Supplementary Material for PCCP

Supplementary Information

A comparison of the reactivity of germylene and dimethylgermylene with some methylgermanes. Direct kinetic and quantum chemical studies.

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Table S1 Estimated entropy changes and decomposition A factors for 1,1-dimethydigermane decomposition (reaction (-3))

T/K	ΔS^o/J K^{-1} mol^{-1} [a]	T/K	log(A_{-3}/s^{-1}) [b]
300	131.0	296	14.98
400	130.1	337	14.91
500	128.4	386	14.82
600	127.2	447	14.72
		553	14.53

[a] Values from Ge_2H_6 decomposition (see ref. 15). [b] Calculated via $\Delta S^o = R\ln(A_{-3}/A_3)$ with correction for standard state change.

Table S2 Temperature dependent parameters for RRKM calculations for 1.1-dimethyldigermane decomposition: RRKM(1), E_o = 154.8 kJ mol^{-1}.

T/K	553	447	386
Log (A/s^{-1})	14.53	14.72	14.82
$\tilde{\nu}$ (TS)/cm^{-1}	500(2)	470(2)	470(2)
	190(1)	150(1)	120(1)
	173(1)	130(1)	110(1)
Z_{LJ}/10^{-10} cm^3 molecule^{-1} s^{-1}	4.56	4.30	4.21

Table S3 Temperature dependent parameters for RRKM calculations for 1,1-dimethyldigermane decomposition: RRKM(2), E_o = 146.4 kJ mol^{-1}.

T/K	553	447	386
Log (A/s^{-1})	14.83	15.02	15.12
$\tilde{\nu}$ (TS)/cm^{-1}	470(2)	440(2)	390(2)
	135(2)	110(1)	98(1)
		98(1)	90(1)
Z_{LJ}/10^{-10} cm^3 molecule^{-1} s^{-1}	4.56	4.30	4.21

For RRKM(3), E_o = 138.1 kJ mol^{-1}. The other temperature dependent parameters are as in Table S3.

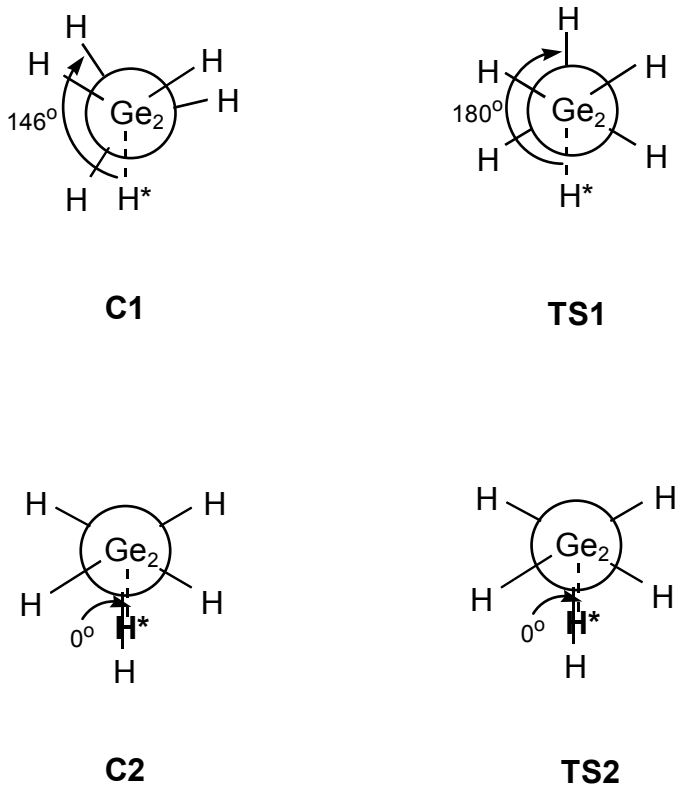


Fig. S1 G2MP2B3 calculated conformations of complexes and transition states in reaction (1), $GeH_2 + GeH_4$. Note: C1 has *right*- and *left*-handed forms; only one is shown.

