Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information
For

Elucidating the Molecular Mechanisms of Criegee-Amine Chemistry in the Gas-phase and Aqueous Surface Environments

Manoj Kumar,[1,2] and Joseph S. Francisco[1,2,*]

[1]Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE, USA 68588
[2]*Department of Earth and Environmental Sciences, University of Pennsylvania, Philadelphia, Pennsylvania, USA* 19104-6316.

*Email: jfrancisco3@unl.edu; frjoseph@sas.upenn.edu

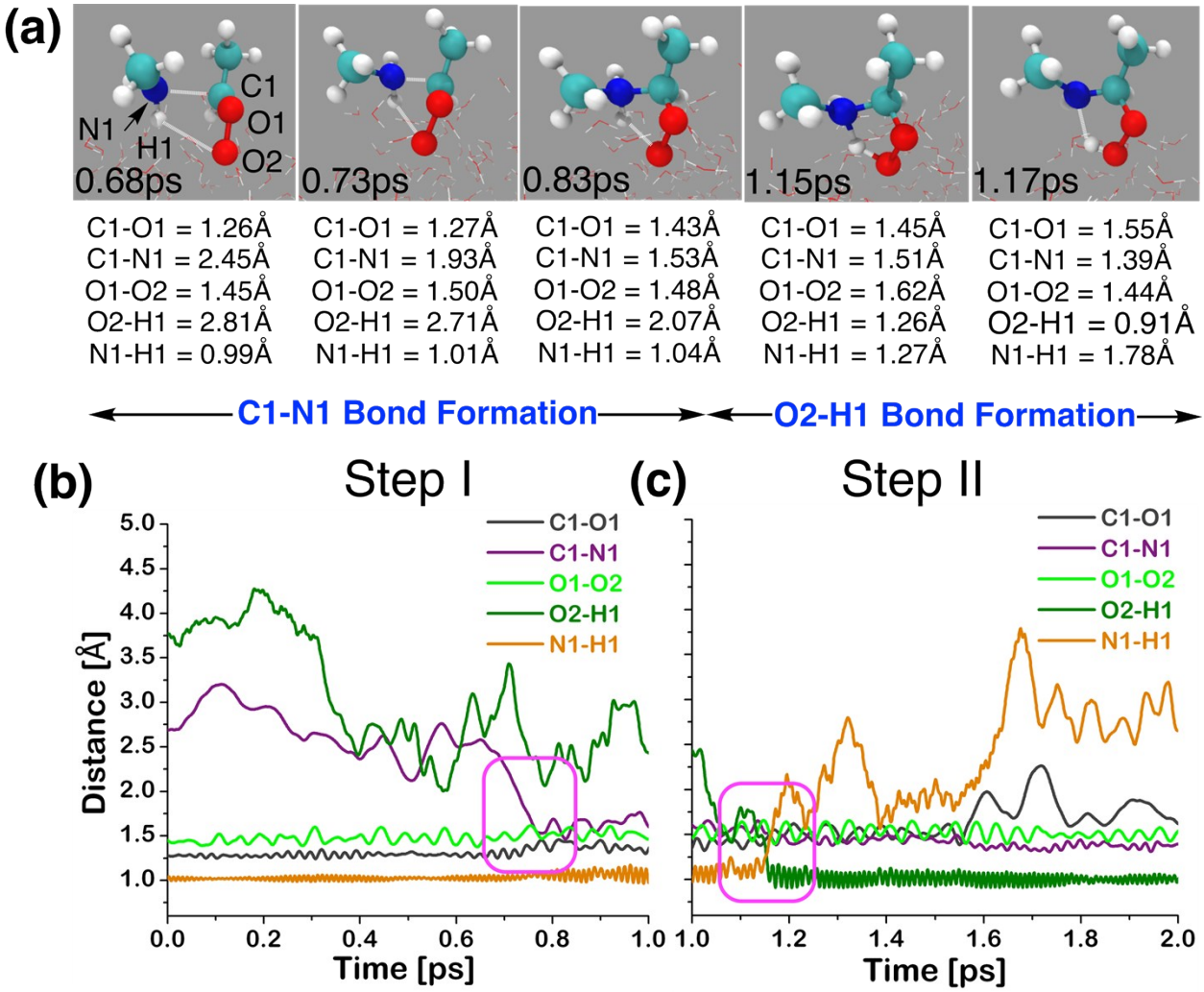

Figure S1. (a) Snapshot structures taken from the BOMD simulations, which illustrates the stepwise mechanism for the direct adduct formation between *anti*-CH_3CHOO and methylamine (CH_3NH_2) on the water droplet. (b) Time evolution of key bond distances (C1-O1, C1-N1, O1-O2, O2-H1, and N1-H1) involved in the C1-N1 bond formation. (C) Time evolution of key bond distances involved in the proton transfer from CH_3NH_2 to the terminal oxygen of *anti*-CH_3CHOO. Pink rectangles illustrate the formation of C1-N1 and O2-H1 bonds.

