Electronic Supporting Information

A Comparative Study of Methanol Activation by Different Small Mixed Silicon Clusters Si_2M with M = H, Li, Na, Cu, Ag

Tran Dieu Hang, [≠,#] Huynh Minh Hung[≠,#] and Minh Tho Nguyen[%,&,#,*]

[%] *Computational Chemistry Research Group, Ton Duc Thang University, 700000 Ho Chi Minh City, Vietnam*

[&] *Faculty of Applied Sciences, Ton Duc Thang University, 700000 Ho Chi Minh City, Vietnam*

[≠] *Department of Chemistry, Quy Nhon University, 590000 Binh Dinh, Vietnam*

[#] *Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium*

nguyenminhtho@tdt.edu.vn; minh.nguyen@kuleuven.be

Table S1. Mulliken net charges q (electrons) on the Si and X atoms of the Si_2X clusters with X = H, Li, Na, Cu, Ag (B3LYP/6-311+G(d))

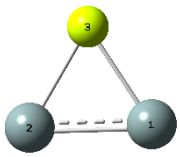	**Si_2H**	**Si_2Li**	**Si_2Na**	**Si_2Cu**	**Si_2Ag (APT)**
q (Si_1)	0.06	-0.07	-0.10	-0.006	0.02
q (Si_2)	0.06	-0.07	-0.10	-0.006	0.02
q (X)	-0.12	0.14	0.21	0.012	-0.04

Table S2. Cartesian Coordinates of the most stable complexes, transition states and resulting products of all methanol activation pathways (B3LYP/6-311+G(d))

Structure	Geometry (Cartesian Coordinates, angstrom)			
cp.H.c	14	-1.888786000	-0.611918000	0.047923000
	14	-0.283483000	1.057436000	-0.010265000
	1	-3.027723000	0.396385000	0.094746000
	8	1.132603000	-0.369280000	-0.266600000
	6	2.513657000	-0.280843000	0.155390000
	1	3.122634000	-0.919909000	-0.480383000
	1	2.799018000	0.758890000	0.030525000
	1	2.608643000	-0.569403000	1.200658000
	1	0.766429000	-1.263916000	-0.172306000
ts-H.c,2	14	0.178252000	1.192211000	0.008721000
	14	1.665020000	-0.595286000	0.025545000
	1	3.164087000	-0.518132000	0.052063000
	6	-2.300355000	-0.473348000	0.081234000
	1	-2.690593000	-1.167476000	-0.660584000
	1	-2.804982000	0.486011000	-0.007565000
	8	-0.896653000	-0.282309000	-0.165239000
	1	-0.051801000	-1.183079000	-0.112198000
	1	-2.447163000	-0.875703000	1.083066000
2	14	-0.059530000	0.895384000	-0.012472000
	14	1.962566000	-0.319074000	0.032051000
	1	3.260310000	0.395244000	-0.126202000
	6	-2.490070000	-0.355584000	-0.004232000
	1	-2.865467000	-0.886265000	-0.879440000
	1	-2.834380000	0.682300000	-0.040480000
	8	-1.068653000	-0.440097000	0.015107000
	1	2.173361000	-1.774107000	-0.216484000
	1	-2.886681000	-0.831234000	0.893026000
cp.Li.a	14	-1.875338000	1.055514000	-0.059628000
	14	-1.875334000	-1.055510000	-0.059664000
	3	0.456178000	0.000004000	0.490294000
	8	2.335589000	-0.000056000	0.584943000
	6	3.221213000	0.000039000	-0.554776000
	1	3.843254000	0.894254000	-0.553992000
	1	2.591711000	0.000074000	-1.440024000
	1	3.843305000	-0.894140000	-0.554097000
	1	2.850616000	-0.000047000	1.396430000

