

Supporting Information

Reactions of Gas-phase Uranyl Formate/Acetate Anions: Intra-complex Hydride Attack to Convert Carboxylates to Aldehydes

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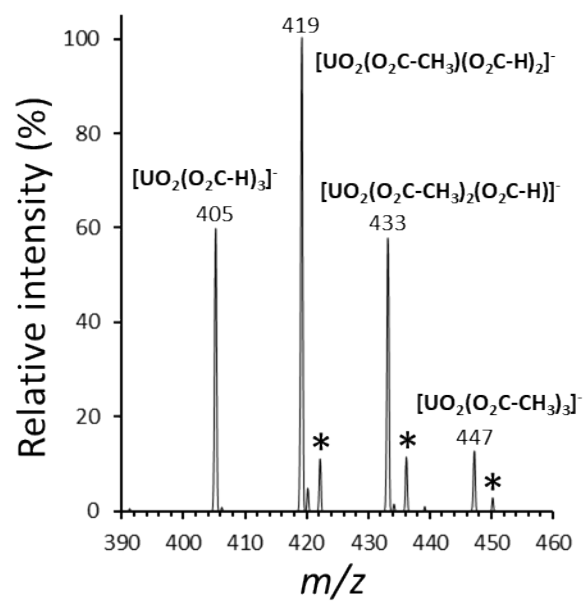


Figure S1.