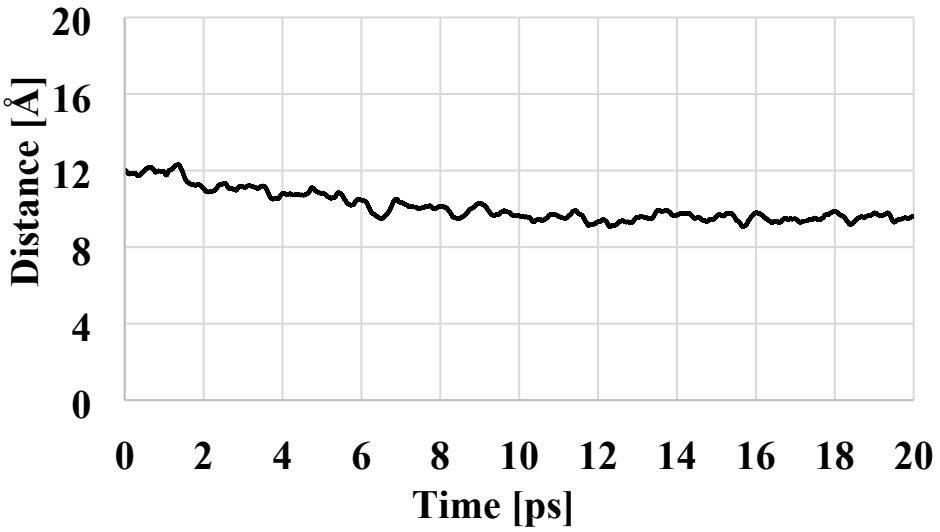

Figure S2. Distance between the centre of the mass of the *anti*-CH_3CHOO-CH_3NH_2 adduct, and that of the water droplet over the simulated time scale of 20 ps.