ts-Li.a,7	14	1.358128000	1.070409000	-0.131070000
	14	1.358582000	-1.070141000	-0.131476000
	3	-0.488840000	-0.000484000	1.769478000
	8	-1.535170000	-0.000578000	0.450191000
	6	-2.578700000	0.000200000	-0.479859000
	1	-2.196139000	0.001924000	-1.508669000
	1	-3.216282000	0.884757000	-0.365325000
	1	-3.215293000	-0.885401000	-0.367916000
	1	-0.186144000	-0.000156000	-0.113261000
7	14	0.057854000	-1.014920000	-0.000101000
	14	1.986497000	0.354127000	0.000210000
	3	0.076497000	1.792768000	-0.000537000
	8	-1.063791000	0.379008000	-0.000141000
	6	-2.478911000	0.185278000	0.000184000
	1	-2.913705000	0.645111000	0.889423000
	1	-2.712659000	-0.880993000	0.000586000
	1	-2.914050000	0.644507000	-0.889200000
	1	3.073804000	-0.679555000	-0.000702000
cp.Na.a	14	-1.713092000	-0.360502000	-1.057942000
	14	-1.713374000	-0.360085000	1.057966000
	11	0.268178000	1.595028000	-0.000311000
	8	1.854752000	-0.017119000	0.000302000
	6	3.116859000	-0.686734000	0.000034000
	1	3.233425000	-1.306507000	-0.890704000
	1	3.889574000	0.078658000	-0.000074000
	1	3.233765000	-1.306589000	0.890670000
	1	1.124648000	-0.665303000	0.000570000
ts-Na.a,8	14	-1.703482000	-0.155377000	-0.958943000
	14	-1.092323000	-0.620408000	1.061301000
	11	0.467445000	1.860428000	0.205458000
	8	1.450123000	0.038256000	-0.072368000
	6	2.397644000	-0.964648000	-0.290043000
	1	1.924973000	-1.914717000	-0.578135000
	1	3.093121000	-0.696320000	-1.097606000
	1	2.999160000	-1.162945000	0.607659000
	1	-0.004718000	-0.347890000	-0.305762000
8	14	2.109476000	-0.388428000	0.307170000
	14	0.065703000	-0.917879000	-0.329123000
	11	0.346370000	1.906270000	-0.190171000
	8	-1.214754000	0.200924000	0.019451000

	6	-2.538757000	-0.218509000	0.340570000
	1	-2.896622000	-0.961555000	-0.376386000
	1	-2.576881000	-0.651925000	1.343251000
	1	-3.199945000	0.647741000	0.306812000
	1	-0.638550000	-2.011270000	-1.073472000
cp.Cu.c	14	-0.952093000	1.550327000	-0.276605000
	14	0.392261000	0.189902000	0.965272000
	29	-1.479549000	-0.708128000	-0.119732000
	6	3.462991000	-0.204133000	-0.120753000
	1	3.748098000	0.823812000	0.104265000
	1	4.102788000	-0.607783000	-0.905042000
	1	3.559088000	-0.808584000	0.776577000
	8	2.081583000	-0.288052000	-0.518968000
	1	1.903983000	0.294273000	-1.268666000
ts-Cu.c,13	14	-0.270343000	1.521066000	0.192923000
	14	0.481267000	-0.584088000	0.953771000
	8	1.594979000	-0.270532000	-0.532710000
	6	3.024284000	-0.148806000	-0.363297000
	1	3.469195000	0.002979000	-1.343984000
	1	3.398842000	-1.071076000	0.075214000
	1	3.267039000	0.691828000	0.288714000
	1	1.054479000	0.832435000	-0.863516000
	29	-1.553380000	-0.362647000	-0.267885000
13	14	-0.812315000	1.569394000	-0.082255000
	14	0.619144000	0.001539000	1.000129000
	29	-1.361652000	-0.674383000	-0.205012000
	6	2.755532000	-0.111059000	-0.852156000
	1	2.178450000	-0.479469000	-1.701734000
	1	3.723758000	-0.607696000	-0.829092000
	1	2.903178000	0.963312000	-0.965835000
	8	2.086059000	-0.401956000	0.371298000
	1	0.165238000	1.569913000	-1.265660000
cp.Ag.b	14	-0.297847000	1.830402000	-0.336409000
	14	0.837530000	0.359231000	1.002176000
	47	-1.339628000	-0.476947000	-0.060870000
	8	2.330452000	-0.422508000	-0.503310000
	6	3.725751000	-0.541527000	-0.161127000
	1	3.765724000	-1.125536000	0.753600000
	1	4.172941000	0.437016000	0.013835000
	1	4.258638000	-1.062965000	-0.955333000