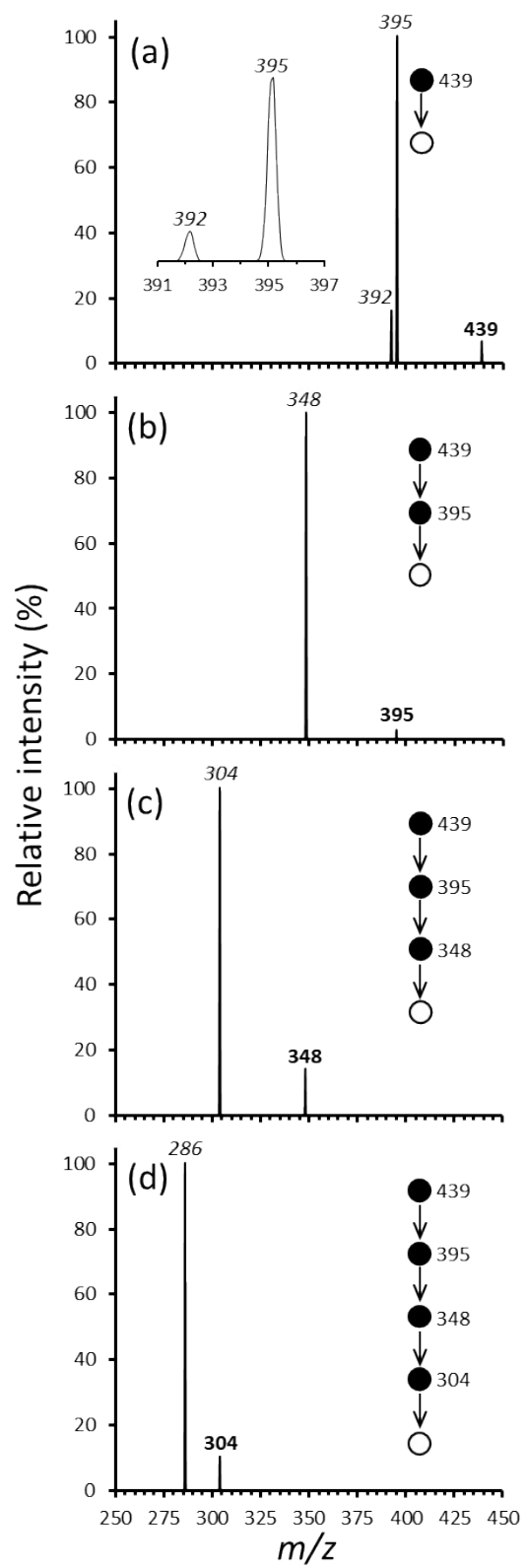


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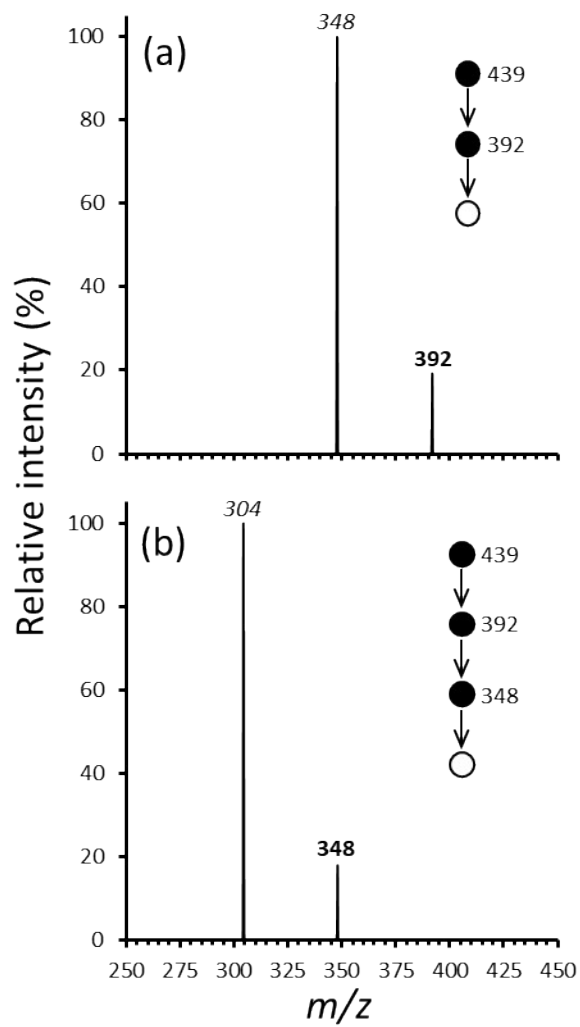


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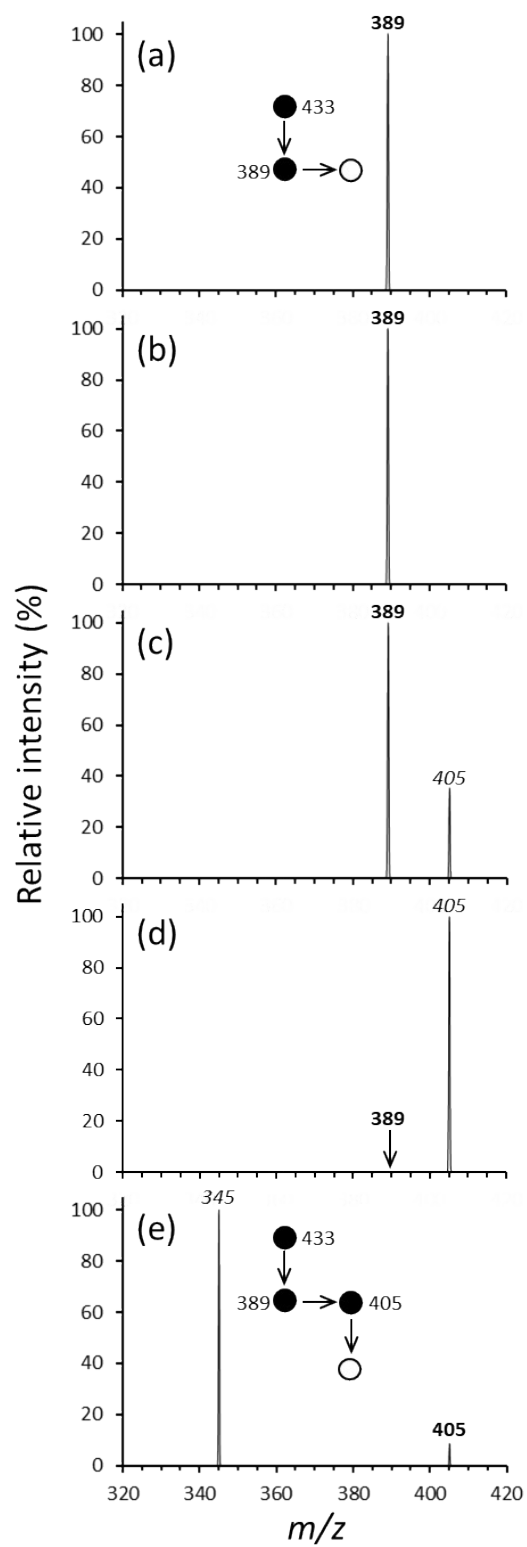


