

SUPPORTING INFORMATION

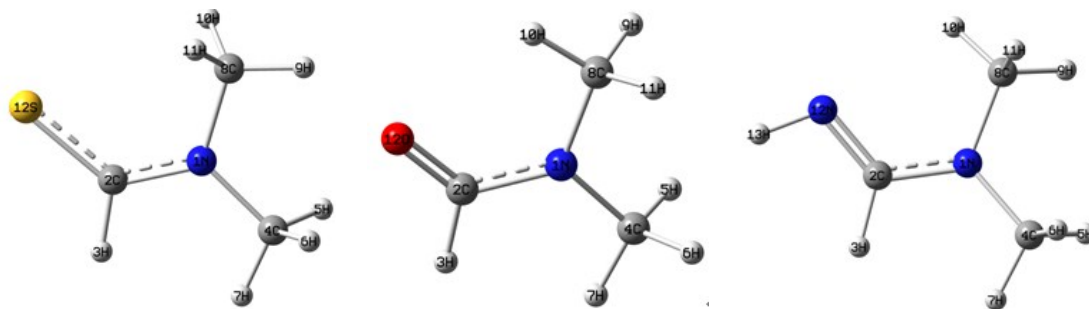
Reversibility of imido-based ionic liquids: a theoretical and experimental study

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Table S1 The averages of ESP calculated on the surface corresponding to individual atoms and the minimal/maximal value calculated on the whole molecular surfaces (in kcal/mol).



Minimal value	-35.04	Minimal value	-43.69	Minimal value	-43.71
Maximal value	26.57	Maximal value	22.17	Maximal value	21.75
N1	3.49	N1	-1.17	N1	-13.98
C2	-7.48	C2	-2.80	C2	-9.61
H3	4.19	H3	6.44	H3	10.25
H5	19.79	H5	14.28	H5	9.44
H6	19.80	H6	14.30	H6	8.94
H7	21.32	H7	16.82	H7	12.63
H9	18.66	H9	9.86	H9	5.76
H10	2.15	H10	-2.97	H10	-9.88
H11	2.12	H11	9.86	H11	-0.50
S12	-26.37	O12	-33.06	N12	-32.54
				H13	-0.27

Note: the atoms have zero surface area are not shown in the table.

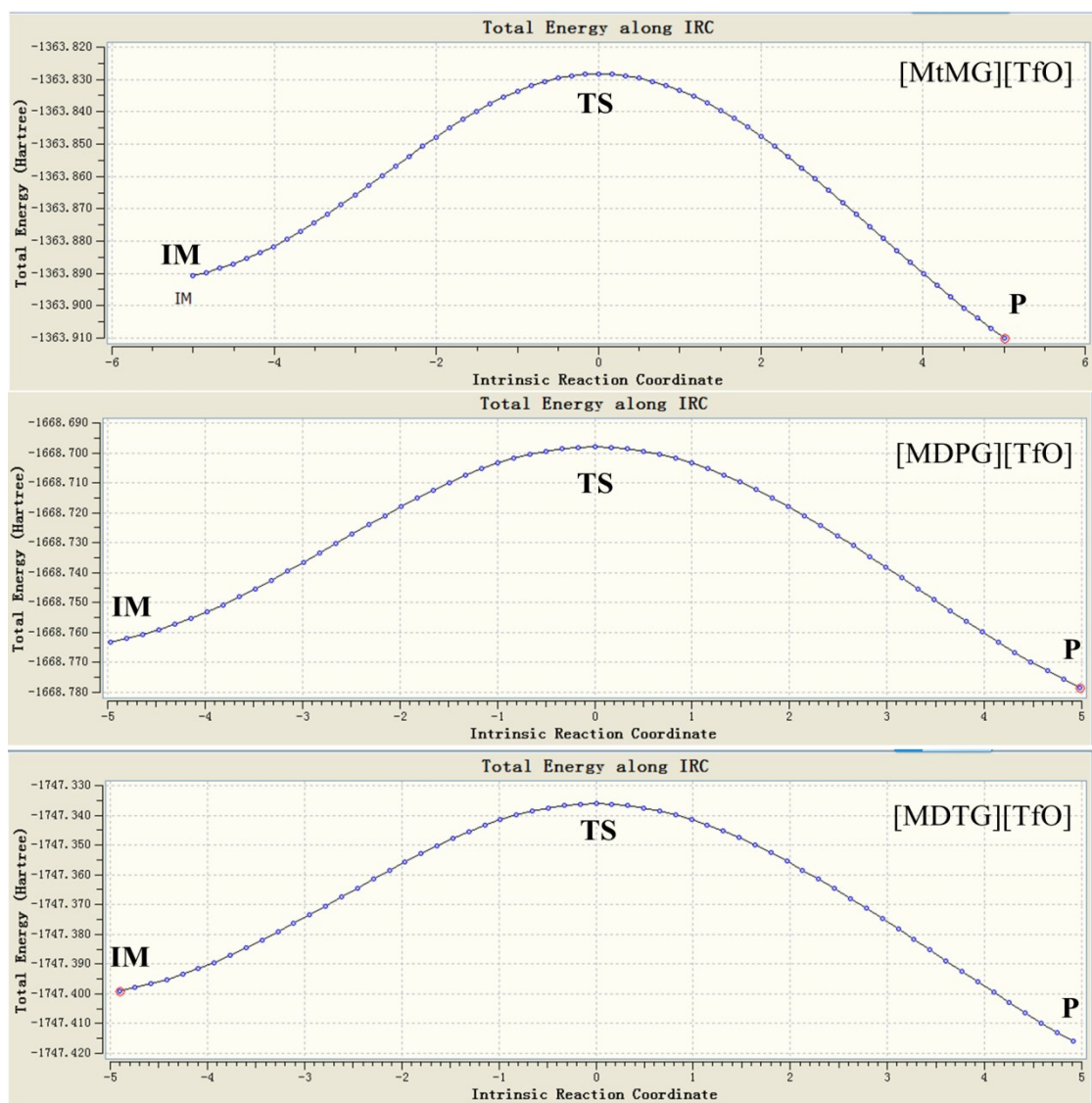


Fig. S1 Total energy along IRC of [MtMG][TfO], [MDPG][TfO], [MDTG][TfO].

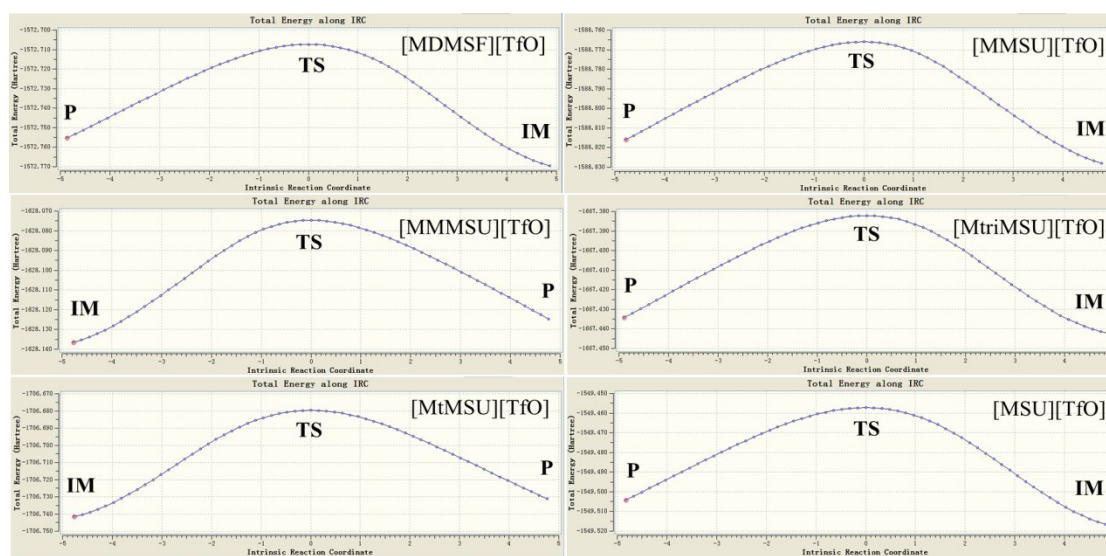


Fig. S2 Total energy along IRC of [MDMSF][TfO], [MMSU][TfO], [MMMSU][TfO], [MtriMSU][TfO], [MtMSU][TfO], [MSU][TfO].