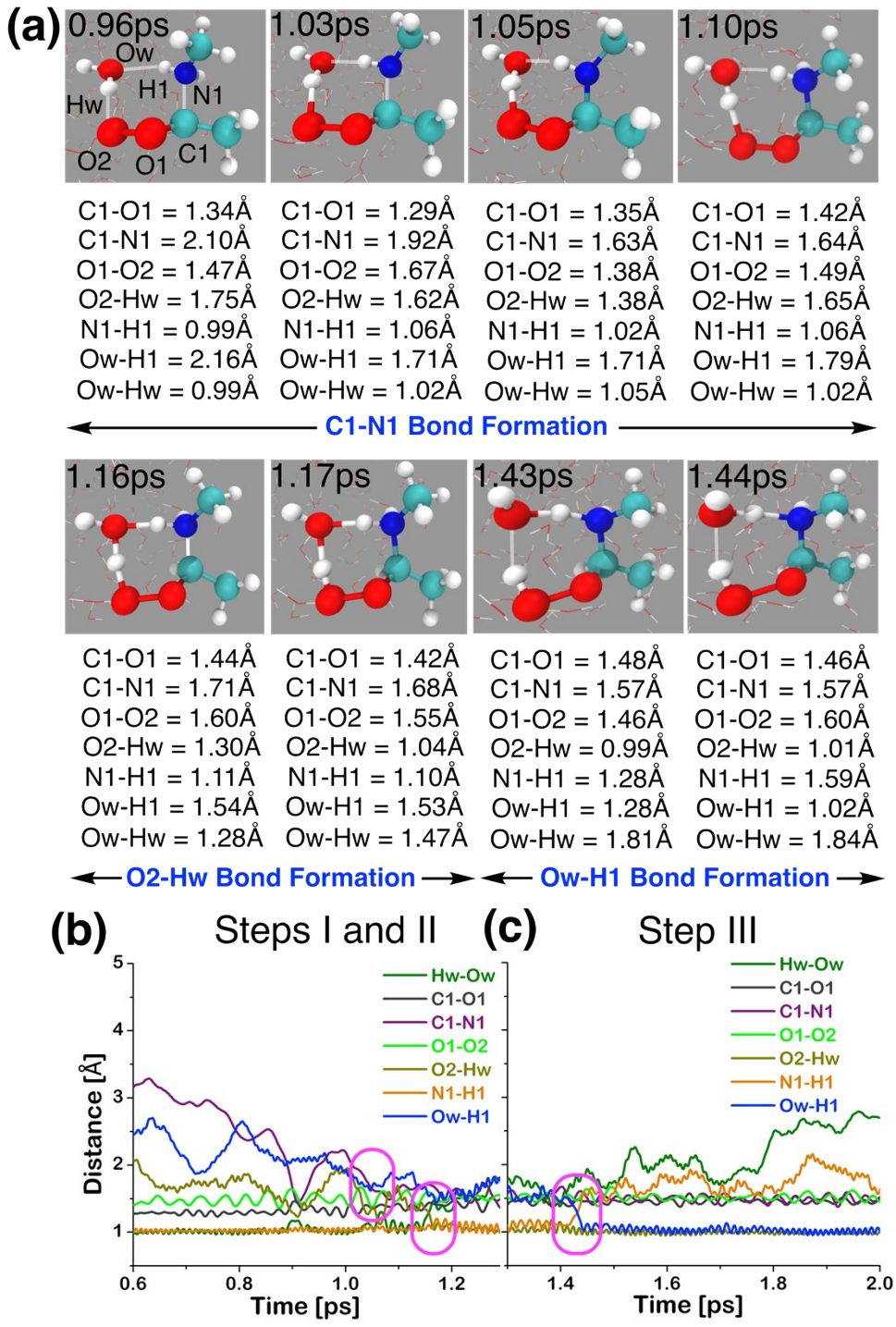

Figure S3. (a) Snapshot structures taken from the BOMD simulations, which illustrates the interfacial water-mediated stepwise mechanism for the adduct formation between *anti*-CH_3CHOO and methylamine (CH_3NH_2) on the water droplet. (b) and (c) Time evolution of key bond distances involved in the interfacial water-mediated stepwise adduct formation between *anti*-CH_3CHOO and CH_3NH_2.

Table S1. M06-2X/aug-cc-pVTZ optimized geometries of key species involved in the reactions of CH_2OO, *anti*-CH_3CHOO, *syn*-CH_3CHOO, and $(CH_3)_2COO$ with ammonia (NH_3), methylamine (CH_3NH_2), and dimethylamine ($(CH_3)_2NH$), respectively.

CH_2OO

C	-1.05385700	0.20328600	-0.00002400
H	-1.97278200	-0.36663900	-0.00007100
O	1.16734800	0.19259000	0.00005300
O	-0.00744200	-0.45988300	-0.00003800
H	-0.98332100	1.28526600	0.00009400

anti-CH_3CHOO

C	0.36995200	0.40017600	-0.00023100
H	0.09656700	1.45275400	0.00003900
O	-1.83974300	0.07624000	0.00014600
O	-0.56632800	-0.41241600	-0.00013700
C	1.76274200	-0.09329600	0.00002400
H	2.28776100	0.28953900	-0.87655500
H	2.28546100	0.28503900	0.88013300
H	1.78261400	-1.17920700	-0.00245500

NH_3

N	0.000011	-0.000003	-0.111988
H	0.795810	0.500877	0.261319
H	0.035905	-0.939513	0.261312
H	-0.831789	0.438657	0.261286

CH_3NH_2

N	0.049408	-0.755833	0.000000
H	-0.436468	-1.113412	0.811683
H	-0.436468	-1.113412	-0.811683
C	0.049408	0.704891	0.000000
H	0.587547	1.061824	0.877072
H	0.587547	1.061824	-0.877072
H	-0.944462	1.164663	0.000000

$(CH_3)_2NH$

N	-0.000037	0.568129	-0.148481
H	-0.000060	1.336753	0.507833
C	1.204634	-0.223964	0.020244
H	1.262863	-0.961016	-0.782205
H	2.083149	0.415404	-0.048947
H	1.240758	-0.767435	0.975345
C	-1.204539	-0.223942	0.020188

H	-2.083108	0.415571	-0.046401
H	-1.264384	-0.959735	-0.783279
H	-1.239532	-0.769007	0.974432

CH_2OO+NH_3 Reaction

Int_1

C	-0.584991	1.069973	0.230908
H	-0.666736	2.031054	-0.261254
O	-0.875100	-1.130137	0.183013
O	-1.022608	0.101595	-0.398383
H	-0.175018	0.920738	1.220423
H	1.254461	-0.801320	0.029532
N	1.902673	-0.017385	-0.041339
H	2.658995	-0.184929	0.609701
H	2.301193	-0.035356	-0.971521

