the B3LYP level of theory with LanL2DZ and SDD as basis sets. These two basis sets produced nearly identical optimized geometries, and both compared favorably with available experimental data. Single-point calculations were run on these optimized geometries using a variety of methods and basis sets. The CCSD(T) method with LanL2DZ produced reaction energies nearest to available experimental data. After the reactions had been successfully modeled, transition state optimizations were run on two types of disassociation reactions. These were done with varying degrees of success. Transitions states for reactions that produce hydrogen chloride from a molybdenum chloride species and a hydrogen atom have been found for all of the molybdenum chloride compounds. However, the transition states for the unimolecular disassociation of these molybdenum chlorides have been considerably more difficult to find. These unimolecular transition states will hopefully be completed in the near future.

Reactions:	Unimolecular Decomposition:
$MoCl_6 + 1/2H_2$ ---------- > $MoCl_5 + HCl$	$MoCl_6$ ---------- > $MoCl_5 + Cl$
$MoCl_5 + 1/2H_2$ ---------- > $MoCl_4 + HCl$	$MoCl_5$ ---------- > $MoCl_4 + Cl$
$MoCl_4 + 1/2H_2$ ---------- > $MoCl_3 + HCl$	$MoCl_4$ ---------- > $MoCl_3 + Cl$
$MoCl_3 + 1/2H_2$ ---------- > $MoCl_2 + HCl$	$MoCl_3$ ---------- > $MoCl_2 + Cl$
$MoCl_2 + 1/2H_2$ ---------- > $MoCl + HCl$	$MoCl_2$ ---------- > $MoCl + Cl$
$MoCl + 1/2H_2$ ---------- > $Mo + HCl$	$MoCl$ ---------- > $Mo + Cl$