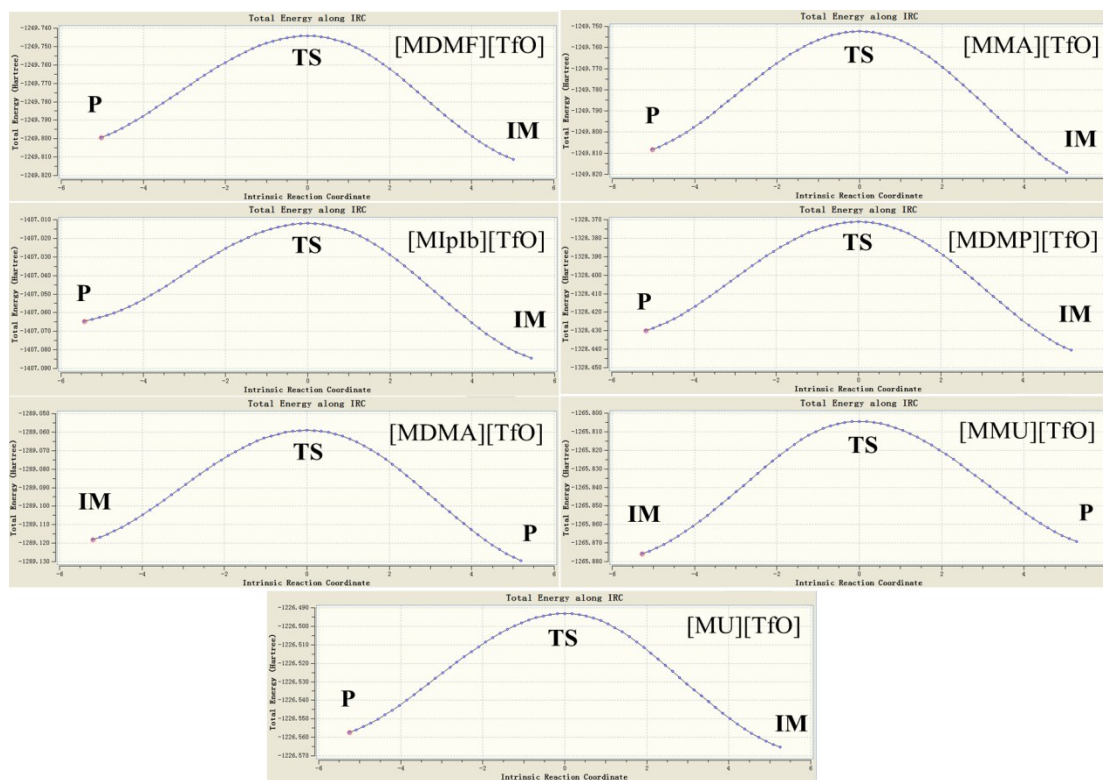


Fig. S3 Total energy along IRC of [MDMF][TfO], [MMA][TfO], [MIPb][TfO], [MDMP][TfO], [MDMA][TfO], [MMU][TfO], [MU][TfO].

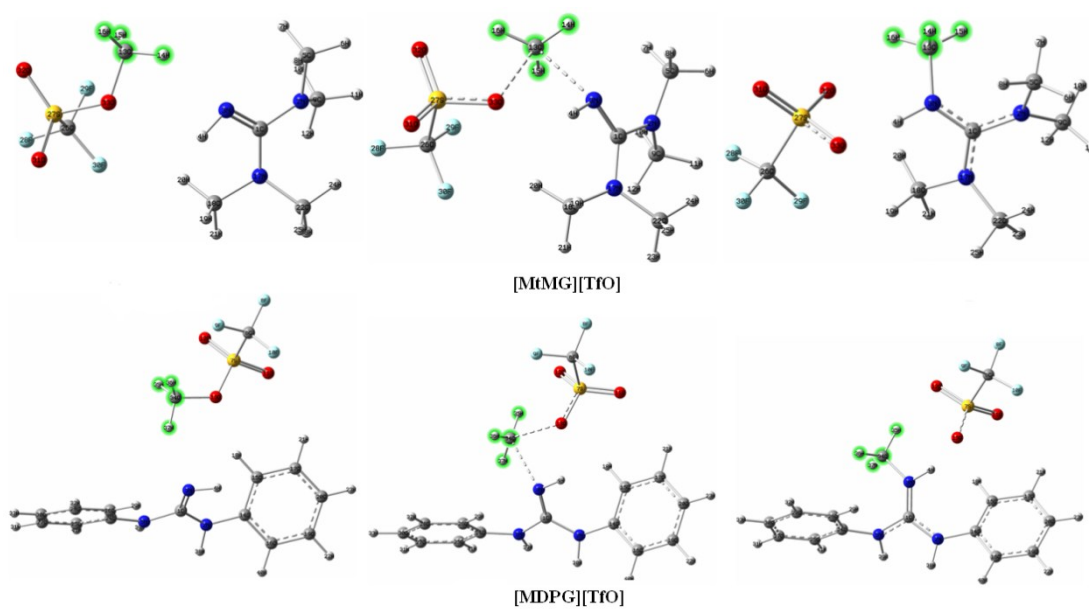


Fig. S4 The most stable structures of [MtMG][TfO] and [MDPG][TfO].