TS

C	-0.095015	1.001887	0.262884
H	0.228913	1.940241	-0.172510
O	-1.160201	-0.925900	0.172501
O	-0.893592	0.326302	-0.414353
H	0.023694	0.778915	1.315014
H	2.392383	-0.483889	0.587030
N	1.631846	-0.303861	-0.054738
H	0.938504	-1.055057	0.009618
H	1.994018	-0.267717	-0.998473

Int_2

C	0.558771	0.613347	0.269953
H	0.982810	1.563140	-0.061899
O	-1.402846	-0.535147	0.153387
O	-0.712523	0.601819	-0.337311
H	0.443123	0.611965	1.354803
H	1.892219	-0.919676	0.611323
N	1.318672	-0.545909	-0.128349
H	-0.858603	-1.255236	-0.201531
H	1.880070	-0.392285	-0.952574

$CH_2OO+CH_3NH_2$ Reaction

Int_1

C	1.013248	1.018549	-0.344554
O	1.347598	-1.161243	-0.138210

O	1.643671	0.131091	0.240416
H	-0.606807	-0.631637	0.772167
N	-1.215342	0.170224	0.624552
H	-1.635256	0.419726	1.509454
C	-2.229466	-0.156310	-0.373665
H	-1.730689	-0.458909	-1.294648
H	-2.899700	-0.968898	-0.080003
H	-2.832853	0.724093	-0.591398
H	0.392467	0.759966	-1.191396
H	1.187399	2.031880	-0.004376

TS

C	0.913939	1.003978	-0.357540
O	1.392943	-1.143268	-0.128202
O	1.618270	0.176521	0.234911
H	-0.568579	-0.642290	0.789215
N	-1.168834	0.160769	0.612865
H	-1.565465	0.470028	1.489637
C	-2.202816	-0.190467	-0.355368
H	-1.722307	-0.552788	-1.264228
H	-2.887106	-0.969685	-0.009649
H	-2.788057	0.692004	-0.610368
H	0.346885	0.696630	-1.225686
H	1.010024	2.033616	-0.035203

Int_2

C	-0.090961	0.752552	0.261144
H	0.049659	1.828242	0.111053
O	-1.731851	-0.817184	0.163749
O	-1.408362	0.524771	-0.167066
H	0.007168	0.510524	1.322631
N	0.825754	-0.079973	-0.482270
H	-1.064664	-1.303022	-0.347125
H	0.962443	0.297460	-1.410879
C	2.103238	-0.301868	0.180703
H	2.731931	-0.929586	-0.447212
H	2.650707	0.621069	0.404558
H	1.930526	-0.829678	1.118310

$CH_2OO+(CH_3)_2NH$ Reaction

Int_2

C	-0.323291	-0.271997	0.811991
H	-0.065055	0.188671	1.776175

O	-2.022223	-0.332558	-0.694582
O	-1.534030	0.341842	0.455918
H	-0.470799	-1.346946	0.935508
N	0.673246	-0.046356	-0.208633
H	-1.293247	-0.193289	-1.320510
C	1.763558	-1.002089	-0.134121
H	2.450312	-0.831593	-0.961997
H	2.333137	-0.916325	0.803139
H	1.373668	-2.015921	-0.213429
C	1.155414	1.326002	-0.190628
H	1.743409	1.539688	0.714368
H	1.783568	1.506328	-1.061892
H	0.308218	2.008115	-0.225070

anti-$CH_3CHOO+NH_3$ Reaction

Int_1

C	0.717314	0.074935	0.383154
O	-0.930054	1.550418	0.098089
O	0.224860	0.935047	-0.359057
H	-1.807578	-0.363996	-0.009303
N	-1.572083	-1.358102	-0.037048
H	-2.214460	-1.840797	0.578404
H	-1.766125	-1.683604	-0.976057
C	1.891871	-0.694569	-0.067296
H	2.217852	-0.366055	-1.049710
H	2.702106	-0.591750	0.655294
H	1.607742	-1.748129	-0.099321
H	0.251489	-0.064864	1.352627

TS

C	-0.422580	-0.285081	0.363128
O	1.746221	-0.637058	0.111501
O	0.425342	-0.868297	-0.363344
H	-0.140462	-0.103465	1.394873
H	0.202144	2.442655	0.562572
N	0.236819	1.650702	-0.065133
H	1.175056	1.222186	-0.058451
H	0.002234	1.947200	-1.003536
C	-1.851803	-0.357898	-0.037701
H	-2.285278	-1.266642	0.383673
H	-2.393308	0.496946	0.359125
H	-1.944328	-0.393082	-1.120146

