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Silyl and σ-silane ruthenium complexes: Chlorine substituent effects on the catalysed silylation of ethylene.

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Supplementary Information

DFT calculations

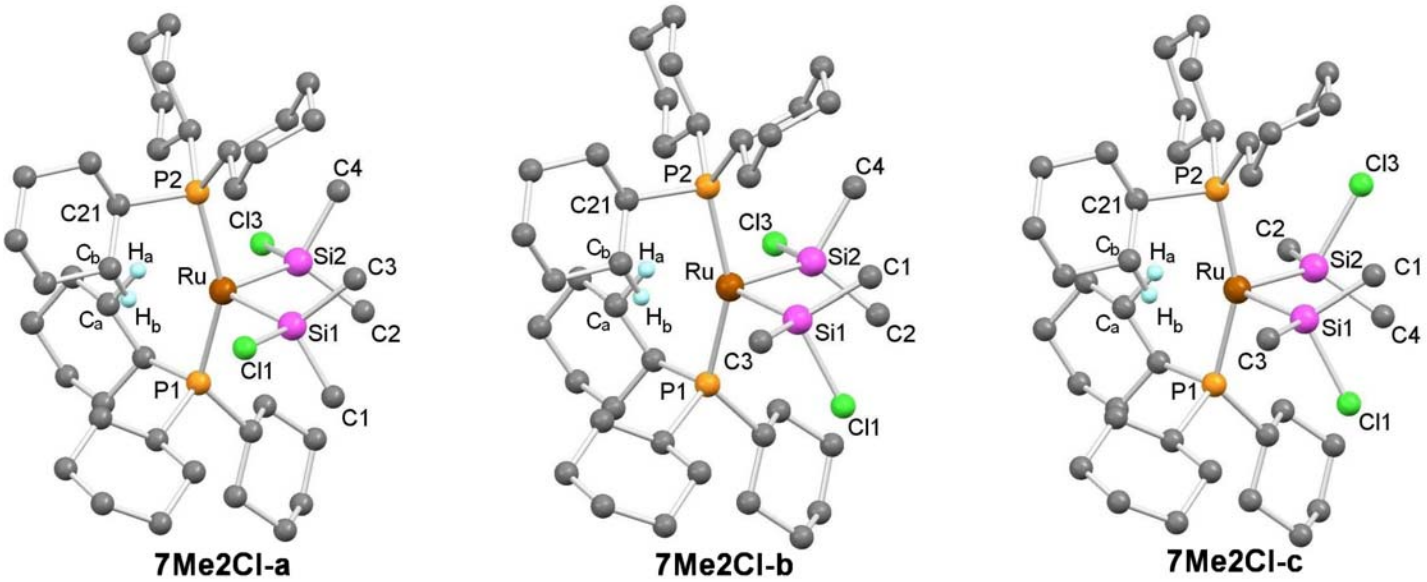

Figure. Optimized structures of three **7Me$_2$Cl** rotamers.