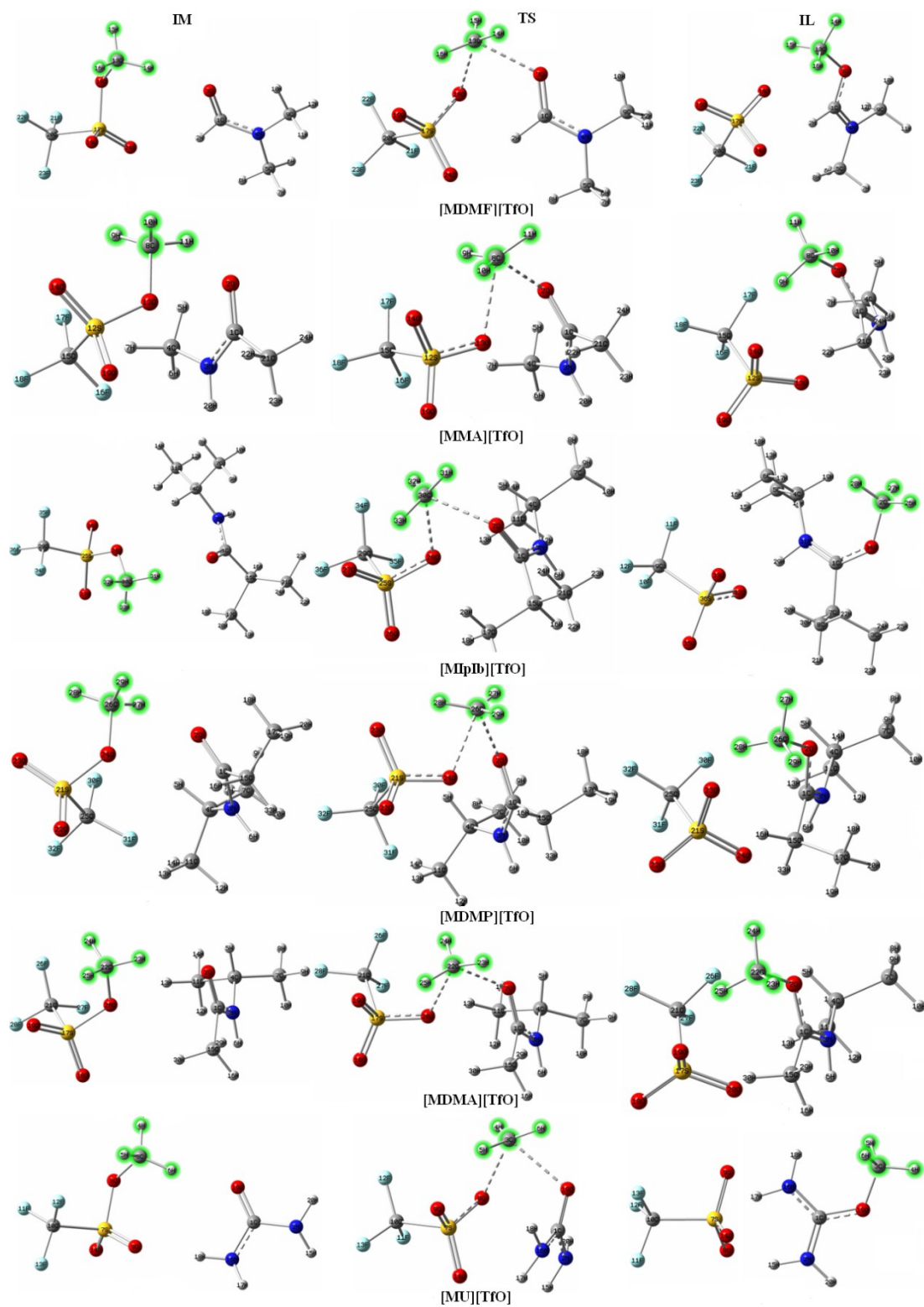


Fig. S5 The most stable structures of [MDMF][TfO], [MMA][TfO], [MIPb][TfO], [MDMP][TfO], [MDMA][TfO] and [MU][TfO].

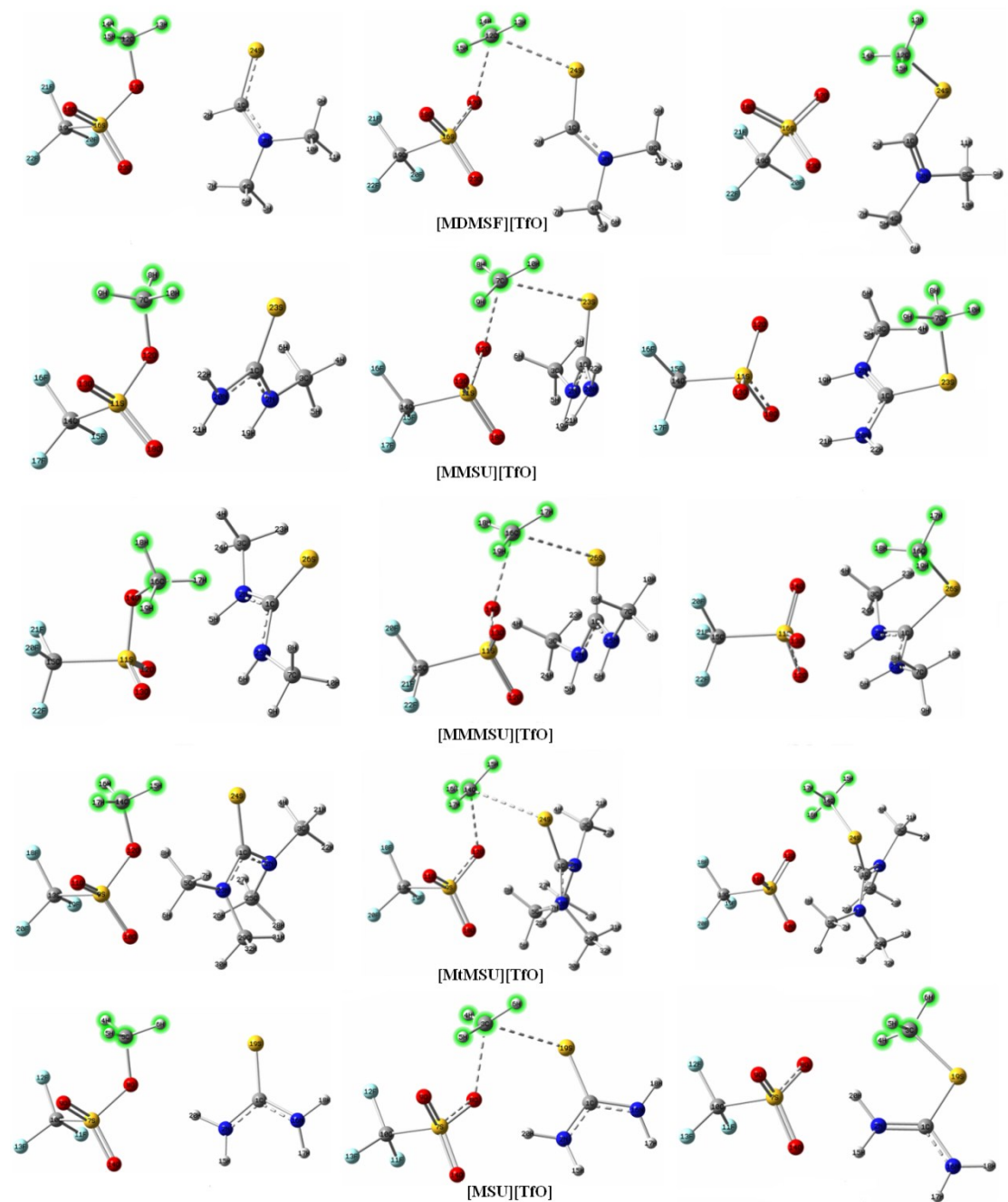


Fig. S6 The most stable structures of [MDMSF][TfO], [MMMSU][TfO], [MMSU][TfO], [MtMSU][TfO] and [MSU][TfO].

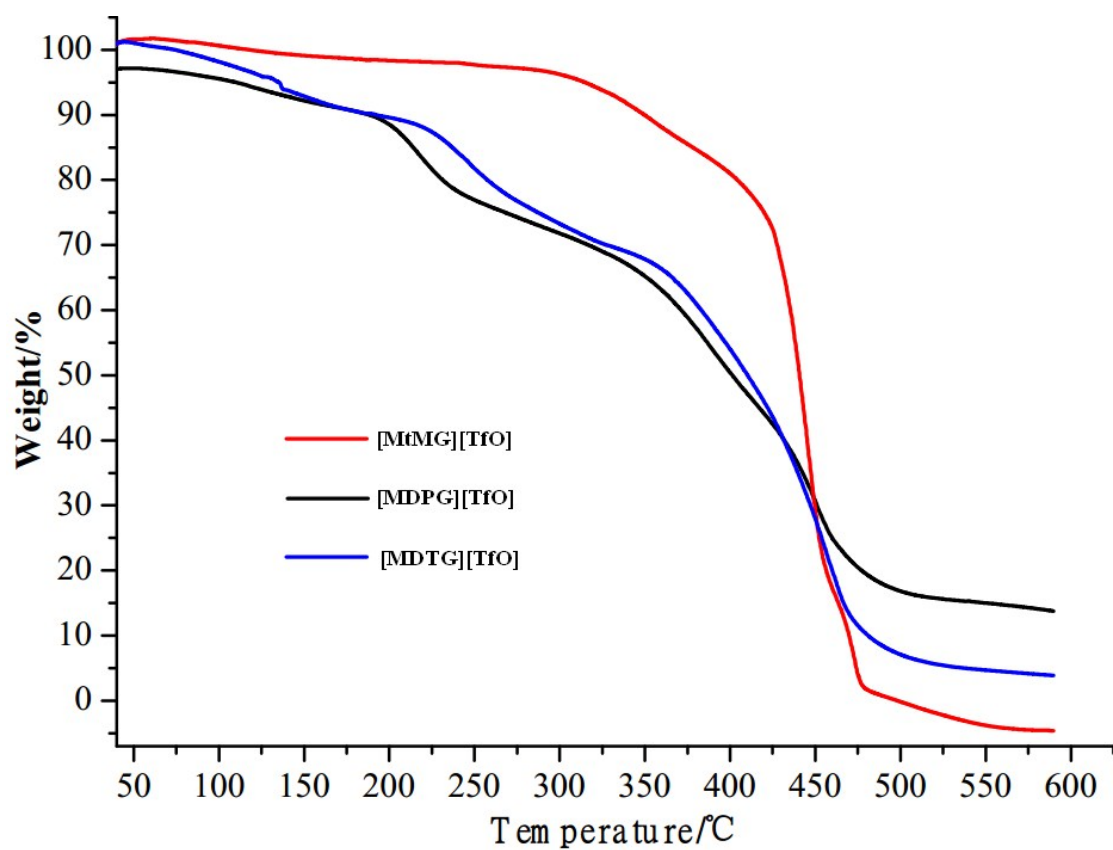


Fig. S7 TG curves of [MtMG][TfO], [MDPG][TfO] and [MDTG][TfO].