Int_2

C	-0.383084	0.029594	0.334113
O	1.878407	-0.230590	0.108446
O	0.621742	-0.754022	-0.282348
H	-0.206520	0.028050	1.412497
H	-0.510861	2.072539	0.573359
N	-0.264711	1.396332	-0.133847
H	1.823826	0.670671	-0.248556
H	-0.820295	1.564048	-0.962554
C	-1.685768	-0.656763	-0.019585
H	-1.677752	-1.691809	0.315768
H	-2.516947	-0.134860	0.451450
H	-1.826549	-0.643056	-1.100983

anti-$CH_3CHOO+CH_3NH_2$ Reaction

Int_1

C	-1.040579	-0.247216	-0.372859
O	-0.395260	1.872364	-0.131622
O	-1.227898	0.821162	0.224947
H	1.134479	0.645984	0.704355
N	1.454102	-0.319041	0.632053
H	1.806023	-0.599548	1.537524
C	-1.818039	-1.442580	0.005145
H	-2.494167	-1.220508	0.825457
H	-2.377640	-1.807645	-0.857108
H	-1.115027	-2.223234	0.299830
H	-0.318700	-0.239953	-1.182590
C	2.502778	-0.405038	-0.381345
H	2.794689	-1.444496	-0.528823
H	2.110544	-0.029890	-1.327057
H	3.401393	0.173363	-0.148198

TS

C	0.800735	0.351505	-0.352147
O	0.809480	-1.857681	-0.163316
O	1.347044	-0.612807	0.223272
H	-0.912590	-0.975812	0.559704
N	-1.239276	-0.006378	0.559786
H	-1.409535	0.288306	1.511818
C	1.214895	1.728445	0.006622
H	1.664030	1.747815	0.995795
H	1.941869	2.084447	-0.726143
H	0.350040	2.387421	-0.027130

C	-2.406212	0.167125	-0.294418
H	-2.697664	1.216616	-0.319314
H	-2.146729	-0.135079	-1.309277
H	-3.271250	-0.423591	0.016642
H	0.248061	0.135968	-1.260592

Int_2

C	0.091485	0.399543	-0.254382
O	1.789631	-1.126503	-0.166535
O	1.426677	0.204872	0.159779
H	1.118058	-1.626124	0.326855
N	-0.764232	-0.511058	0.482221
H	-0.932809	-0.140052	1.410099
C	-0.193005	1.869589	-0.023279
H	-0.028603	2.113153	1.026950
H	0.459950	2.491623	-0.631921
H	-1.228838	2.089734	-0.279228
H	0.007603	0.136871	-1.313589
C	-2.020088	-0.824871	-0.184372
H	-2.611409	-1.482722	0.449067
H	-2.626548	0.056527	-0.424339
H	-1.808595	-1.354121	-1.113194

anti-CH_3CHOO+$(CH_3)_2NH$ Reaction

Int_2

C	0.343631	0.451296	-0.424856
O	1.954551	-1.149696	-0.154198
O	1.551819	0.152742	0.240130
H	1.154762	-1.661612	0.055276
N	-0.670886	-0.499625	0.005970
C	0.067422	1.913486	-0.127112
H	0.099200	2.100796	0.944733
H	0.816416	2.537159	-0.609572
H	-0.916857	2.191156	-0.504541
H	0.484623	0.293438	-1.497951
C	-1.767505	-0.628522	-0.933917
H	-2.405073	-1.458978	-0.631823
H	-2.392898	0.274861	-0.983552
H	-1.380814	-0.838889	-1.930393
C	-1.145363	-0.279849	1.363308
H	-1.807843	0.592780	1.442571
H	-1.700536	-1.157435	1.693020
H	-0.294849	-0.138738	2.028450

syn-$CH_3CHOO+NH_3$ Reaction

Int_1

C	0.891581	0.297930	0.685769
O	0.212041	-1.299340	-0.712303
O	0.502628	-0.877990	0.558828
H	-1.662379	-0.313654	-0.396343
N	-2.131049	0.458475	0.075954
C	1.091610	1.187868	-0.460483
H	0.113578	1.359057	-0.916672
H	1.545258	2.124950	-0.155388
H	1.691195	0.661674	-1.206056
H	1.076732	0.575118	1.718158
H	-2.828998	0.822421	-0.560651
H	-2.634537	0.064966	0.861360