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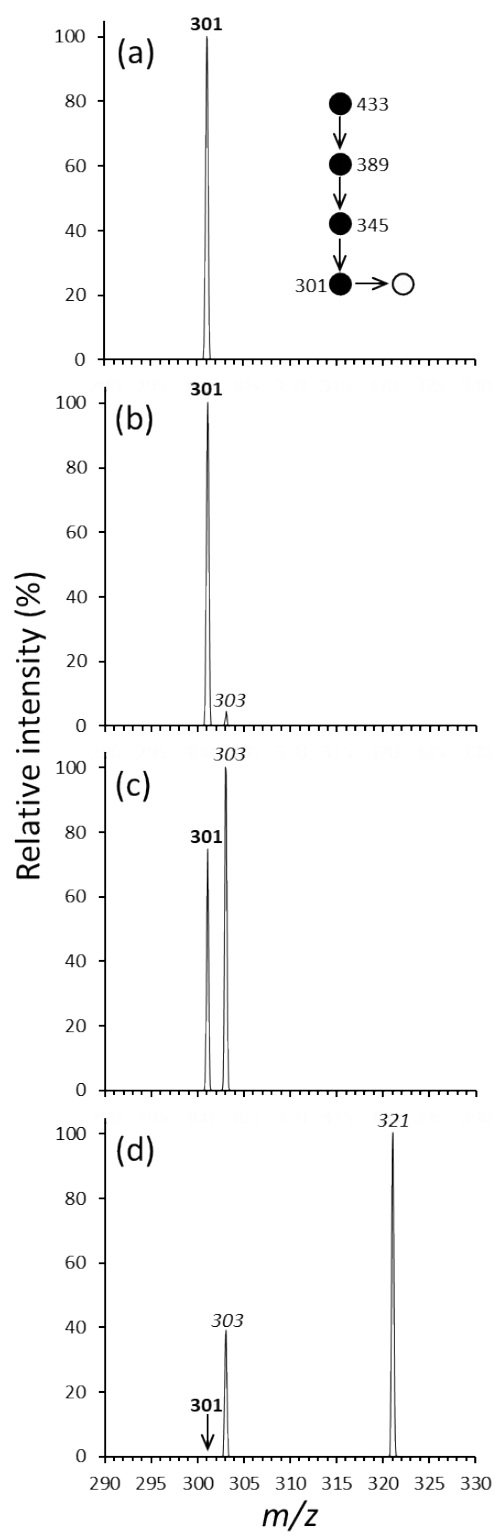