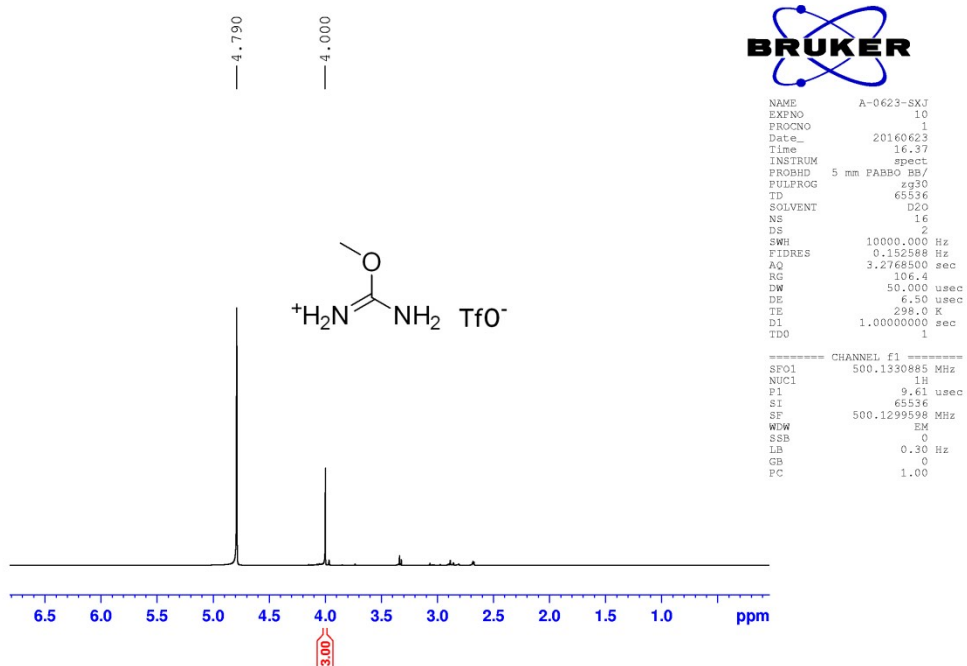


Fig. S8 ^1H NMR spectrum of ionic liquid [MU][TfO].

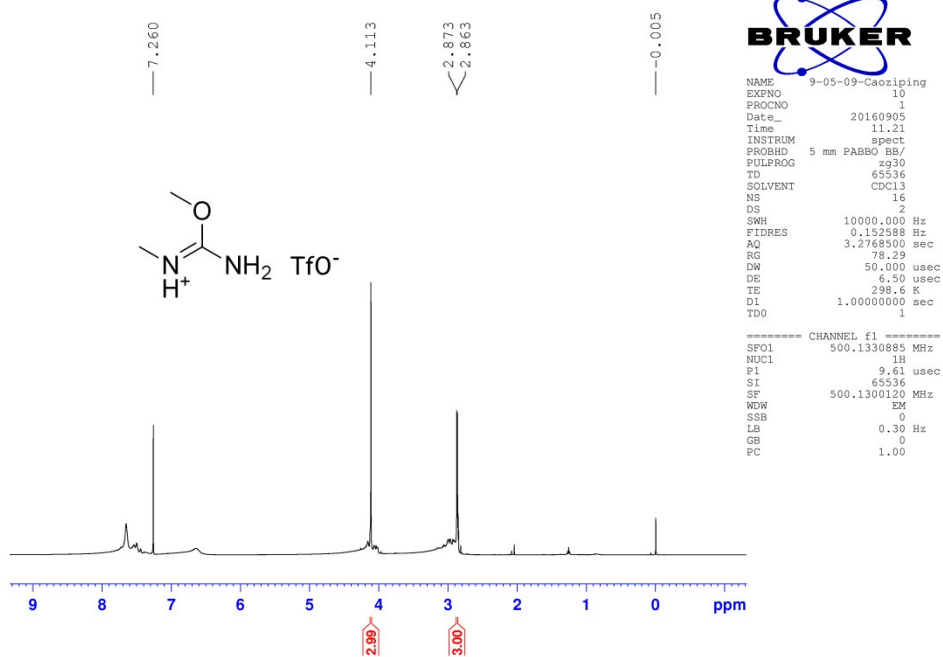


Fig. S9 ^1H NMR spectrum of ionic liquid [MMU][TfO].

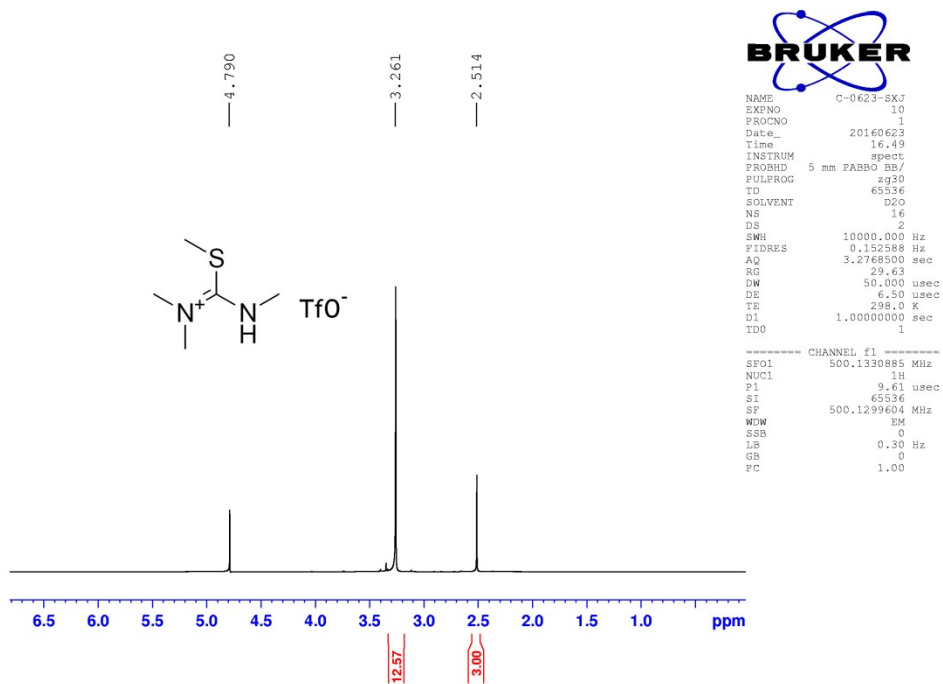


Fig. S10 ^1H NMR spectrum of ionic liquid [MtriMSU][TfO].