	1	2.211522000	0.142374000	-1.278729000
ts-Ag.b,16	14	0.023834000	1.751189000	-0.126919000
	14	0.958330000	-0.079000000	0.953641000
	47	-1.389852000	-0.342167000	-0.093968000
	8	2.130461000	-0.504999000	-0.482307000
	6	3.552361000	-0.428146000	-0.300838000
	1	3.841292000	-1.051895000	0.546836000
	1	3.865287000	0.600603000	-0.109859000
	1	4.035609000	-0.791459000	-1.205722000
	1	1.472714000	0.522817000	-0.725376000
16	14	-0.189898000	1.821792000	-0.270063000
	14	1.059161000	0.251289000	1.027080000
	47	-1.254999000	-0.445016000	-0.070138000
	8	2.385551000	-0.496803000	0.404260000
	6	2.951873000	-0.607268000	-0.898122000
	1	3.846692000	-1.222211000	-0.822172000
	1	3.219352000	0.375291000	-1.287540000
	1	2.244978000	-1.077542000	-1.583688000
	1	0.708602000	1.435118000	-1.453672000
cp.H.b	14	-1.761851000	-0.815157000	-0.045510000
	14	-0.611228000	1.114077000	-0.014035000
	1	-0.841013000	-0.049930000	1.186443000
	6	2.110862000	-0.874820000	0.022702000
	1	2.101824000	-1.186260000	1.066939000
	1	1.461606000	-1.527302000	-0.553391000
	8	1.576454000	0.456502000	-0.125383000
	1	2.100329000	1.089992000	0.377545000
	1	3.123568000	-0.914476000	-0.377045000
ts-H.b,20	14	1.526833000	-0.945632000	-0.146003000
	14	0.986013000	1.186521000	0.027710000
	1	1.659381000	0.120329000	1.146300000
	6	-1.804782000	-0.715497000	0.294313000
	1	-1.871336000	-1.644322000	-0.255528000
	1	-1.882534000	-0.764797000	1.375346000
	8	-2.456857000	0.304532000	-0.339657000
	1	-2.459497000	1.093696000	0.212798000
	1	-0.142303000	-0.320615000	0.128571000
20	14	1.792974000	-0.931752000	-0.041806000
	14	0.879345000	1.093039000	-0.030999000
	1	2.425311000	0.524524000	0.434684000

	6	-2.648483000	-0.783841000	0.008481000
	1	-2.227446000	-1.540192000	-0.631981000
	1	-3.143397000	-1.022863000	0.938023000
	8	-2.095585000	0.454419000	-0.153274000
	1	-2.477982000	1.077717000	0.472665000
	1	0.666627000	-0.229500000	0.981188000
cp.Li.a	14	-1.875338000	1.055514000	-0.059628000
	14	-1.875334000	-1.055510000	-0.059664000
	3	0.456178000	0.000004000	0.490294000
	8	2.335589000	-0.000056000	0.584943000
	6	3.221213000	0.000039000	-0.554776000
	1	3.843254000	0.894254000	-0.553992000
	1	2.591711000	0.000074000	-1.440024000
	1	3.843305000	-0.894140000	-0.554097000
	1	2.850616000	-0.000047000	1.396430000
ts-Li.a,24	14	1.427009000	-1.016934000	0.035267000
	14	1.189473000	1.144029000	-0.090210000
	3	-0.607631000	-0.190686000	1.467348000
	8	-2.230159000	0.065604000	0.492150000
	6	-1.741613000	-0.278233000	-0.802379000
	1	-1.893247000	-1.328118000	-1.011482000
	1	-0.020438000	-0.115446000	-0.633960000
	1	-2.001406000	0.427533000	-1.579533000
	1	-2.601810000	0.953334000	0.469201000
24	14	-2.204947000	-0.738598000	0.011367000
	14	-1.046198000	1.097877000	-0.068967000
	3	0.423162000	-1.180306000	-0.200325000
	8	2.019686000	-0.180061000	-0.087012000
	6	3.374695000	-0.119675000	0.130402000
	1	3.906844000	-1.027170000	-0.096858000
	1	-1.483062000	0.156842000	1.244548000
	1	3.839942000	0.852174000	0.137553000
	1	1.577165000	0.687693000	0.035825000
cp.Na.b	14	-2.299103000	-0.994613000	0.234627000
	14	-2.179011000	1.104062000	-0.014064000
	11	0.425953000	-0.163329000	-0.426139000
	8	2.727969000	-0.199851000	-0.453201000
	6	3.589821000	0.227106000	0.617579000
	1	2.947258000	0.584471000	1.418068000
	1	4.239104000	1.040756000	0.293605000