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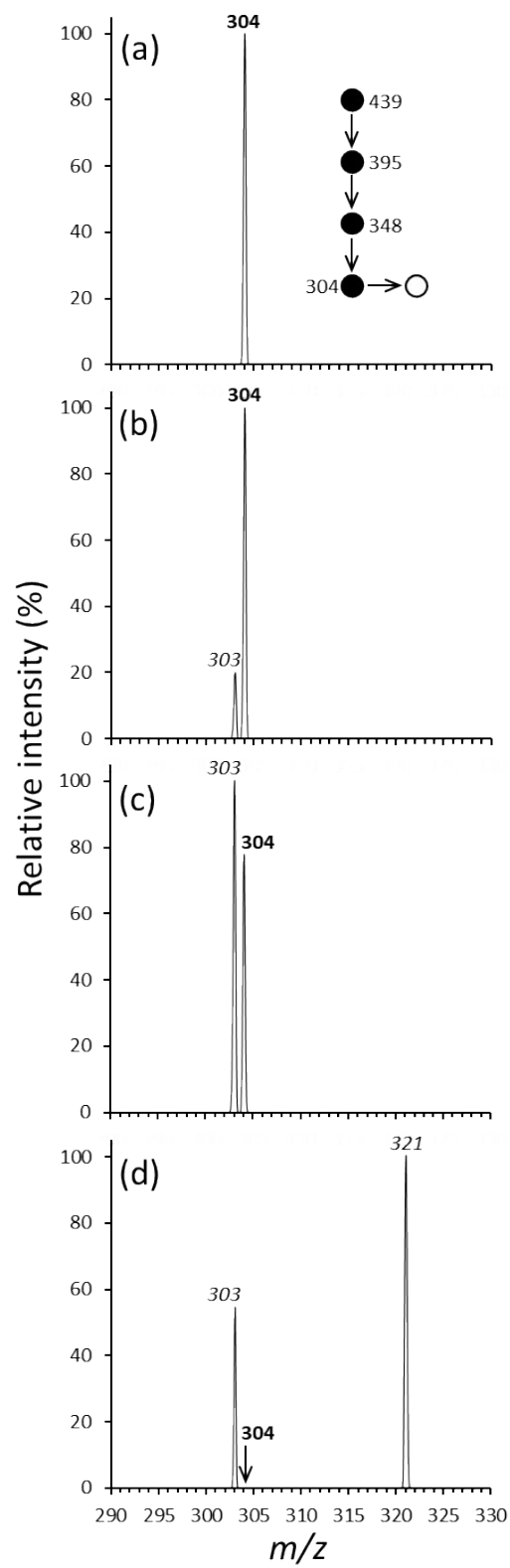


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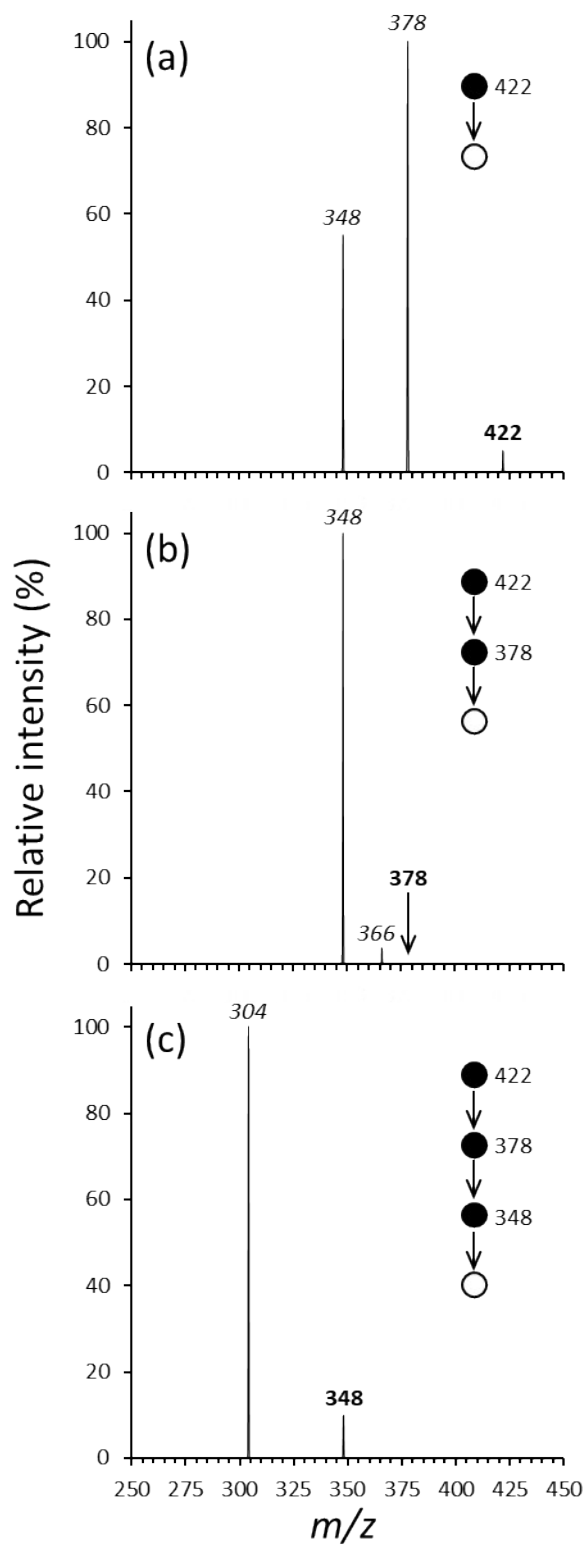


Figure S7.