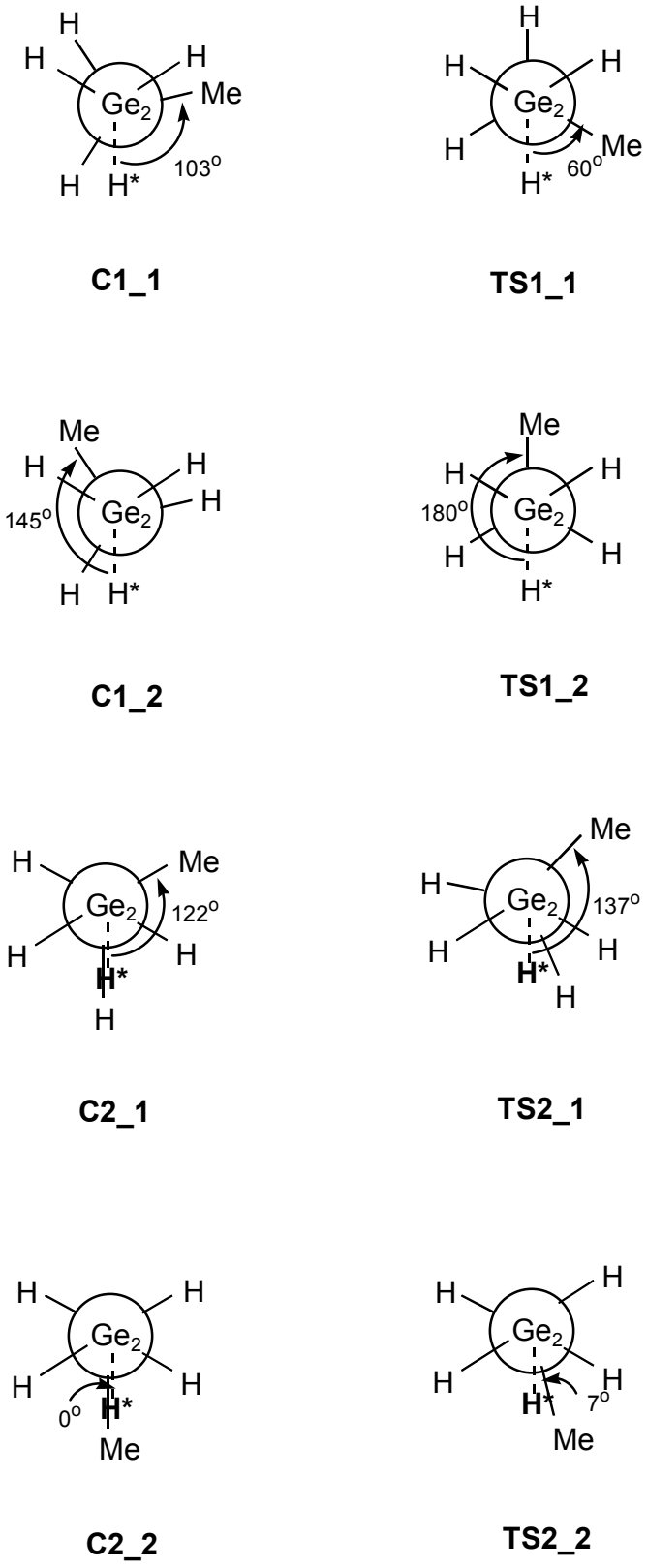


Fig. S2 G2MP2B3 calculated conformations of complexes and transition states in reaction (2), GeH_2 + $MeGeH_3$. Note: C1_1, TS1_1, C1_2, C2_1, TS2_1 and TS2_2 have *right*- and *left*-handed forms; only one of each is shown.

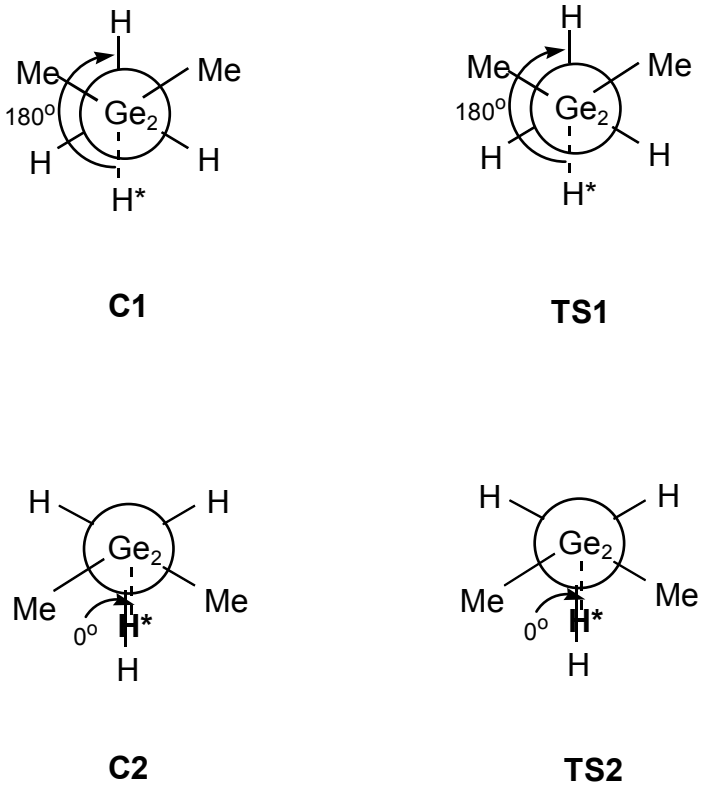
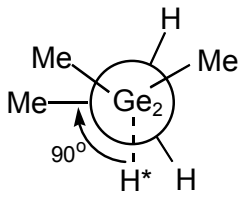
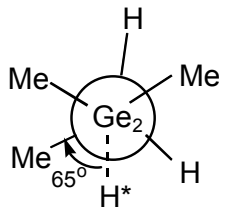


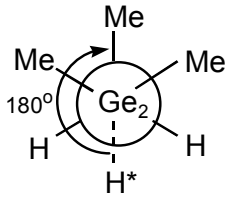
Fig. S3 G2MP2B3 calculated conformations of complexes and transition states in reaction (4), $GeMe_2 + GeH_4$.



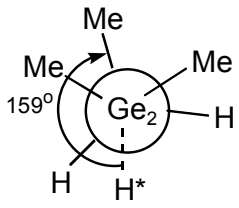
C1_1



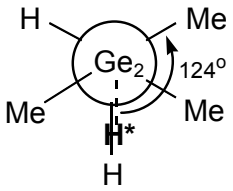
TS1_1



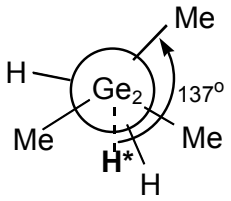
C1_2



TS1_2



C2_1



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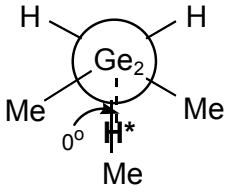
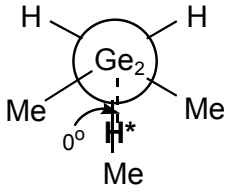


C2_2



TS2_2

Fig. S4 G2MP2B3 calculated conformations of complexes and transition states in reaction (5), $GeMe_2$ + $MeGeH_3$. Note: C1_1, TS1_1, TS1_2, C2_1 and TS2_1 have *right*- and *left*-handed forms; only one of each is shown.