	1	4.190473000	-0.603638000	0.988612000
	1	3.268601000	-0.521066000	-1.180492000
ts-Na.b,28	14	-1.821193000	0.336353000	-0.685791000
	14	-0.791149000	-0.940638000	0.834183000
	11	0.574564000	1.665184000	0.491920000
	8	2.055210000	0.101329000	-0.265106000
	6	1.321117000	-1.122895000	-0.475431000
	1	1.681529000	-1.922670000	0.164868000
	1	-0.101946000	-0.566979000	-0.636040000
	1	1.328937000	-1.414919000	-1.525813000
	1	2.975683000	-0.025733000	-0.518184000
28	14	2.068332000	0.128341000	0.273019000
	14	0.344045000	-1.134436000	-0.461815000
	11	-0.310654000	1.746175000	-0.311616000
	8	-2.021939000	0.358862000	0.152269000
	6	-1.455176000	-0.992037000	0.304236000
	1	-2.121108000	-1.705929000	-0.185807000
	1	1.003010000	0.542368000	1.349535000
	1	-1.409411000	-1.235658000	1.369160000
	1	-2.922004000	0.357945000	0.494468000
cp.Cu.c	14	-0.952093000	1.550327000	-0.276605000
	14	0.392261000	0.189902000	0.965272000
	29	-1.479549000	-0.708128000	-0.119732000
	6	3.462991000	-0.204133000	-0.120753000
	1	3.748098000	0.823812000	0.104265000
	1	4.102788000	-0.607783000	-0.905042000
	1	3.559088000	-0.808584000	0.776577000
	8	2.081583000	-0.288052000	-0.518968000
	1	1.903983000	0.294273000	-1.268666000
ts-Cu.c,30	14	-0.746120000	1.529712000	-0.310375000
	14	0.758325000	0.227562000	0.807918000
	29	-1.456804000	-0.601753000	-0.033388000
	6	2.815349000	0.122264000	-0.326572000
	1	2.740170000	0.775901000	-1.184296000
	1	3.801854000	-0.222049000	-0.049230000
	1	2.216343000	0.426642000	1.289822000
	8	1.873186000	-0.977085000	-0.358823000
	1	1.440498000	-1.048388000	-1.223636000
30	14	-1.053912000	1.450715000	-0.488309000
	14	0.579266000	0.490360000	0.793564000

	29	-1.260892000	-0.791230000	-0.018848000
	6	2.325237000	-0.147899000	0.345884000
	1	3.041003000	0.596387000	0.722607000
	1	2.509722000	-1.073521000	0.906188000
	1	0.635518000	0.516982000	2.293041000
	8	2.463459000	-0.345519000	-1.059037000
	1	3.365579000	-0.617686000	-1.251816000
cp.Ag.a	14	-2.045818000	1.179559000	0.047437000
	14	-2.201587000	-0.962022000	0.242498000
	47	0.121247000	-0.084667000	-0.122802000
	8	2.439197000	-0.184967000	-0.379737000
	6	3.419693000	0.239341000	0.583721000
	1	3.007518000	0.018491000	1.563701000
	1	3.609577000	1.310261000	0.505444000
	1	4.348235000	-0.315954000	0.449976000
	1	2.767998000	-0.035273000	-1.270943000
Ts1-Ag.a,32	14	-0.316907000	1.040393000	1.284900000
	14	-0.014544000	1.584669000	-0.855461000
	47	1.214636000	-0.530913000	-0.062209000
	8	-2.933360000	-1.378900000	0.023837000
	6	-2.993756000	-0.097254000	-0.449620000
	1	-1.418404000	0.646553000	-0.137211000
	1	-3.611311000	0.607361000	0.098823000
	1	-3.033027000	-0.063017000	-1.529646000
	1	-2.955419000	-1.374144000	0.986730000
32	14	2.190161000	-0.956377000	-0.166283000
	14	1.953023000	1.247058000	0.040706000
	8	-3.177078000	0.433942000	-0.443596000
	6	-2.428177000	-0.353870000	0.418935000
	1	2.323950000	0.058334000	1.176135000
	1	-2.594467000	-1.401902000	0.187880000
	1	-2.548309000	-0.112797000	1.473397000
	1	-3.230050000	1.333651000	-0.104856000
	47	-0.254681000	-0.112662000	0.001291000