TS

C	-0.112999	0.438614	0.661231
O	1.361120	-0.589603	-0.655114
O	0.920730	-0.294703	0.666087
H	-2.171591	-0.758731	-0.697592
N	-1.360318	-0.962890	-0.129371
H	-0.561978	-1.241613	-0.716882
H	-1.573014	-1.702675	0.526803
C	-0.346515	1.500068	-0.356930
H	-1.336121	1.931928	-0.228911
H	0.406959	2.272742	-0.185520
H	-0.200883	1.114313	-1.359280
H	-0.538864	0.566621	1.653389

Int_2

C	0.491227	0.056212	0.481177
H	0.881784	0.115753	1.501047
O	-1.572597	-0.186117	-0.515332
O	-0.900705	-0.076698	0.729913
H	1.522362	1.213247	-0.876344
N	0.712156	1.269952	-0.277410
H	-1.347351	0.664354	-0.924931
H	0.783083	2.089533	0.308312
C	1.066187	-1.145955	-0.238573
H	2.154505	-1.090620	-0.251531
H	0.766133	-2.056747	0.274337
H	0.696328	-1.184201	-1.261298

syn-$CH_3CHOO+CH_3NH_2$ Reaction

Int_1

C	-1.145268	-0.247964	0.794269
O	-0.806272	1.290406	-0.781163
O	-0.730026	0.895335	0.528753
H	0.971663	0.041371	-1.030347
N	1.514512	-0.649339	-0.517330
C	-1.764608	-1.112853	-0.213885
H	-1.011796	-1.332757	-0.972988
H	-2.143728	-2.026260	0.232053
H	-2.551046	-0.546201	-0.717475
C	2.463995	0.031276	0.360888
H	1.911824	0.670819	1.049078
H	3.009313	-0.703367	0.952754
H	3.192463	0.659173	-0.160909
H	-1.021708	-0.513701	1.838841
H	2.007092	-1.212386	-1.198053

TS

C	0.629225	0.361393	0.690002
O	1.057872	-1.374525	-0.646849
O	0.652604	-0.894045	0.615483
H	-0.712021	-0.093226	-1.157447
N	-1.173101	0.547363	-0.509810
C	1.477768	1.240138	-0.150681
H	1.405105	0.963442	-1.196525
H	1.216440	2.282210	0.012828
H	2.513947	1.070701	0.155433
C	-2.275666	-0.120000	0.173918
H	-1.867799	-0.965213	0.727609
H	-2.742077	0.567811	0.877351
H	-3.039835	-0.498389	-0.507350
H	0.231542	0.722202	1.634814
H	-1.465372	1.378296	-1.006558

Int_2

C	0.149309	0.478392	0.419738
O	1.238803	-1.349394	-0.466373
O	0.698218	-0.796014	0.724476
H	0.459090	-1.346627	-1.045607
N	-0.931558	0.298408	-0.519984
C	1.185141	1.448228	-0.108557

H	1.511285	1.149077	-1.102482
H	0.768004	2.454139	-0.155255
H	2.047957	1.456762	0.553435
C	-2.168762	-0.187968	0.074394
H	-1.974134	-1.143678	0.558865
H	-2.582540	0.497309	0.823272
H	-2.912618	-0.348338	-0.703281
H	-0.210110	0.795151	1.407867
H	-1.076325	1.128700	-1.075199

syn-CH_3CHOO+$(CH_3)_2NH$ Reaction

Int_1

C	-1.510706	0.048132	-0.816584
O	-1.381458	-0.742452	1.260277
O	-1.410588	-0.960561	-0.094142
H	0.695352	-0.139516	0.793251
N	1.280786	0.098117	-0.003505
C	-1.705915	1.393129	-0.265458
H	-0.841947	1.641366	0.351965
H	-1.843367	2.124400	-1.054942
H	-2.562801	1.361088	0.411993
C	2.279404	1.077024	0.385411
H	2.828009	1.407861	-0.498344
H	1.796669	1.948743	0.827077
H	3.011397	0.686974	1.105948
C	1.880569	-1.117475	-0.526232
H	1.103765	-1.857527	-0.715719
H	2.387454	-0.899230	-1.468219
H	2.617737	-1.561604	0.156238
H	-1.481508	-0.180132	-1.876615

TS

C	-0.981440	0.183629	-0.810590
O	-1.721546	-0.752519	1.078019
O	-1.408212	-0.869995	-0.283312
H	0.533076	-0.280097	0.975782
N	1.081645	-0.049219	0.148143
C	-1.215206	1.528183	-0.242746
H	-0.991862	1.536524	0.819196
H	-0.639781	2.272975	-0.785860
H	-2.283416	1.741590	-0.344010
C	2.031387	1.012611	0.424786
H	2.515365	1.316416	-0.504678

