Ionic Liquids Coordinated Au Catalysts for Acetylene Hydrochlorination: DFT approach towards reaction mechanism and adsorption energy

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Supporting Information

1. Absolute energies of species calculated in DFT study

Table S1(a) Absolute energies in Hartrees of species calculated in DFT study: no IL, $Bmim^+$, $Prmim^+$ and TEA^+.

M=cation	None	Bmim	Prmim	TEA+
M	0.00000000	-423.17912115	-383.86581536	-371.41981872
Au_2Cl_6	-3032.12640122	-3032.12640122	-3032.12640122	-3032.12640122
Au_2Cl_6.M	-3032.12640122	-3455.30544387	-3415.99195844	-3403.54840227
C_2H_2	-77.32564618	-77.32564618	-77.32564618	-77.32564618
HCl	-460.79569406	-460.79569406	-460.79569406	-460.79569406
C_2H_3Cl	-538.18539427	-538.18539427	-538.18539427	-538.18539427
R	-3570.24774143	-3993.42678411	-3954.11329868	-3941.66974251
Abs	-3109.55239989	-3532.63916672	-3493.32555691	-3480.88247214
IM1	-3109.55137291	-3532.69612014	-3493.38437255	-3480.89472579
TS1	-3109.49523516	-3532.66363890	-3493.35005624	-3480.87637298
IM2	-3109.48896646	-3532.68093482	-3493.36674310	-3480.91718291
TS2	-3570.24989194	-3993.43410091	-3954.12077199	-3941.67650115
Des	-3570.31375153	-3993.49426656	-3954.18070193	-3941.73905503
P	-3032.19045525	-3455.36957640	-3416.05627061	-3403.61027397

Table S1(b) Absolute energies in Hartrees of species calculated in DFT study: TEP^+, $TMBA^+$ and $TEBA^+$.

M=cation	TEP^+	$TMBA^+$	$TEBA^+$
M	-658.00581526	-445.22171114	-563.16616756
Au_2Cl_6	-3032.12640122	-3032.12640122	-3032.12640122
Au_2Cl_6.M	-3690.13184482	-3477.34684434	-3595.28694618
C_2H_2	-77.32564618	-77.32564618	-77.32564618
HCl	-460.79569406	-460.79569406	-460.79569406
C_2H_3Cl	-538.18539427	-538.18539427	-538.18539427
R	-4228.25318506	-4015.46818458	-4133.40828642
Abs	-3767.46683521	-3554.67727160	-3672.61983966
IM1	-3767.53307675	-3554.74149794	-3672.63428318
TS1	-3767.52953908	-3554.68296095	-3672.61740291
IM2	-3767.54272918	-3554.74204314	-3672.68183982
TS2	-4228.31507865	-4015.47394236	-4133.40990957
Des	-4228.37862707	-4015.53482692	-4133.47621512
P	-3690.19627051	-3477.41216639	-3595.35662281

Table S2 Absolute energies in Hartrees of PrmimCl-related species calculated in DFT study: with and without chlorine anions.

M=$Prmim^+$	Without Cl^-	With Cl^-	Energy difference
M	-383.86581536	-843.39181232	-459.52599696
Au_2Cl_6.M	-3415.99195844	-3875.51795543	-459.52599699
R	-3954.11329868	-4413.63929560	-459.52599692
Abs	-3493.32555691	-3952.85155391	-459.52599700
IM1	-3493.38437255	-3952.91036951	-459.52599696
TS1	-3493.35005624	-3952.87605319	-459.52599695
IM2	-3493.36674310	-3952.89274008	-459.52599698
TS2	-3954.12077199	-4413.64676899	-459.52599700
Des	-3954.18070193	-4413.70669889	-459.52599696
P	-3416.05627061	-3875.58226756	-459.52599695

