THEORETICAL STUDIES OF ELECTRONIC SPECTRA AND BONDING OF AlCl/AlF($X^1\Sigma^+$, $a^3\Pi$, $A^1\Pi$) WITH EXCITED STATES EXHIBITING RECOUPLED PAIR BONDING

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Ground electronic state rotational lines of AlCl and AlF have been observed in the circumstellar envelope of IRC +10216, and electronic transitions of AlF have been observed in sunspot umbra. We have performed high-level *ab initio* MRCI+Q and RCCSD(T) calculations with large correlation consistent basis sets up to augmented sextuple zeta quality including core-valence correlation effects on the ground state ($X^1\Sigma^+$) and two lowest excited states ($a^3\Pi$, $A^1\Pi$) of AlF and AlCl. Theoretical spectroscopic constants as well as vibrational and rotational spectra will be presented and compared with experiment. We will also discuss the nature of the bonding in these states. The excited states are formed via recoupled pair bonds, in which the Al $3s^2$ pair of electrons is decoupled to allow one of its electrons to recouple with a halogen to form a bond.