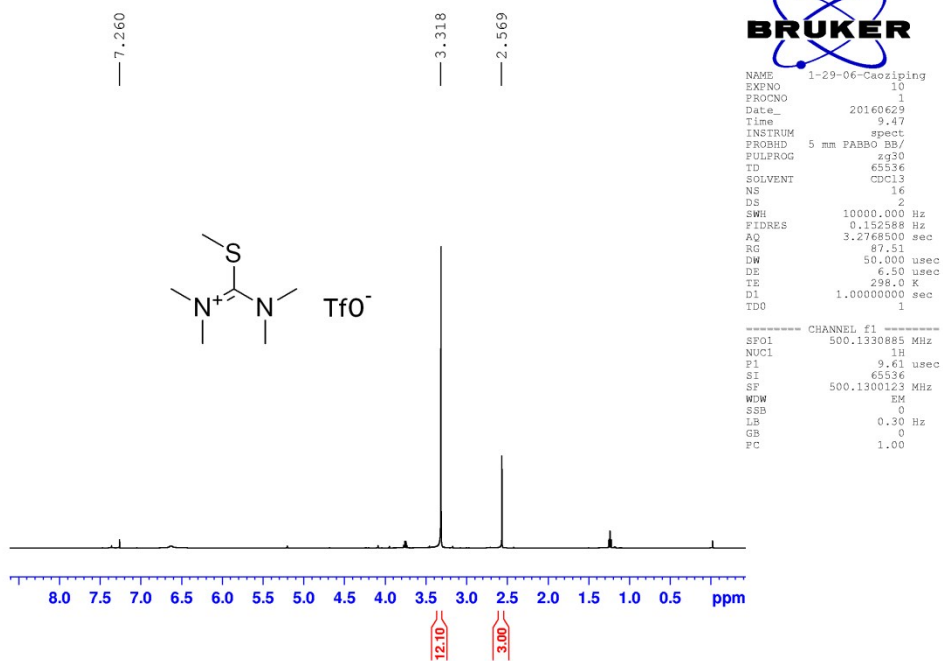


Fig. S11 ¹H NMR spectrum of ionic liquid [MtMSU][TfO].

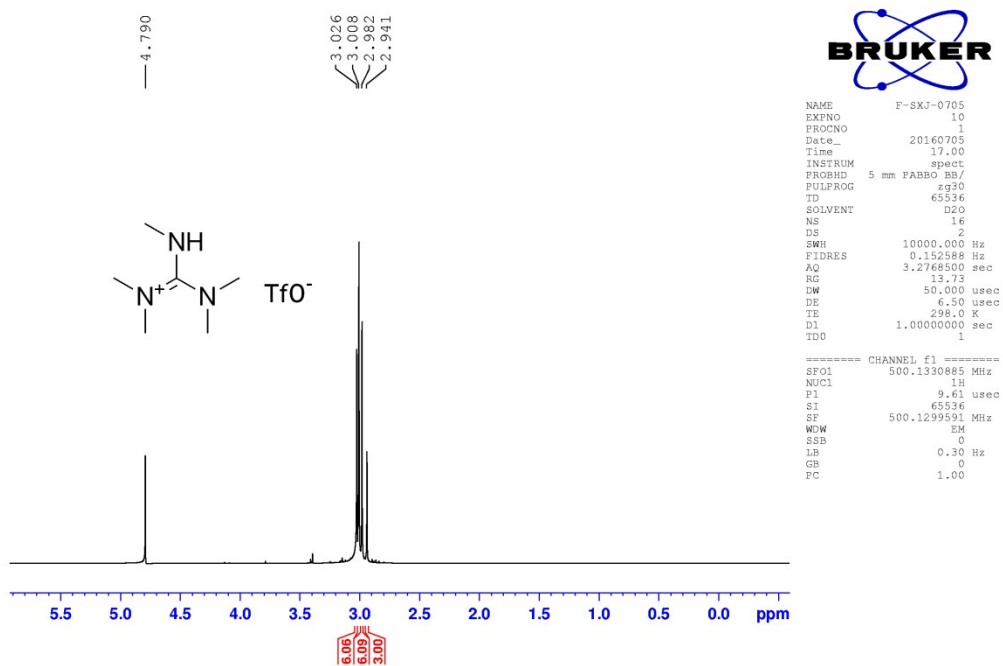


Fig. S12 ^1H NMR spectrum of ionic liquid [MtMG][TfO].

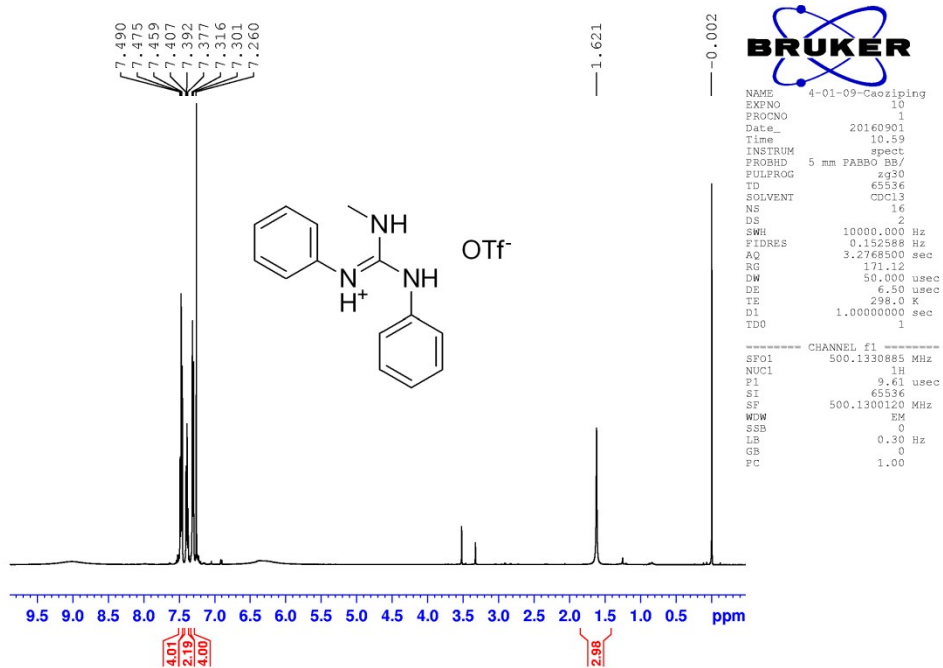


Fig. S13 ^1H NMR spectrum of ionic liquid [MDPG][TfO].

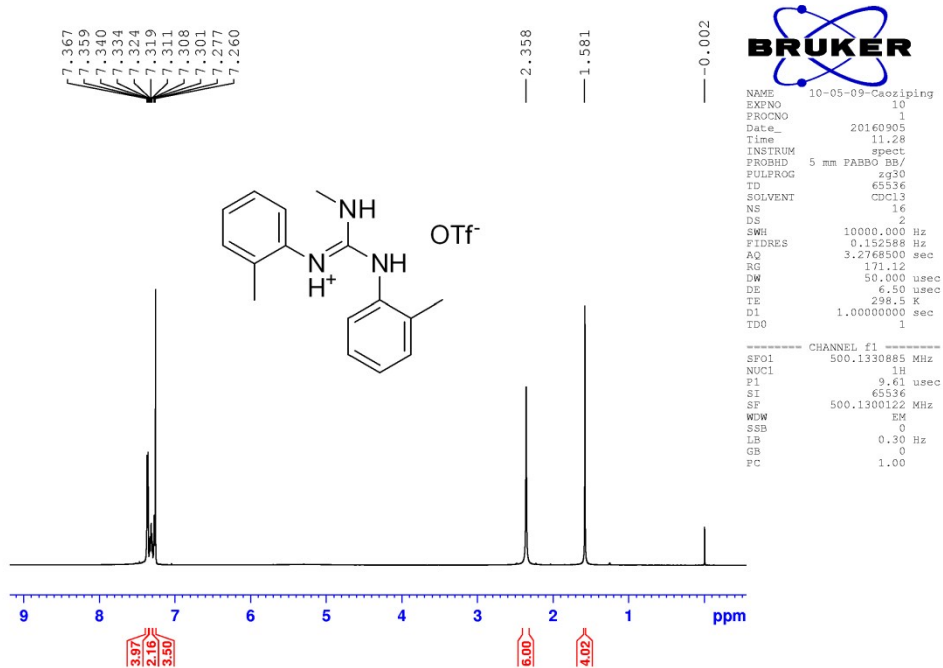


Fig. S14 ^1H NMR spectrum of ionic liquid [MDTG][TfO].

Cartesian coordinates and imaginary frequencies for all the transition states.

