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A fragment-based ab initio study of some organometallics having interesting nonlinear optical effects GURU DAS, MLBP/AFRL, WPAFB, OH 45433, JEANE-PHILLIPPE BLAUDEAU, ASC/HP, WPAFB,OH 45433 — The *Ab initio* Fragment Orbital Theory (AFOT), which is essentially an approximate *ab initio* scheme that builds wavefunctions from those of its constituent fragments, is applied to study the singlet and triplet excited states of some Platinum containing organometallic compounds. These molecules have interesting nonlinear optical properties. AFOT is programmed as an extension onto GAMESS-US. Relativistic Effective Core Potential (RECP) theory of the Stevens et al. (SBK) variety is used. The results are compared with the corresponding Time-Dependent-Density-Functional-Theory (TDDFT) results.

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