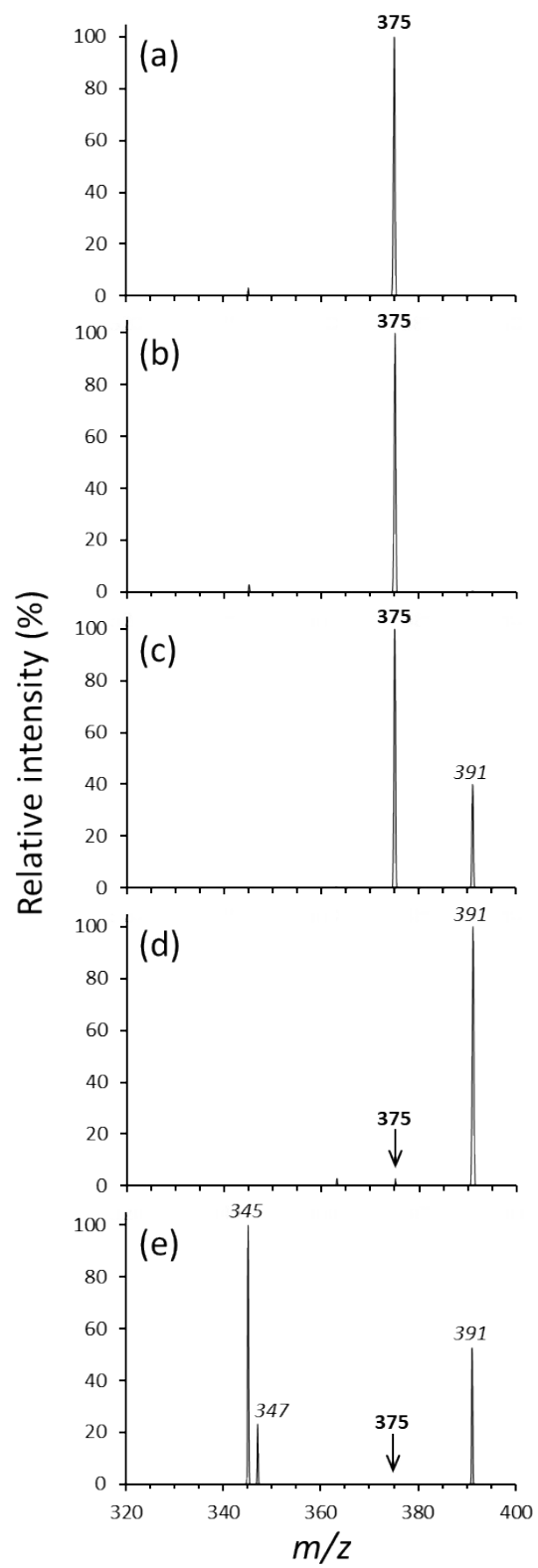


Figure S8.

