ELECTRONIC SUPPLEMENTARY INFORMATION

Table 1S. Total MP2 energies of the calculated structures (Hartree).

Structure	Energy
Ia	–704.200075
Ib	–704.200039
IIa	–2817.087340
IIb	–2817.087717
IIIa	–539.359196
IIIb	–539.359765
Cl^-	–459.724492
Br^-	–2572.613175
I^-	–294.887430
CH_3NO_2	–244.450706

Table 2S. Cartesian coordinates (Å) of the calculated equilibrium structures.

CH_3NO_2

O	2.104054	-1.792136	0.123440
O	1.239624	-0.633414	1.785122
N	1.181335	-1.175524	0.673153
C	-0.123848	-1.112837	-0.049182
H	-0.703819	-1.989014	0.268178
H	-0.627287	-0.188656	0.250515
H	0.085690	-1.157156	-1.122235

Ia

Cl	-2.506640	-3.417484	0.322978
O	2.117091	-1.780509	0.128321
O	1.256375	-0.627014	1.783102
N	1.178665	-1.172087	0.669388
C	-0.122784	-1.120219	-0.043422
H	-0.746333	-1.994892	0.250213
H	-0.620219	-0.192323	0.257430
H	0.092956	-1.161693	-1.116041

Ib

Cl	-3.480322	-0.904306	0.131718
O	1.616663	-2.353689	0.311555
O	1.771149	-0.167510	0.279286
N	1.110137	-1.219129	0.312331
C	-0.383265	-1.114005	0.316663
H	-0.792426	-1.983011	0.835584
H	-0.665329	-0.171426	0.789599
H	-0.724418	-1.117345	-0.724765

IIa

Br	-2.690786	-3.458552	0.258116
O	2.158262	-1.728461	0.113048

O	1.299321	-0.568245	1.764803
N	1.215031	-1.136782	0.663617
C	-0.103203	-1.136999	-0.021819
H	-0.688235	-2.024143	0.294258
H	-0.628681	-0.225042	0.278330
H	0.087404	-1.187997	-1.098384

IIb

Br	-3.618142	-0.894732	0.129770
O	1.635156	-2.355217	0.314535
O	1.789493	-0.168412	0.280609
N	1.129755	-1.220474	0.313660
C	-0.362776	-1.115497	0.315994
H	-0.773123	-1.984662	0.834352
H	-0.645994	-0.173106	0.789342
H	-0.702179	-1.118320	-0.726290

IIIa

I	-2.888316	-3.532576	0.206643
O	2.199272	-1.670726	0.092601
O	1.339987	-0.513393	1.747201
N	1.251513	-1.098607	0.655403
C	-0.080713	-1.147056	-0.002602
H	-0.628496	-2.043980	0.339619
H	-0.629801	-0.248616	0.295374
H	0.085666	-1.211270	-1.082271

IIIb

I	-3.817386	-0.880893	0.126242
O	1.661904	-2.357385	0.318682
O	1.816141	-0.169748	0.283600
N	1.158102	-1.222396	0.315799
C	-0.334351	-1.117549	0.314938
H	-0.744876	-1.987232	0.833021
H	-0.617743	-0.174977	0.788647
H	-0.669603	-1.120242	-0.728957