H	1.511064	1.875175	0.839373
H	2.813538	0.707513	1.129958
C	1.690535	-1.255524	-0.384914
H	2.443004	-1.680161	0.288624
H	0.915436	-2.002311	-0.551954
H	2.175307	-1.027303	-1.335573
H	-0.676840	0.050933	-1.844735

Int_2

C	-0.307675	0.286586	-0.587817
O	-1.818196	-0.698578	0.843198
O	-1.344165	-0.676235	-0.496524
H	-1.000814	-0.892154	1.330848
N	0.798912	-0.169186	0.239449
C	-0.802680	1.676396	-0.239641
H	-0.960276	1.778624	0.831972
H	-0.099288	2.436583	-0.574297
H	-1.752279	1.834030	-0.746287
C	1.399164	-1.374260	-0.319562
H	0.627122	-2.116909	-0.505855
H	1.922421	-1.166886	-1.264838
H	2.117230	-1.784529	0.388784
H	-0.050270	0.236193	-1.657430
C	1.815383	0.839307	0.489359
H	2.272339	1.211716	-0.440175
H	1.401486	1.681351	1.037428
H	2.603686	0.396610	1.096279

$(CH_3)_2COO+NH_3$ Reaction

Int_1

C	0.774030	0.038941	-0.011803
O	-0.813506	1.569954	-0.416749
O	0.081949	0.620874	-0.873885
H	-1.973080	-0.196489	0.015028
N	-1.929536	-1.200419	0.193527
H	-2.671683	-1.424868	0.844499
H	-2.164360	-1.659222	-0.678387
C	0.691406	0.436343	1.403069
H	-0.319837	0.221555	1.751391
H	1.427647	-0.092497	2.000766
H	0.809721	1.519294	1.465803
C	1.647518	-1.055103	-0.497518
H	1.608079	-1.132908	-1.579949

H	2.672465	-0.894059	-0.162955
H	1.292530	-1.985585	-0.048305

TS

C	-0.391276	-0.244337	-0.022086
O	1.826749	-0.483619	-0.267901
O	0.526148	-0.587239	-0.844958
H	0.103671	2.230162	0.960538
N	0.220690	1.660813	0.133317
H	1.182275	1.278739	0.070183
H	0.005080	2.198174	-0.696286
C	-1.756459	-0.181379	-0.632445
H	-2.207024	-1.173711	-0.575280
H	-2.385517	0.511488	-0.078630
H	-1.693394	0.117126	-1.675710
C	-0.283118	-0.590999	1.429891
H	-1.058416	-0.083211	1.999149
H	-0.437233	-1.670220	1.506810
H	0.707660	-0.367084	1.806726

Int_2

C	0.364357	0.019576	0.025090
O	-1.938818	-0.118212	-0.204798
O	-0.703695	-0.660235	-0.638013
H	0.538309	0.598615	1.997718
N	0.183247	-0.175205	1.455143
H	-1.889730	-0.287816	0.750320
H	0.613182	-1.031710	1.778432
C	0.347156	1.504025	-0.298420
H	1.238712	1.985335	0.104256
H	0.331916	1.638686	-1.377954
H	-0.538101	1.974779	0.122955
C	1.598490	-0.672484	-0.530530
H	2.492799	-0.239684	-0.084402
H	1.563579	-1.737303	-0.299988
H	1.646692	-0.553593	-1.611687

$(CH_3)_2COO+CH_3NH_2$ Reaction

Int_1

C	1.198910	-0.207892	0.082227
O	0.430276	1.883964	-0.162151
O	1.041522	0.761338	-0.690011
H	-1.311522	0.652199	-0.508910

N	-1.694171	-0.291360	-0.550849
H	-1.882345	-0.482680	-1.526602
C	0.845080	-0.091882	1.506876
H	-0.230339	0.077188	1.575863
H	1.132386	-0.984457	2.054502
H	1.317774	0.806249	1.907968
C	1.751665	-1.445193	-0.517192
H	1.993000	-1.294234	-1.565103
H	2.635122	-1.766147	0.035419
H	0.994808	-2.226625	-0.420706
C	-2.930184	-0.370009	0.223803
H	-3.330552	-1.382203	0.177442
H	-2.712826	-0.154073	1.270308
H	-3.713527	0.321745	-0.101215

