Supplementary Material to:

Ab-initio Molecular Dynamics study of the S_N2 reaction $Cl^- + ClCH_2CN$

By
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$ClCH_3+Cl^-$									
		BLYP			MP2			B3LYP	
Exp.	I	M	T	I	M	T	I	M	T
		72.8	172.8		62.7	201.4		72.4	188.4
		72.8	175.5		62.7	201.4		72.4	188.4
		102.3	189.1		103.8	229.3		100.9	203.9
732.8	666.1	471.9	-274.1	785.5	708.5	-557.9	709.4	573.6	-345.5
1017.26	997.1	922.6	841.4	1065.8	1029.6	980.8	1030.2	976.7	900.1
1017.26	997.1	922.6	843.1	1065.8	1029.6	980.8	1030.2	976.7	900.1
1354.95	1345.2	1246.1	965.6	1442.1	1385.1	1078.4	1388.4	1314.9	1030.1
1452.12	1440.5	1416.7	1368.1	1493.7	1470.4	1415.5	1478.5	1457.7	1400.5
1452.12	1440.5	1416.7	1368.1	1493.7	1470.4	1415.5	1478.5	1457.7	1400.5
2967.8	2998.7	3050.9	3115.2	3116.1	3159.7	3228.9	3071.1	3119.6	3190.1
3039.25	3092.7	3170.0	3305.8	3223.3	3279.6	3439.2	3168.9	3236.1	3388.7
3039.25	3092.7	3170.0	3306.7	3223.3	3279.6	3439.2	3168.9	3236.1	3388.7

Table 1: Vibrational frequencies at the stationary points for the reaction $Cl^- + ClCH_3$. The calculations are performed with the 6-311+G(d,p) basis set. I, M and T label the isolated molecule, the ion-dipole complex and the transition state respectively. We have not accluded the frequency computed using PW since they were determined by a finite differences algorithm and are affected by a large uncertainity.

$ClCH_2CN+Cl^-$									
		BLYP			MP2			B3LYP	
Exp.	I	M	T	I	M	T	I	M	T
		50.0	129.5		56.4	154.9		53.5	143.8
		89.8	144.0		84.3	167.0		90.2	153.0
		157.4	174.2		158.1	194.9		158.5	196.9
198	181.0	201.2	181.7	186.3	205.8	236.3	188.9	208.8	201.9
352	339.0	378.0	376.6	322.5	360.0	368.2	354.6	393.5	391.4
492	461.0	455.7	448.9	482.1	493.4	399.9	486.3	492.0	469.4
746	677.0	632.2	-239.7	787.0	762.1	-569.8	727.7	692.9	-331.2
907	889.0	880.3	800.9	943.8	946.7	944.7	919.3	916.2	876.5
930	920.0	923.0	885.9	965.1	962.5	1001.0	953.4	952.1	953.9
1184	1164.0	1168.3	975.7	1240.1	1255.8	1002.6	1207.7	1217.7	1000.8
1270	1255.0	1279.6	999.5	1355.3	1404.7	1020.0	1303.1	1337.9	1024.3
1421	1422.0	1403.1	1383.6	1479.0	1478.0	1419.7	1461.6	1448.9	1417.4
2256	2257.0	2220.7	2223.2	2197.2	2188.0	2175.7	2361.5	2332.8	2335.4
2963	3012.0	2588.6	3180.4	3137.1	2837.8	3294.6	3090.3	2736.3	3262.1
3010	3063.0	3046.8	3299.7	3200.4	3169.3	3436.3	3143.6	3125.7	3389.5

Table 2: Vibrational frequencies at the stationary points for the reaction $Cl^- + ClCH_2CN$. The calculations are performed with the 6-311+G(d,p) basis set. I, M and T label the isolated molecule, the ion-dipole complex and the transition state respectively. We have not accluded the frequency computed using PW since they were determined by a finite differences algorithm and are affected by a large uncertainity.