Supporting Information for the Paper:
A DFT Computational Study of the Mechanism of Allyl Chloride Carbonylation Catalyzed by Palladium Complexes

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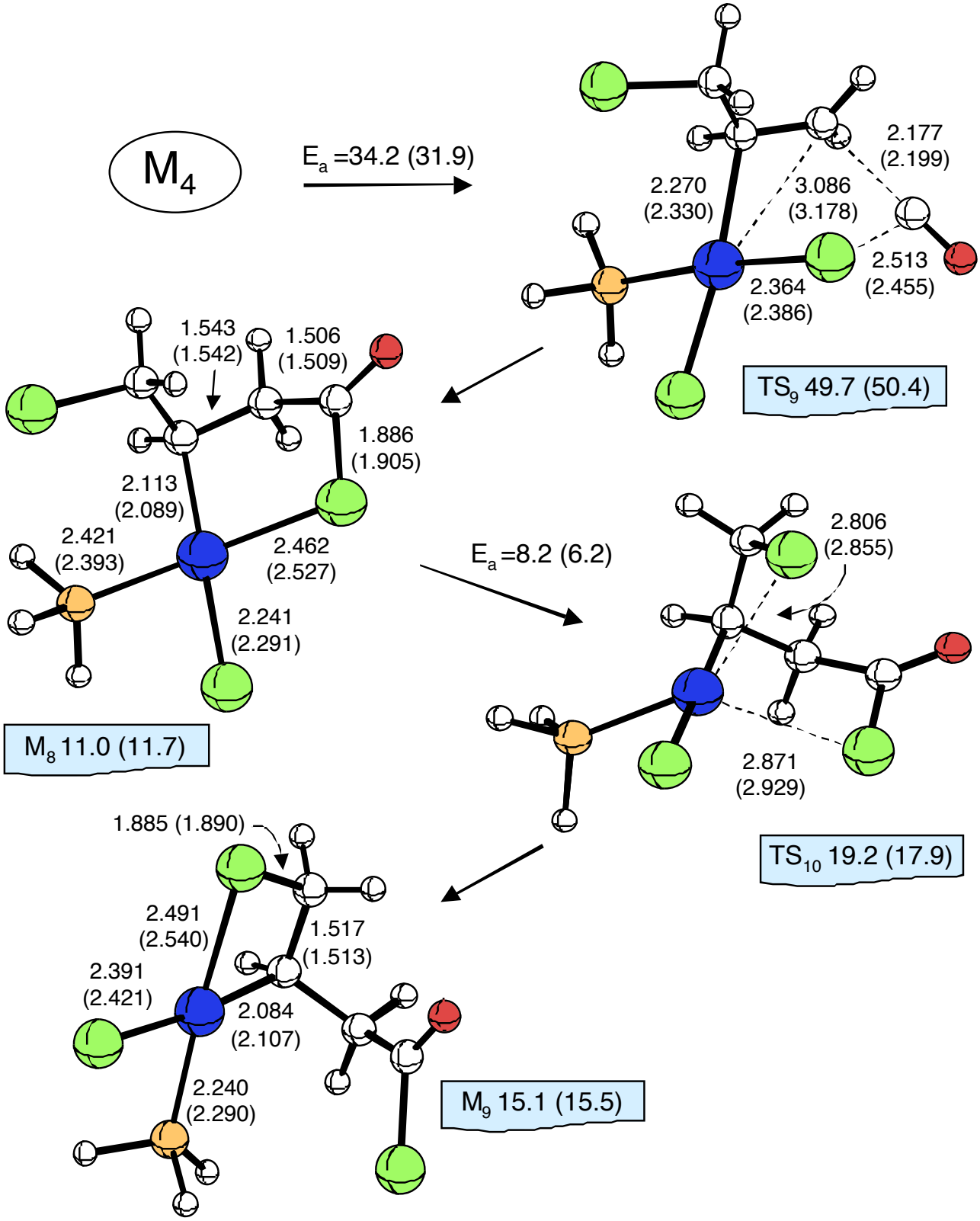

Figure 1S. Schematic representation of the structures of TS_9, M_8, TS_{10} and M_9. The energies (kcal mol^{-1}) are relative to non-interacting *trans*-$Cl_2Pd(PH_3)_2$ and allylchloride (asymptotic limit). E_a = activation barriers. Values in parenthesis: DZVP basis. The absolute energy of the asymptotic limit is: -2425.525368 a.u. (sdd/6-31G* basis) and –7237.198999 a.u. (DZVP basis). Bond lengths are in Ångstroms and angles in degrees.