TS

C	-0.669960	0.406970	0.069139
O	-1.086769	-1.797855	-0.083423
O	-1.307512	-0.483720	-0.576434
H	0.817431	-1.189576	-0.539366
N	1.202076	-0.240426	-0.609785
H	1.250628	0.014260	-1.588195
C	-0.374465	0.245410	1.521937
H	-0.029264	-0.759786	1.734561
H	0.337486	0.999480	1.850795
H	-1.318487	0.392894	2.053278
C	-0.799257	1.787011	-0.490601
H	-0.995757	1.747459	-1.558915
H	-1.630689	2.291716	0.004938
H	0.107572	2.355403	-0.294192
C	2.475348	-0.077807	0.077413
H	2.773002	0.970525	0.065440
H	2.358027	-0.385117	1.114990
H	3.279770	-0.671168	-0.363313

Int_2

C	-0.086066	0.382270	0.015630
O	-1.854375	-1.114858	-0.051215
O	-1.408460	0.165001	-0.470893
H	-1.154722	-1.682097	-0.416340
N	0.745906	-0.645510	-0.605022
C	0.233674	1.788152	-0.470889
H	0.085310	1.850261	-1.548921
H	-0.413646	2.518188	0.012234

H	1.270302	2.032021	-0.239165
C	2.076954	-0.838337	-0.045916
H	2.630433	-1.519781	-0.688681
H	2.656388	0.088456	0.047334
H	2.006245	-1.296456	0.938583
C	-0.040417	0.289822	1.532028
H	-0.833016	0.915766	1.937095
H	-0.199651	-0.732680	1.866230
H	0.915532	0.647531	1.912726
H	0.813286	-0.435225	-1.594200

$(CH_3)_2COO+(CH_3)_2NH$ Reaction

Int_1

C	-1.371412	0.234383	0.193119
O	-0.975987	-1.468828	-1.210400
O	-1.193303	-0.120161	-0.991949
H	1.012954	-0.819356	-0.440531
N	1.452948	-0.066051	0.084098
C	-1.480955	-0.770687	1.264400
H	-0.558819	-1.349992	1.289735
H	-1.675450	-0.299242	2.223013
H	-2.270281	-1.474358	0.991029
C	-1.472362	1.693212	0.432513
H	-1.465410	2.241873	-0.504935
H	-2.372791	1.922951	1.002173
H	-0.608604	1.984522	1.034962
C	2.568545	-0.582763	0.856346
H	2.960704	0.204418	1.503008
H	2.233744	-1.402968	1.490777
H	3.396986	-0.945243	0.232468
C	1.862066	0.978392	-0.838651
H	1.014840	1.271953	-1.458172
H	2.199547	1.851738	-0.276044
H	2.680967	0.672743	-1.503741

TS

C	0.920896	0.407407	0.150424
O	1.346875	-1.693546	-0.527359
O	1.294272	-0.743884	0.517885
H	-0.716127	-1.057519	-0.637179
N	-1.144899	-0.255467	-0.171256
C	1.121106	0.875130	-1.247941
H	0.801426	0.123673	-1.960806

H	0.617399	1.826349	-1.404617
H	2.197682	1.011276	-1.384352
C	-2.094745	0.437922	-1.018563
H	-2.400873	1.367871	-0.534557
H	-1.630325	0.681936	-1.972731
H	-2.997034	-0.152969	-1.213651
C	-1.682323	-0.661206	1.114003
H	-2.536544	-1.338968	1.015119
H	-0.900575	-1.168232	1.678143
H	-2.009746	0.221388	1.667578
C	0.773101	1.405203	1.249439
H	1.663795	2.035768	1.280495
H	-0.085779	2.043989	1.049311
H	0.653609	0.906413	2.207662

Int_2

C	0.334420	0.384493	0.214658
O	1.734837	-1.199313	-0.735749
O	1.345939	-0.583452	0.483092
H	0.871697	-1.481782	-1.084394
N	-0.803289	-0.352468	-0.350711
C	0.070416	1.001319	1.583820
H	-0.078647	0.230891	2.337143
H	0.919183	1.614050	1.880896
H	-0.817223	1.633268	1.541508
C	-1.806093	0.466890	-1.008954
H	-2.583284	-0.187281	-1.402053
H	-2.285848	1.181276	-0.323593
H	-1.378507	1.015989	-1.843245
C	-1.430183	-1.261128	0.601386
H	-2.054794	-0.736411	1.336772
H	-2.065030	-1.958910	0.056245
H	-0.664884	-1.826292	1.128995
C	0.853140	1.434891	-0.757187
H	1.842883	1.738742	-0.422581
H	0.935955	1.036950	-1.765668
H	0.205108	2.310111	-0.766134