[MtMG][TfO]

Imaginary frequency: -526.48

C	-2.38368600	-0.06089600	0.41639400
N	-3.30943000	-0.70975400	-0.38053700
N	-1.56222200	-0.76082100	1.14807300
H	-0.99628700	-0.20056600	1.77661100
C	-3.61505200	-2.11089100	-0.13386000
H	-4.66718500	-2.29616400	-0.38137000
H	-3.00046600	-2.78723800	-0.74612200
H	-3.44499000	-2.33884000	0.91874400
C	-3.64943400	-0.22937100	-1.71470300
H	-3.28134500	-0.93172500	-2.47658400
H	-4.73612300	-0.13578900	-1.83901100
H	-3.18706300	0.74147800	-1.89230800
C	0.01076200	-2.18345400	0.22637400
H	-0.73381300	-2.78741600	0.71836600
H	-0.23636900	-1.79373200	-0.75142000
H	1.04351500	-2.45765100	0.39270200
N	-2.42548400	1.32234300	0.37912600
C	-1.28878300	2.08418100	0.88843600
H	-1.33662600	2.22249100	1.97969700
H	-0.35256100	1.58726900	0.63283600
H	-1.30019600	3.07461700	0.42225600
C	-3.70041700	2.03643000	0.43134100
H	-3.72784800	2.83847600	-0.31616900
H	-4.52660000	1.35037200	0.24682400
H	-3.84181100	2.48886700	1.42360200
C	2.43779800	0.50227700	-0.97950600
S	2.47515100	-0.32616200	0.68795900
F	3.67126300	0.66441900	-1.46163700
F	1.73254500	-0.24702700	-1.85078500
F	1.84668000	1.70612300	-0.89743100
O	3.17982400	0.60517700	1.56679400
O	3.05344100	-1.65398000	0.42628400
O	0.97695700	-0.40863700	0.99932100

[MDPG][TfO]

Imaginary frequency: -541.32

C	-1.75039000	-1.15138400	-0.02653400
N	-1.41718200	-2.47668500	-0.25821400
N	-1.02592900	-0.25135700	0.55280000
H	-0.12559100	-0.58623400	0.88183200
N	-3.01853300	-0.85916300	-0.50644900
C	3.44311700	2.22051400	0.54128300
S	2.47364100	1.22725100	-0.70132500
F	4.55075100	2.70801200	-0.02577100
F	2.69883600	3.24448700	0.98674700
F	3.78938000	1.45895400	1.58510500
O	3.31988000	0.07413400	-1.02374500
O	2.13740400	2.17778500	-1.77579700
O	1.24065700	0.83316700	0.11431200
C	-0.15205700	-3.09161600	-0.05642900
C	1.04350000	-2.45691300	-0.41262800
C	-0.12315700	-4.39217500	0.46459900
C	2.25803700	-3.11468200	-0.21878800
H	1.04657600	-1.45845800	-0.83015000
C	1.09420900	-5.04983700	0.62969400
C	2.29072800	-4.41124600	0.29659700
H	3.17133500	-2.59163700	-0.48441100
H	1.10451800	-6.05990800	1.03010700
H	3.23928300	-4.92144000	0.43660600
C	-3.88410700	0.19999000	-0.14745100
C	-4.91018500	0.53175700	-1.04455200
C	-3.79288000	0.87870200	1.07715000
C	-5.83236400	1.52608000	-0.72452800
C	-4.71759000	1.87731800	1.37957100
H	-3.00030700	0.63161300	1.77168000
C	-5.74063000	2.20874700	0.48877400
H	-6.62057000	1.76802400	-1.43205400
H	-4.63651100	2.39703800	2.33051500
H	-6.45474600	2.98826700	0.73659900
C	-0.61395000	1.79874600	-0.41261200
H	0.11527100	2.20932700	-1.09898800
H	-0.71111300	2.25816400	0.56024000
H	-1.52188400	1.42035600	-0.85600900
H	-2.20419900	-3.11357100	-0.23638000
H	-3.32056200	-1.41929300	-1.29205200
H	-1.05238900	-4.88434600	0.74503500
H	-4.98378500	0.00875800	-1.99608600

[MDTG][TfO]

Imaginary frequency: -545.73

C	-0.15600800	-1.38464900	0.17486900
N	0.94722900	-1.63802000	-0.60333400
N	-0.19129200	-1.36153200	1.47398300
H	0.72623700	-1.55236800	1.87471500
N	-1.28911700	-1.16054600	-0.59628800
C	1.15090400	3.48415900	-0.17270200
S	-0.14290600	2.14250900	-0.11190600
F	0.86480600	4.34317000	-1.15488600
F	1.17820300	4.14654600	0.98957200
F	2.35920100	2.95317700	-0.39556800
O	-0.04412500	1.46881900	-1.42087700
O	-1.41441600	2.81307200	0.20714900
O	0.36828400	1.28586500	1.04253200
C	2.30215100	-1.73983700	-0.19066800
C	2.86343600	-0.77988100	0.66134200
C	3.07810500	-2.80796400	-0.68747900
C	4.19769100	-0.89375800	1.04959000
H	2.26111900	0.06584900	0.97602800
C	4.41842900	-2.88246900	-0.29510200
C	4.97949200	-1.94526500	0.57268600
H	4.62765300	-0.14472300	1.70871700
H	5.02796200	-3.69988200	-0.67291700
H	6.02144800	-2.03397600	0.86690400
C	-2.63313600	-1.32966000	-0.18554700
C	-3.64418000	-0.59479900	-0.84659700
C	-2.97951400	-2.27328900	0.79497000
C	-4.97399500	-0.82584000	-0.47683800
C	-4.31295900	-2.47000800	1.14586200
H	-2.19861000	-2.83910500	1.28741000
C	-5.32113700	-1.74447500	0.51205000
H	-5.75316500	-0.26044300	-0.98245500
H	-4.55867300	-3.20122900	1.91146700
H	-6.36339800	-1.89350100	0.77916900
C	-1.11676400	0.57116500	2.46363200
H	-1.40605100	1.57787900	2.19966500
H	-0.37711100	0.44739700	3.24231200
H	-1.86529800	-0.19764600	2.36022100
H	0.73773600	-1.91250500	-1.55390000
C	2.48603500	-3.84028900	-1.61745000
H	1.57096200	-4.28246200	-1.20479800
H	2.22639700	-3.41567900	-2.59817000

H	3.19781900	-4.65013300	-1.80033100
H	-1.12537600	-0.47902600	-1.33282800
C	-3.32174300	0.41375200	-1.92432100
H	-2.72874400	1.25107000	-1.54087500
H	-2.75754900	-0.03234800	-2.75550000
H	-4.24327700	0.82393500	-2.34714100

[MDMSF][TfO]

Imaginary frequency: -459.10

C	2.28017500	0.00517100	0.01207700
H	1.28225100	-0.30858500	0.30707800
N	3.17668200	-0.96967800	0.02140200
C	2.76984100	-2.33335500	0.37772700
H	2.96098900	-3.00750200	-0.46484900
H	3.34864800	-2.67722000	1.24207000
H	1.70586100	-2.34522000	0.61967900
C	4.57526000	-0.78837200	-0.35473500
H	4.79449800	0.27583200	-0.44208100
H	5.21666500	-1.23709100	0.41073400
H	4.77242100	-1.28061100	-1.31423900
C	0.12648100	2.86859100	0.22697300
H	0.98181500	3.26959400	0.74936800
H	-0.02520800	3.17310500	-0.79893300
H	-0.74006300	2.63432000	0.82936200
S	-1.30778300	0.04343500	0.56667500
O	-0.49781600	0.86634500	-0.42637000
O	-1.89432400	0.85927500	1.64247700
C	-2.74226600	-0.52306700	-0.48111900
F	-2.30418900	-1.25188000	-1.51432600
F	-3.41263600	0.53469500	-0.95302400
F	-3.57182600	-1.26943600	0.25489100
O	-0.60957400	-1.19948800	0.95293600
S	2.49653200	1.61830500	-0.40503500

[MMSU][TfO]