2.Structures of species calculated in DFT study

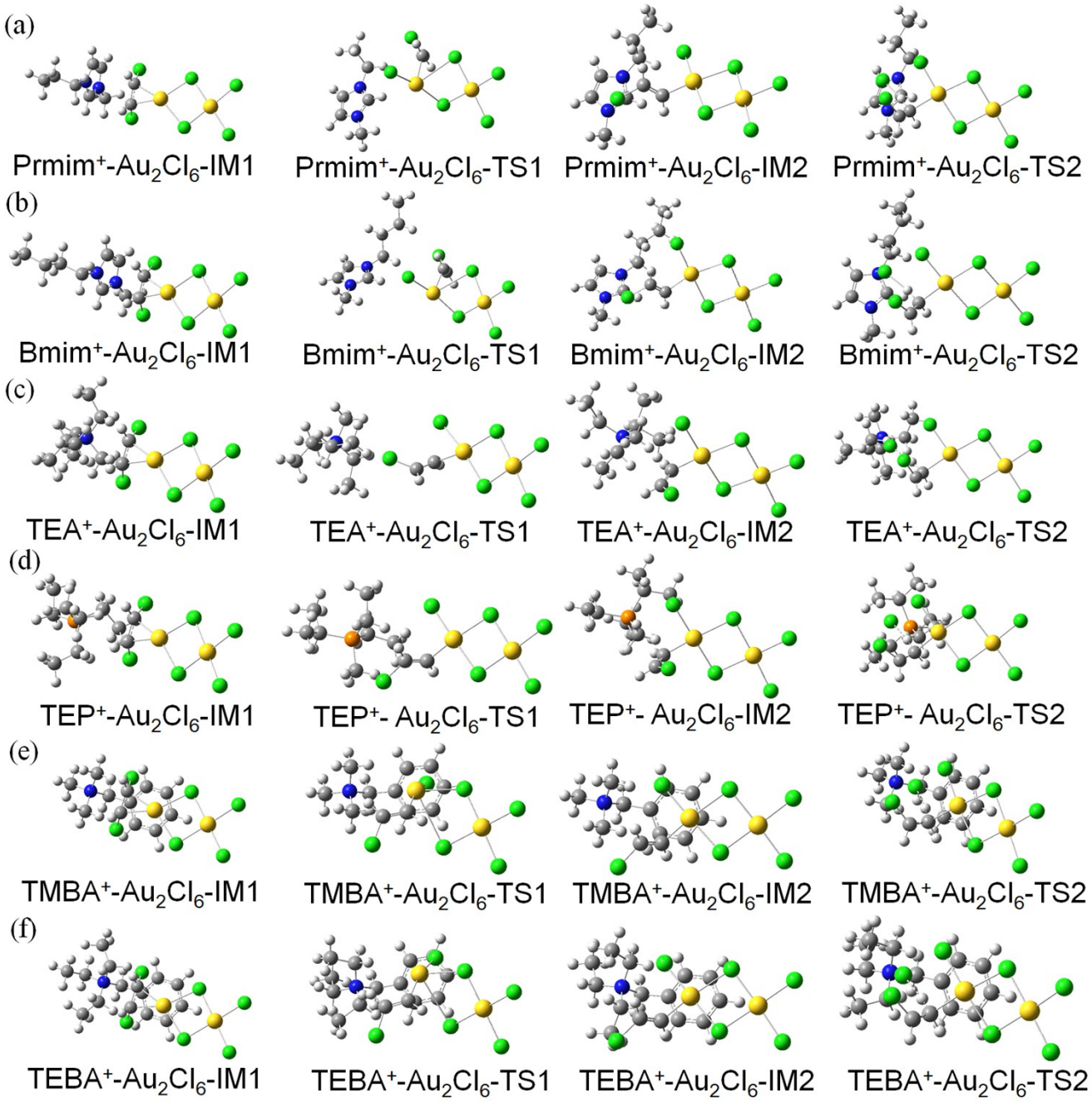

Fig. S1 Structure of intermediates in various Au_2Cl_6-IL systems during energy profile calculation.