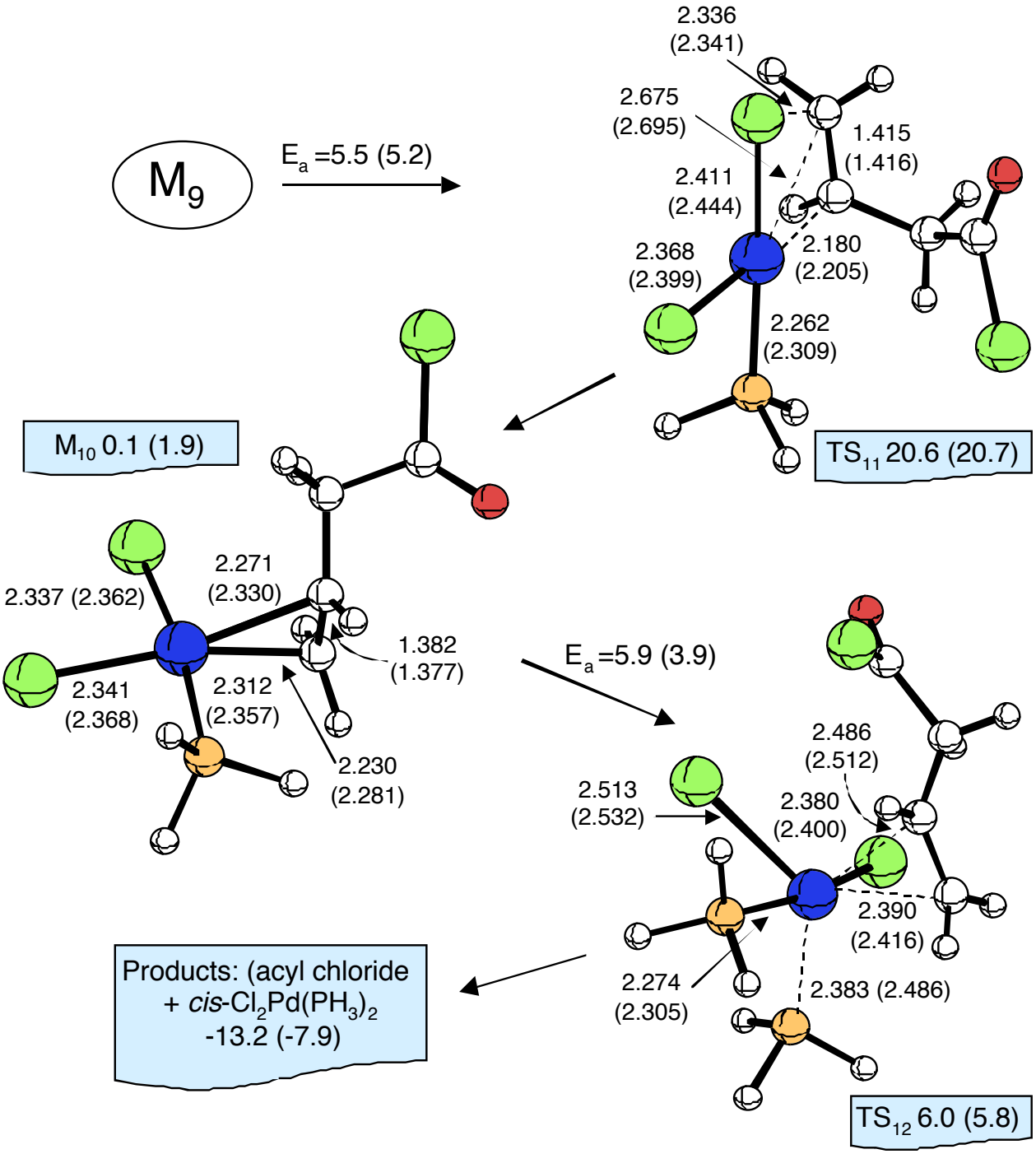

Figure 2S. Schematic representation of the structures of TS_{11}, M_{10} and TS_{12}. The energies (kcal mol^{-1}) are relative to non-interacting *trans*-$Cl_2Pd(PH_3)_2$ and allylchloride (asymptotic limit). E_a = activation barriers. Values in parenthesis: DZVP basis. The absolute energy of the asymptotic limit is: -2425.525368 a.u. (sdd/6-31G* basis) and –7237.198999 a.u. (DZVP basis). Bond lengths are in Ångstroms and angles in degrees.