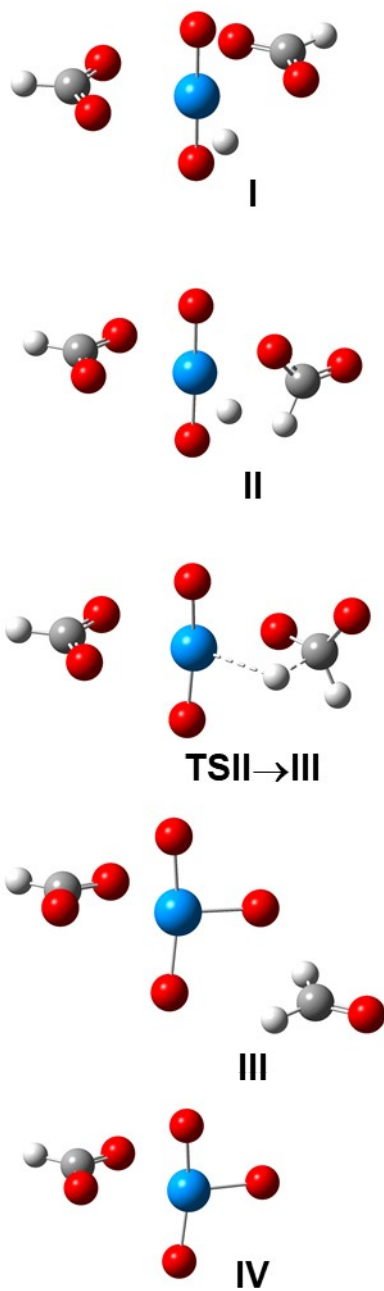
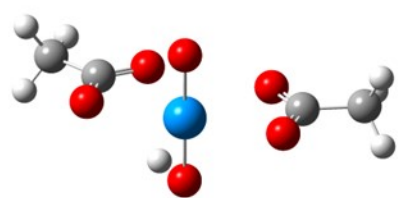
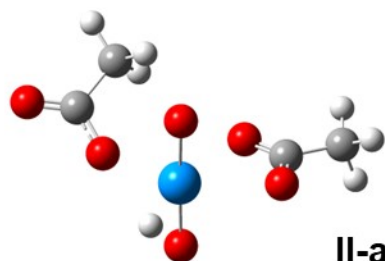


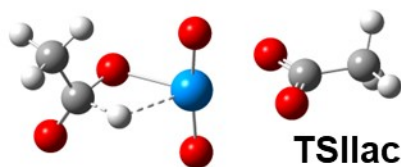
Figure S9.



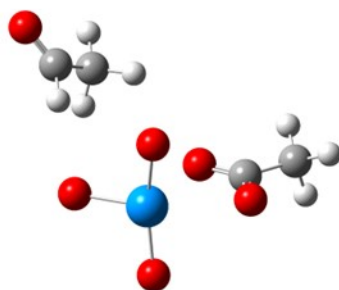
I-ac



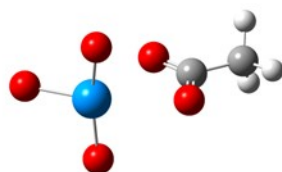
II-ac



TSIIac→IIIac



III-ac



IV-ac

Figure S10.