Imaginary frequency: -484.19

C	2.39521800	0.36682400	-0.55109300
N	2.04492100	1.61816500	-0.23350800
C	2.03635800	2.14943200	1.12450200
H	2.99762900	1.96049200	1.60249400
H	1.86833300	3.22700400	1.06228700
H	1.24018300	1.68166900	1.71391100
C	0.91158200	-2.37379900	1.04213200
H	0.73059700	-2.10344000	2.07260800
H	0.06925800	-2.60924100	0.40579300
H	1.86556700	-2.80849800	0.79016900
S	-0.98127700	-0.28911800	-0.50713800
O	-0.01267300	-0.39752500	0.66103500
O	-1.28444000	-1.59291600	-1.11935200
C	-2.55160900	0.26628400	0.32774000
F	-2.35896300	1.44175900	0.93748500
F	-2.92259400	-0.63831200	1.24144500
F	-3.52572600	0.39808800	-0.57522400
O	-0.64555500	0.82657000	-1.42252200
H	1.39760500	2.06256700	-0.87776100
N	2.12371900	-0.04154700	-1.81312100
H	1.29936600	0.34448000	-2.26968500
H	2.32144100	-1.01178000	-2.01311200
S	3.17422300	-0.69431100	0.55672400

[MtriMSU][TfO]

Imaginary frequency: -475.80

C	2.20322200	-0.33520200	0.09929600
N	1.87766000	-1.62669600	-0.12813400
C	1.51989300	-2.12244800	-1.45540300
H	0.42807500	-2.19248400	-1.53728800
H	1.29114400	-0.27985800	1.87984100
C	2.48864300	1.42666700	1.82421400
H	1.79283000	2.20136100	1.47960200
H	2.49603800	1.42187700	2.91731800
H	3.48731900	1.66149500	1.45539500
S	-1.25762900	0.60170600	0.45104400
O	-0.81625600	-0.17028600	1.63340600
O	-1.76068700	1.96447300	0.67940900
O	-0.26974000	0.52073100	-0.70413300
C	-2.68957200	-0.38742300	-0.21478600
C	0.56091400	2.39181200	-1.49454600
H	1.48193800	2.90357000	-1.26303700
H	0.44589000	1.98536900	-2.48916800
H	-0.32444100	2.69606900	-0.95422200
F	-3.16627400	0.17719800	-1.32944700
F	-2.28447200	-1.63478200	-0.50512600
F	-3.66669000	-0.45246400	0.69241500
H	1.89439800	-1.44060000	-2.21473700
H	1.96181000	-3.11327500	-1.60059800
N	2.09267700	0.09712100	1.37771900
S	2.77548300	0.71260100	-1.14925000
C	1.50623300	-2.51455500	0.97586600
H	2.16645900	-2.34060800	1.82921500
H	0.46450700	-2.35974800	1.28273100
H	1.63041500	-3.54708700	0.64125500

[MtMSU][TfO]

Imaginary frequency: -481.16

C	-2.24166700	0.14654900	-0.04945400
N	-2.25868800	0.26404200	1.30503800
C	-2.47678000	1.55903600	1.94234600
H	-1.53432700	2.11365600	2.03511300
C	-1.95616100	-1.42336100	-1.93809400
H	-1.52810100	-2.43008400	-1.92099600
H	-2.80671600	-1.40011400	-2.63055000
H	-1.19301800	-0.72607300	-2.27629400
S	1.33694100	-0.34383400	-0.36777600
O	0.86874100	-1.67480800	0.05195300
O	1.50970100	-0.09822000	-1.80937100
O	0.58893100	0.77857200	0.34495400
C	3.04655700	-0.17504600	0.35203600
C	0.39910200	2.60926600	-0.85917900
H	-0.37677400	3.35918400	-0.85167400
H	1.20560900	2.74374900	-0.15479400
H	0.62366000	2.09022800	-1.78127200
F	3.50137000	1.07341900	0.13999700
F	3.02721200	-0.39868500	1.67170600
F	3.88735700	-1.04005500	-0.22097500
H	-3.18388000	2.15284500	1.36438300
H	-2.88299900	1.38047000	2.94353800
N	-2.38336500	-1.09146700	-0.57753300
S	-2.09861100	1.51905400	-1.07874000
C	-1.55327000	-0.69943700	2.16310400
H	-1.02116600	-1.42992300	1.55711100
H	-0.80050500	-0.15149100	2.73920600
H	-2.24169600	-1.19653100	2.85689200
C	-3.08791700	-2.17134300	0.11106600
H	-2.39864300	-2.94402700	0.47048900
H	-3.65688700	-1.77148000	0.95054100
H	-3.78508600	-2.63239400	-0.59778300

[MSU][TfO]

Imaginary frequency: -449.45

C	3.22167300	-0.57296800	-0.15077900
N	2.20906600	-1.39825900	0.09234600
C	0.74571600	2.26477300	0.58918300
H	0.50200400	2.63628100	-0.39651700
H	-0.06511000	2.02342900	1.26335900
H	1.67409900	2.58834200	1.03581700
S	-1.22786600	-0.26304300	0.68918600
O	0.01906100	0.26805500	-0.03526400
O	-1.64441200	0.62651600	1.78451900
C	-2.53937300	-0.07545400	-0.62020700
F	-2.23828900	-0.81593800	-1.69225500
F	-2.62643000	1.20936900	-0.99434400
F	-3.72194200	-0.46795200	-0.13909700
O	-1.11760400	-1.70394100	0.94142200
H	2.35155900	-2.35787100	0.37864900
N	4.48100600	-1.07380300	-0.14375400
H	4.64408600	-2.06960400	-0.21856400
H	5.23540100	-0.46147200	-0.41666500
S	2.99183200	1.10067600	-0.46314200
H	1.25950500	-1.00924500	0.09374900

[MDMF][TfO]

Imaginary frequency: -476.87

C	2.33461500	0.16999800	0.02951100
H	1.44153400	-0.33897200	0.39877700
O	2.31149000	1.37475800	-0.29509000
N	3.42707300	-0.60176400	-0.04737000
C	3.36675500	-2.00720700	0.33834100
H	3.62936300	-2.64629000	-0.51296300
H	4.06835000	-2.20819200	1.15658300
H	2.35448300	-2.25260800	0.66696900
C	4.69777900	-0.08301000	-0.53614100
H	4.57502300	0.97242200	-0.77774400
H	5.47241900	-0.19704800	0.23119800
H	5.01001400	-0.63068200	-1.43303200
C	0.55518000	2.68402200	-0.01714100
H	1.45474400	3.07682400	0.43151800
H	0.39951200	2.88196700	-1.06776300
H	-0.31450600	2.59191800	0.62099700
S	-1.16324700	0.09847000	0.53378800
O	-0.32892000	0.75383900	-0.56014800
O	-1.67430400	1.07524900	1.51213200
C	-2.64964600	-0.48274300	-0.42997300
F	-2.27936200	-1.34738800	-1.38130400
F	-3.26045600	0.55858300	-1.00767700
F	-3.51022300	-1.08748900	0.39483200
O	-0.53904300	-1.13037500	1.05763000

[MMA][TfO]

Imaginary frequency: -474.22

C	2.76404700	-0.13462000	-0.01397000
O	2.31846900	-0.17203100	1.15590600
N	2.93474300	1.04808900	-0.62253500
C	2.39334500	2.28459900	-0.06580700
H	2.77815400	2.44003500	0.94439400
H	2.70142700	3.11676800	-0.70124100
H	1.30060200	2.23294300	-0.02678700
C	0.71092200	-1.50603000	1.76923300
H	0.22483800	-0.65508700	2.22296400
H	0.08301100	-2.21547200	1.25049500
H	1.62036700	-1.86356000	2.22700000
S	-1.29375000	-0.77517900	-0.54695300
O	0.19822000	-0.66971100	-0.25351400
O	-1.92605200	-1.84998200	0.23671800
C	-1.92194400	0.80047000	0.22368400
F	-1.31080000	1.86924900	-0.31646700
F	-1.66679800	0.80494100	1.54888200
F	-3.23775100	0.92805400	0.04749600
O	-1.60060000	-0.65389100	-1.97204700
H	3.25609500	1.05047400	-1.58020600
C	3.14422000	-1.37833900	-0.77980000
H	2.21939600	-1.87478100	-1.08829500
H	3.74331100	-1.16482700	-1.66980800
H	3.70389700	-2.05201400	-0.12524200