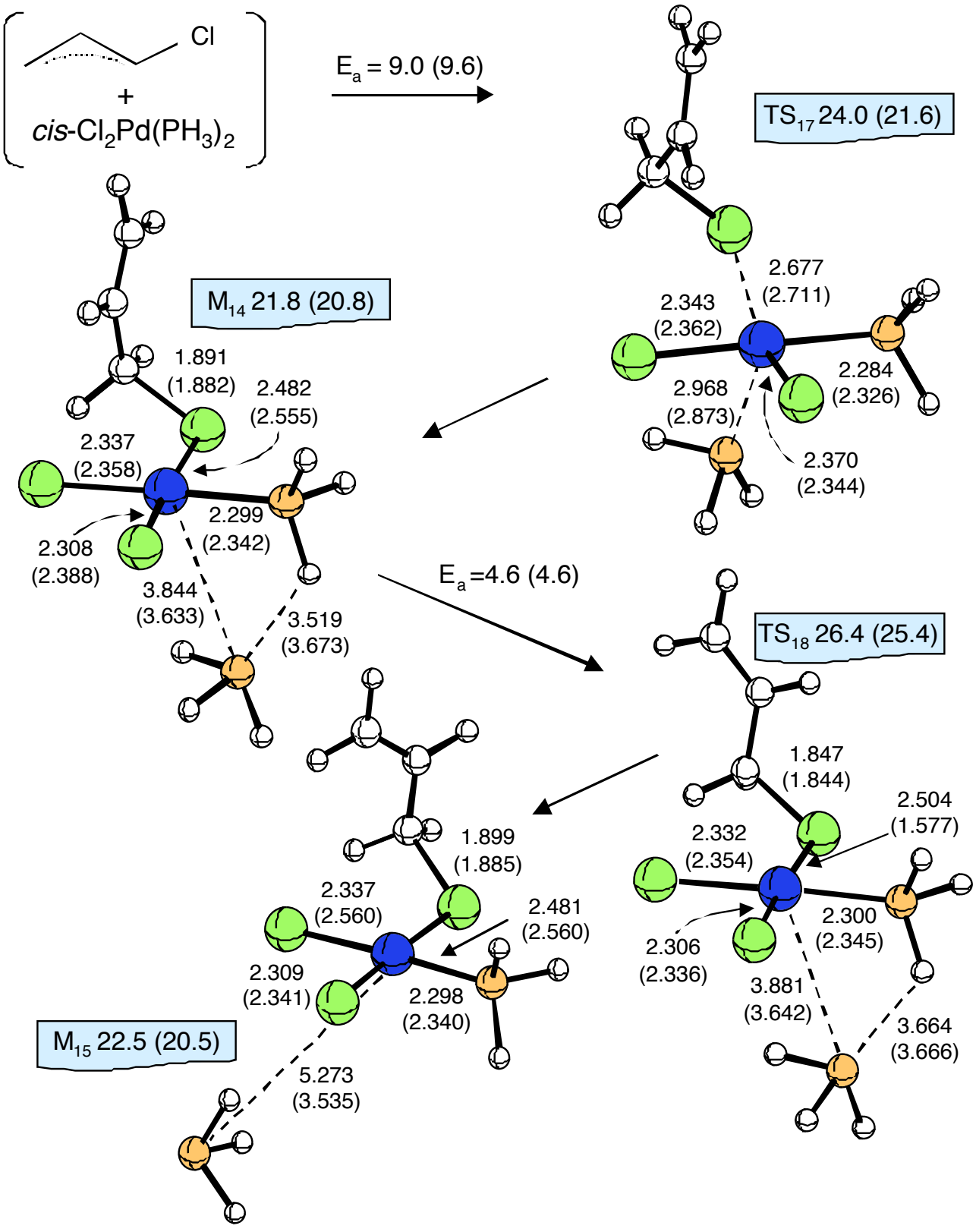

Figure 3S. Schematic representation of the structures of TS_{17}, M_{14}, TS_{18} and M_{15}. The energies (kcal mol^{-1}) are relative to non-interacting *trans*-$Cl_2Pd(PH_3)_2$ and allylchloride (asymptotic limit). E_a = activation barriers. Values in parenthesis: DZVP basis. The absolute energy of the asymptotic limit is: -2425.525368 a.u. (sdd/6-31G* basis) and –7237.198999 a.u. (DZVP basis). Bond lengths are in Ångstroms and angles in degrees.