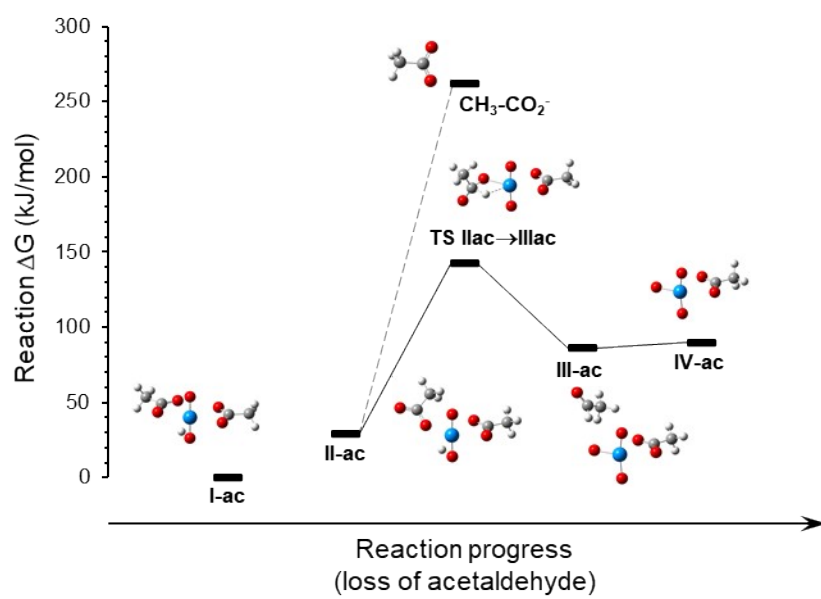


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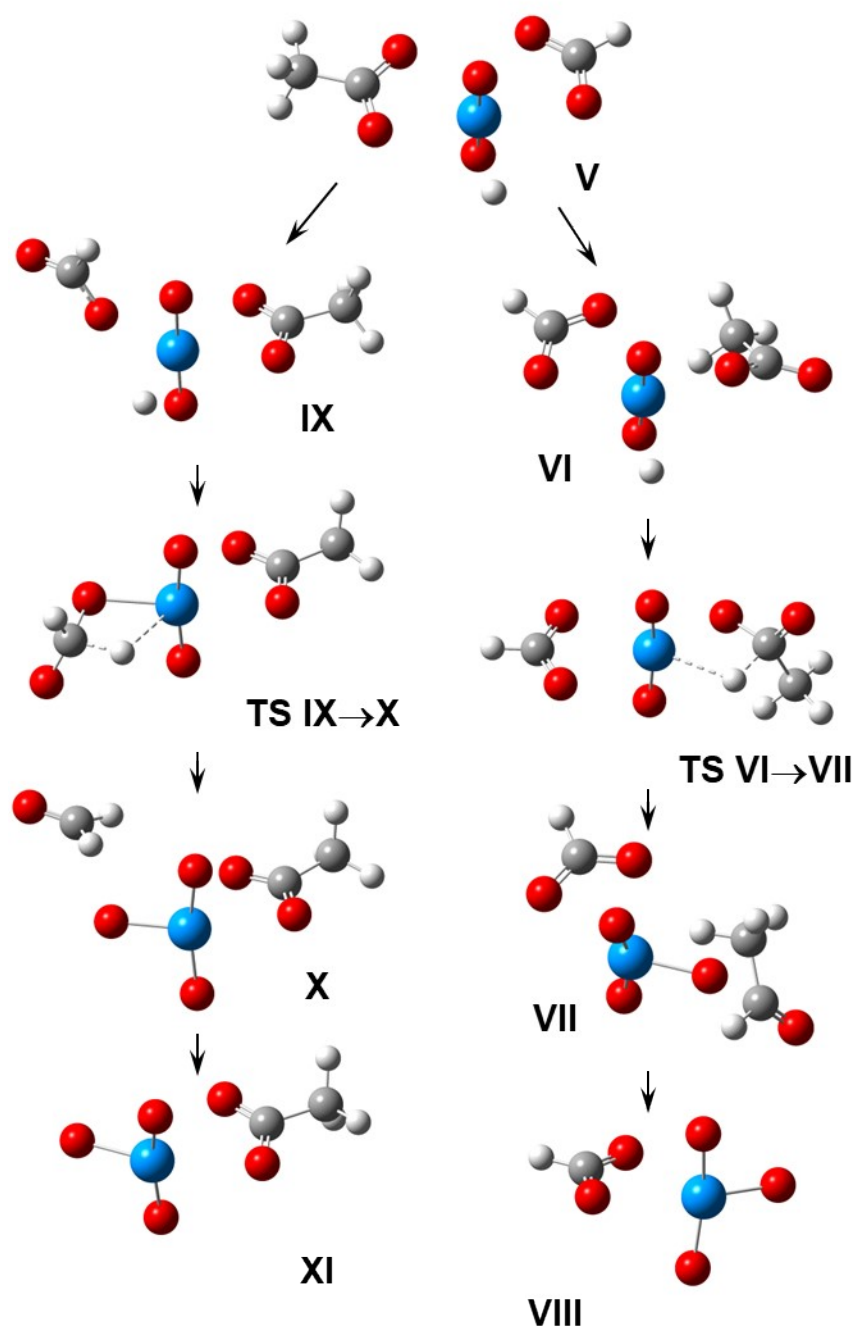