[Mlplb][TfO]

Imaginary frequency: -455.50

C	2.30176700	-0.25317100	0.06312500
O	1.99797600	-0.41116000	1.27066500
N	2.22336300	0.92613800	-0.56951300
C	1.72484400	2.18397800	0.00115900
H	1.22132000	1.90821700	0.92898500
H	2.45921800	0.93740200	-1.55391800
C	2.89969000	3.11649000	0.32792600
H	2.53444800	4.03989500	0.79098200
H	3.59901600	2.63638500	1.01990900
H	3.44936300	3.39154300	-0.58066400
C	0.71146000	2.82174000	-0.95303700
H	1.17413200	3.05348900	-1.92179700
H	-0.13975000	2.15742500	-1.11692500
H	0.34292500	3.76419600	-0.53390200
C	2.87898500	-1.42321800	-0.72947600
H	3.08805400	-1.08281800	-1.75341800
C	1.86716500	-2.57959200	-0.79030000
H	0.92911100	-2.27602400	-1.26243000
H	2.29332100	-3.41196900	-1.36107100
H	1.63971200	-2.93622200	0.21897900
C	4.20501000	-1.86544300	-0.08308800
H	4.63047300	-2.70809100	-0.63817200
H	4.94289800	-1.05481600	-0.07605400
H	4.03463400	-2.18174600	0.95046200
S	-1.74434600	-0.97307600	-0.11142200
O	-1.80544300	-1.54094700	-1.46005700
O	-2.17440700	-1.79907000	1.03047800
O	-0.42684800	-0.25856000	0.16164400
C	-2.93149900	0.46187800	-0.12229800
C	0.07746800	-0.25676300	2.33670900
H	0.93525300	-0.11322300	2.97382000
H	-0.59809800	0.57702500	2.21285300
H	-0.34571900	-1.24726600	2.24303500
F	-2.85590500	1.12013000	1.05400000
F	-2.62124700	1.32758300	-1.10067500
F	-4.18772300	0.04954900	-0.29748900

[MDMP][TfO]

Imaginary frequency: -458.26

C	-1.84704800	0.78731700	-0.19275200
O	-1.47129700	0.96594600	0.98925800
N	-2.30673200	-0.41500000	-0.57596400
C	-2.34664000	-1.60199600	0.29417000
H	-1.53818800	-1.45883800	1.01431300
H	-2.65994800	-0.51069700	-1.51938800
C	-3.68099500	-1.68169500	1.04590600
H	-3.68201800	-2.54038200	1.72642700
H	-3.84310000	-0.77551400	1.63751900
H	-4.52128900	-1.79943000	0.35066500
C	-2.05961700	-2.84759300	-0.54640700
H	-2.82269200	-2.99120200	-1.32341500
H	-1.07905000	-2.77380500	-1.02388400
H	-2.06763300	-3.73865300	0.08938100
C	-1.85810700	1.89606600	-1.22720000
H	-0.81306100	2.17359700	-1.39288000
C	-2.67394200	3.11059900	-0.75988500
H	-2.29547400	3.49468300	0.19192500
H	-2.61360800	3.91369800	-1.50090700
H	-3.73077200	2.85616800	-0.62154800
S	2.27470900	0.58247000	-0.07987100
O	3.09421500	0.75641000	-1.27847400
O	2.89480500	0.77135400	1.24430100
O	0.92648600	1.28971000	-0.17700100
C	1.76807600	-1.20961900	-0.11039900
C	0.23135900	2.19624800	1.71748400
H	-0.60598800	2.14850700	2.39482700
H	1.14749400	1.69084800	2.00175700
H	0.32348800	3.07990100	1.10141300
F	0.97969100	-1.49744400	0.94309900
F	1.07604200	-1.48290900	-1.23179700
F	2.83865600	-2.00507100	-0.06523000
H	-2.24807300	1.52208300	-2.18133700

[MDMA][TfO]

Imaginary frequency: -446.15

C	-2.21332900	1.23580000	0.03046400
O	-1.68967000	1.11376700	1.16087600
N	-3.03961700	0.28704000	-0.44067900
C	-3.24773100	-1.01917600	0.20729100
H	-3.06566900	-0.84630900	1.27078300
H	-3.41223400	0.40814300	-1.37389800
C	-4.69937400	-1.45914300	0.00321700
H	-4.87805000	-2.41326200	0.50916000
H	-5.40049900	-0.72005100	0.40481500
H	-4.92372200	-1.60601900	-1.06163200
C	-2.23562700	-2.04699600	-0.31475600
H	-2.38226300	-2.23165700	-1.38615300
H	-1.21043000	-1.69877500	-0.16412100
H	-2.36134700	-3.00038200	0.21094700
C	-1.97652900	2.44171500	-0.84692100
H	-2.67667600	2.50144200	-1.68512400
S	1.93658000	0.52047200	-0.58907600
O	2.11636700	0.25033700	-2.01528000
O	2.82817700	1.48820700	0.07519700
O	0.47606200	0.75210000	-0.21057300
C	2.27513000	-1.09754200	0.26797900
C	0.28427200	1.86643300	1.70924900
H	-0.45646200	2.52353400	2.13810100
H	0.47602700	0.93593000	2.22329400
H	1.10632600	2.30960800	1.16442400
F	2.07926500	-0.96542300	1.59608700
F	1.44589200	-2.05235500	-0.18081900
F	3.53360500	-1.49202700	0.06446900
H	-2.06430200	3.35093300	-0.24531400
H	-0.95587600	2.37642800	-1.23385900

[MMU][TfO]

Imaginary frequency: -503.74

C	-2.56014900	0.08801600	-0.40510500
N	-2.66895100	-1.24917500	-0.23812800
C	-2.72103500	-1.84325900	1.08952400
H	-3.35615100	-1.22499500	1.72404000
H	-3.15354600	-2.84397100	1.01361700
H	-1.72072500	-1.90246100	1.53433200
C	-1.04757600	2.02811200	1.44205800
H	-0.62272100	1.59095600	2.33379800
H	-0.36554600	2.41305200	0.69252800
H	-2.03412000	2.45464100	1.51105400
S	0.74664300	0.18659500	-0.44007700
O	-0.13091400	0.11950300	0.80400800
O	0.91168600	1.56827300	-0.93168400
C	2.41195900	-0.31289700	0.22715100
F	2.35409000	-1.54162200	0.75034800
F	2.79235500	0.54585200	1.18239200
F	3.31707900	-0.29833200	-0.75408300
O	0.41274800	-0.85230400	-1.43291600
H	-2.31799400	-1.83275700	-0.98674400
N	-2.25931900	0.52640400	-1.67025600
H	-1.59794100	-0.03360900	-2.20082200
H	-2.05198800	1.51595900	-1.71160600
O	-2.80584200	0.89254400	0.53059700

[MU][TfO]

Imaginary frequency: -506.01

C	2.72381400	-0.36363000	-0.14223400
N	2.64165600	-1.28554300	-1.14008500
C	1.36428100	2.37380900	-0.06126100
H	0.80348600	2.66801400	-0.93631000
H	0.81115500	2.17118000	0.84893000
H	2.38858100	2.69866700	0.01413600
S	-0.50689300	-0.17601900	0.34846100
O	0.25186500	0.57853800	-0.73434800
O	-0.45129400	0.51288800	1.65313400
C	-2.27176500	-0.02567600	-0.22737100
F	-2.42313900	-0.61449400	-1.41733100
F	-2.60260800	1.26751300	-0.33932800
F	-3.08709400	-0.60739000	0.65526800
O	-0.22951300	-1.62570600	0.33688500
H	2.09992900	-2.12378000	-0.96388200
N	2.57886800	-0.82013900	1.13420100
H	1.96057300	-1.60961800	1.28781500
H	2.49230200	-0.09388100	1.83242000
O	3.00978100	0.83424500	-0.38951100
H	2.48146800	-0.87191600	-2.04885200