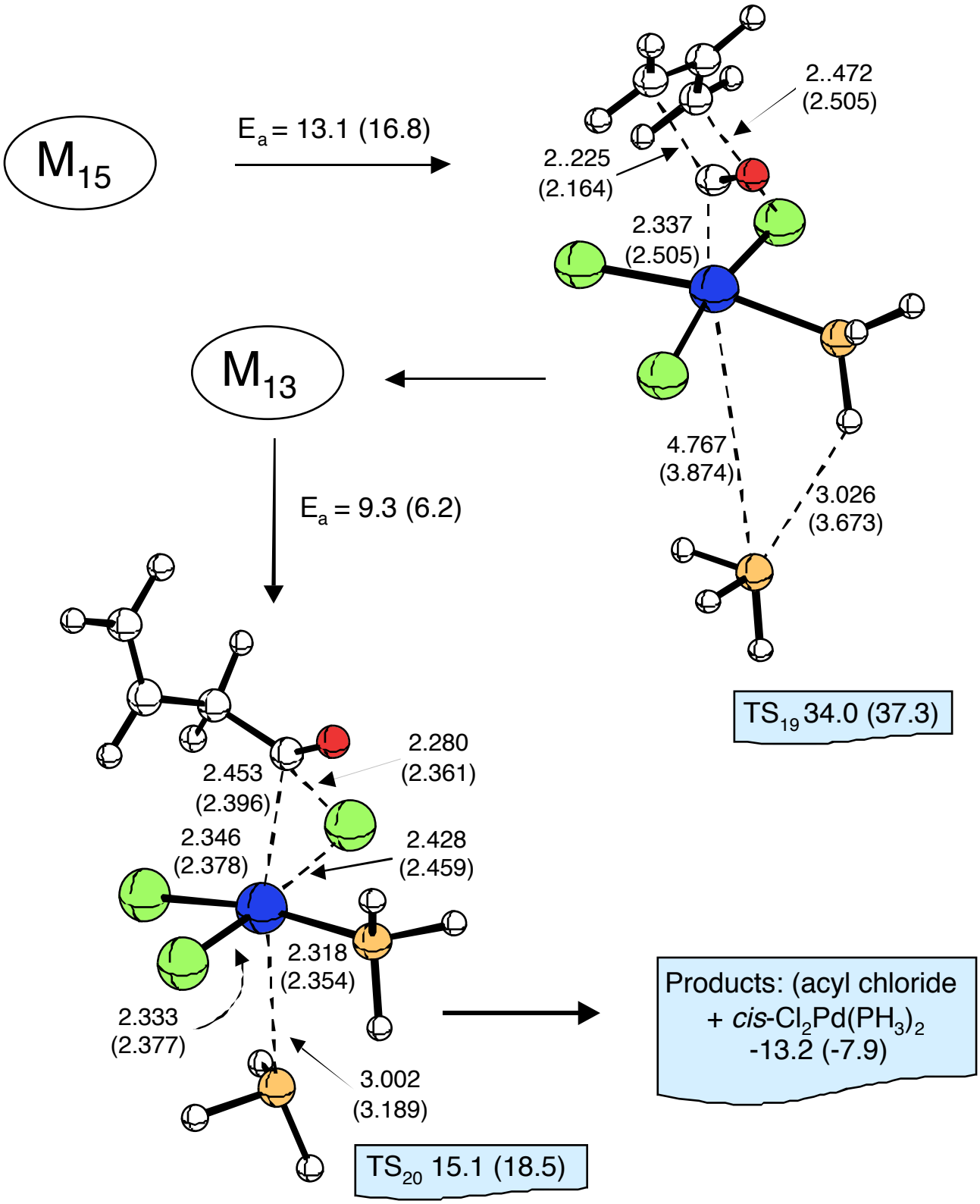

Figure 4S. Schematic representation of the structures of TS_{19} and TS_{20}. The energies (kcal mol^{-1}) are relative to non-interacting *trans*-$Cl_2Pd(PH_3)_2$ and allylchloride (asymptotic limit). E_a = activation barriers. Values in parenthesis: DZVP basis. The absolute energy of the asymptotic limit is: -2425.525368 a.u. (sdd/6-31G* basis) and –7237.198999 a.u. (DZVP basis). Bond lengths are in Ångstroms and angles in degrees.