Figure S12

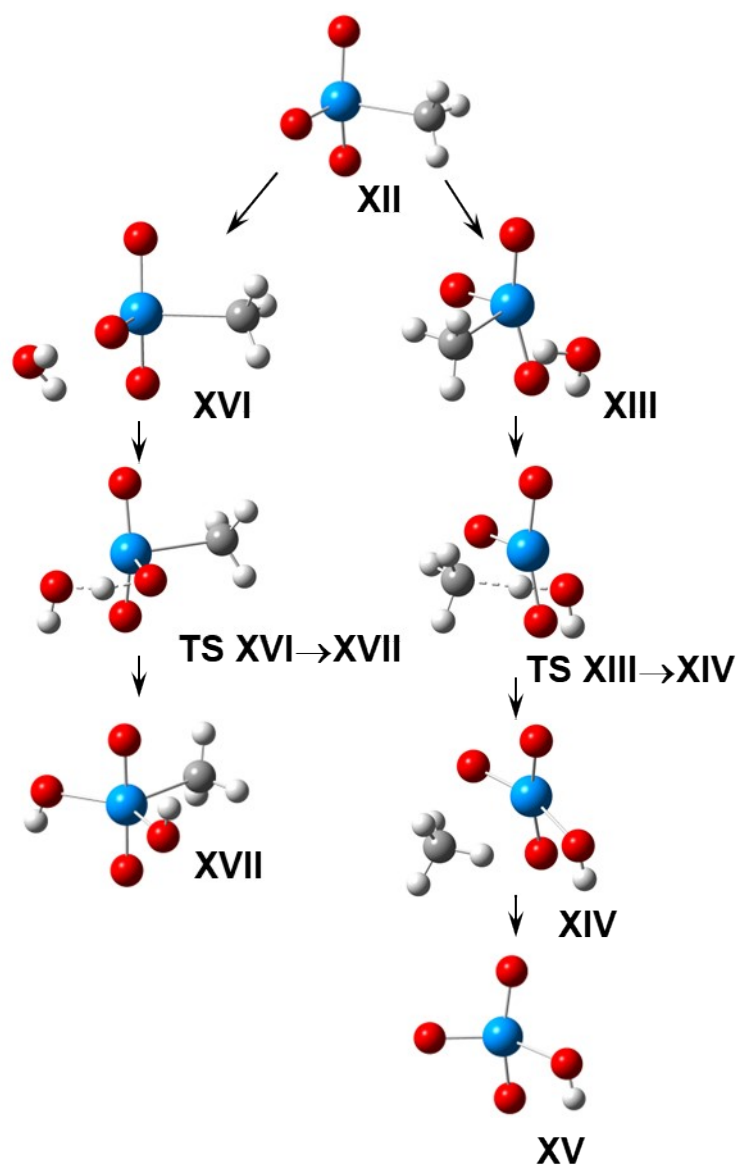


Figure S13.

Table S1.

Structure	Zero-point corrected electronic energy	Thermally corrected free energy
I	-1004.615232	-1004.654507
II	-1004.604059	-1004.644649
TS II->III	-1004.565179	-1004.604376
III	-1004.574499	-1004.615464
IV	-890.057297	-890.092941
formaldehyde	-114.502636	-114.524283

Table S2.

Structure	Zero-point corrected electronic energy	Thermally corrected free energy
I-ac	-1083.221641	-1083.264912
II-ac	-1083.209669	-1083.254063
TS II-ac->III-ac	-1083.1684	-1083.211674
III-ac	-1083.186513	-1083.232462
IV-ac	-929.359691	-929.397871
acetaldehyde	-153.810131	-153.835063

Table S3.

Structure	Zero-point corrected electronic energy	Thermally corrected free energy
V	-1043.918513	-1043.961161
VI	-1043.906032	-1043.947874
TS VI->VII	-1043.864826	-1043.905718
VII	-1043.884324	-1043.929082
VIII	-890.057297	-890.092941
acetaldehyde	-153.810131	-153.835063
IX	-1043.907696	-1043.950918
TS IX->X	-1043.868536	-1043.910748
X	-1043.877684	-1043.922421
XI	-929.359691	-929.397871
formaldehyde	-114.502636	-114.524283

Table S4.

Structure	Zero-point corrected electronic energy	Thermally corrected free energy
XII	-740.656324	-740.690521
H ₂ O	-76.423266	-76.440903
XIII	-817.101013	-817.138227
TSXI II->XIV	-817.100974	-817.137112
XIV	-817.145404	-817.184582
V	-776.660695	-776.694344
CH ₄	-40.480523	-40.497825
XVI	-817.101055	-817.138367
TSXVI->XVII	-817.094361	-817.130389
XVII	-817.143981	-817.180702