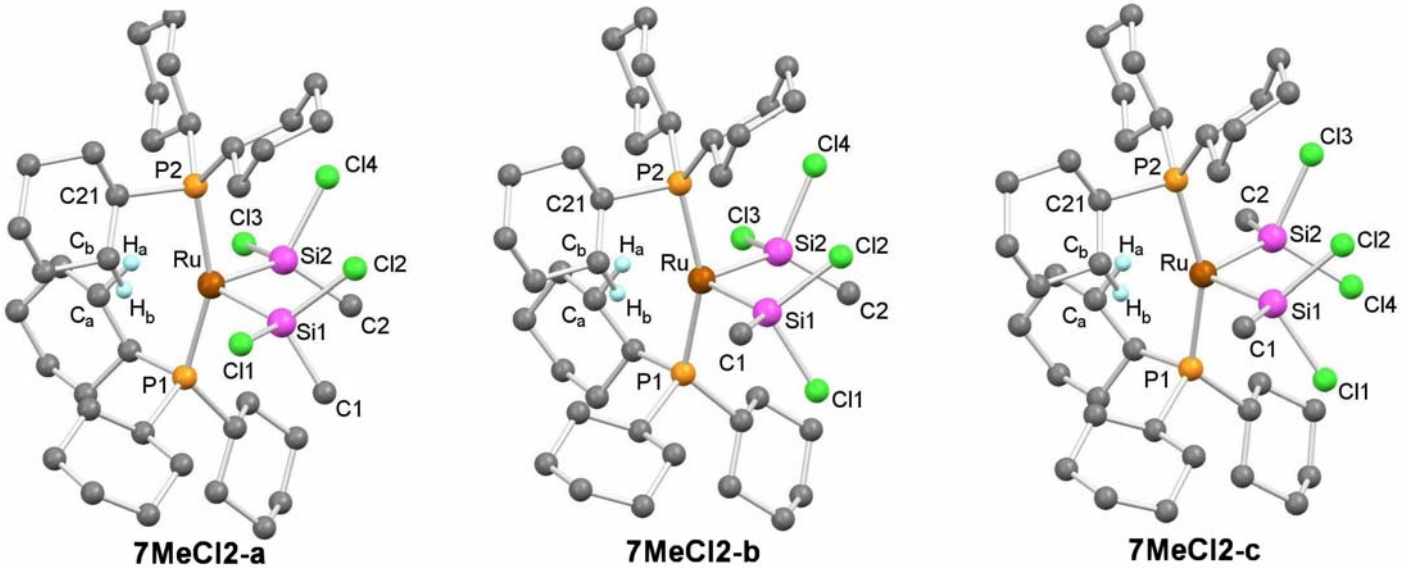

Figure. Optimized structures of three **7MeCl$_2$** rotamers.

Table. Distances (Å) and angles (°) for the optimized geometries of **7Me$_2$Cl** and **7MeCl$_2$** rotamers.

	7Me$_2$Cl-a	**7Me$_2$Cl-b**	**7Me$_2$Cl-c**	**7MeCl$_2$-a**	**7MeCl$_2$-b**	**7MeCl$_2$-c**
Ru – P1	2.535	2.445	2.453	2.428	2.453	2.436
Ru – P2	2.445	2.436	2.421	2.479	2.453	2.457
Ru – Si1	2.317	2.310	2.314	2.279	2.289	2.300
Ru – Si2	2.310	2.311	2.307	2.286	2.292	2.296
Si1 – Cl1	2.206	2.212	2.216	2.185	2.162	2.147
Si1 – Cl2 or C3	1.912	1.925	1.933	2.162	2.178	2.165
Si2 – Cl3	2.198	2.230	2.212	2.197	2.199	2.166
Si2 – Cl4 or C4	1.907	1.913	1.909	2.164	2.167	2.145
Si1 – C1	1.907	1.916	1.910	1.901	1.910	1.918
Si2 – C2	1.907	1.910	1.925	1.899	1.892	1.914
Ru ··· H_a	2.501	2.445	2.392	2.364	2.444	2.397
Ru ··· H_b	2.493	2.372	2.421	2.373	2.347	2.361
Ru ··· C_a	3.305	3.218	3.204	3.134	3.228	3.173
Ru ··· C_b	3.263	3.187	3.189	3.178	3.157	3.175
P1 – Ru – P2	153.95	156.18	156.10	156.89	157.61	158.47
P1 – Ru – Si1	98.77	98.64	98.86	95.60	98.20	96.92
P1 – Ru – Si2	103.18	97.24	99.73	96.79	96.14	96.36
P2 – Ru – Si1	98.42	99.96	95.57	102.64	99.32	99.42
P2 – Ru – Si2	97.98	98.16	99.20	97.93	97.90	96.89
Si1 – Ru – Si2	88.11	87.96	89.75	87.93	89.32	92.30
Ru – P2 – C21	101.06	99.34	100.58	99.03	98.22	98.49
Cl1 – Si1 – Cl2 or C3	101.65	98.77	97.16	102.38	97.27	98.34
Cl1 – Si1 – C1	99.22	95.50	96.10	100.38	100.91	101.62
Cl2 or C3 – Si1 – C1	99.44	105.23	106.24	97.24	99.15	99.42
Cl1 – Si1 – Ru	108.64	115.11	115.51	107.54	118.42	120.36
Cl2 or C3 – Si1 – Ru	123.26	113.88	113.88	119.94	117.08	117.88
C1 – Si1 – Ru	120.73	124.21	123.63	125.74	119.89	115.62
H_a – Ru – Si1	164.95	168.59	168.89	169.43	168.33	168.42
H_b – Ru – Si2	168.86	171.16	169.09	165.70	170.76	167.76
ΔEnergy (kJ.mol^{-1})	**0.0**	**+3.8**	**+8.8**	**0.0**	**+6.3**	**+39.0**