

Secondary organic material formed by methylglyoxal in aqueous aerosol mimics. Part II: Product identification using Aerosol-CIMS

N. Sareen, E. L. Shapiro, A. N. Schwier, and V. F. McNeill*

{Department of Chemical Engineering, Columbia University, New York, New York, USA}

Correspondence to: V. F. McNeill (vfm2103@columbia.edu)

SUPPLEMENTARY MATERIAL

Table S1. B3LYP/ERMLER2 calculated total Gibbs free energies. Labels refer to Table 2 in the text. “cluster” denotes the cluster of the species with I⁻.

Species	G _{tot} (Hartrees)
I ⁻	-111.5214881
I ⁻ H ₂ O	-187.9354270
H ₂ O	-76.3838860
HI	-112.0452540
(a)	-267.0245790
(a) cluster	-378.5773160
(b)	-343.4048790
(b) cluster	-454.9726860
(c)	-457.6584990
(c) cluster	-569.2161910
(d)	-534.0437570
(d) cluster	-645.6083500
(e)	-534.0793570
(e) cluster	-645.6313070
(f)	-534.0829650
(f) cluster	-645.6532510
(g)	-494.3230970
(g) cluster	-605.8775960
(h)	-610.4375880
(h) cluster	-722.0139790
(i)	-610.4236450
(i) cluster	-722.0002230
(j)	-1158.7736880
(j) ionized	-1158.2948550

Table S2. Cartesian coordinates for B3LYP/ERMLER2 optimized geometries. Labels refer to Table 2 in the text. "cluster" denotes the cluster of the species with I⁻.

H₂O

O1	0.1066000000	-1.6372000000	0.0000000000
H2	1.0481000000	-1.3803000000	0.0000000000
H3	-0.4328000000	-0.8238000000	0.0000000000

I⁻H₂O

I1	-0.3414000000	1.9392000000	0.0000000000
O2	0.1066000000	-1.6372000000	0.0000000000
H3	1.0494000000	-1.3800000000	0.0000000000
H4	-0.3685000000	-0.7660000000	0.0000000000

HI

I1	-0.7431000000	0.1665000000	0.0000000000
H2	0.8869000000	-0.1988000000	0.0000000000

(a)

C1	-0.7453000000	0.0567000000	0.0011000000
C2	0.7906000000	-0.0118000000	0.0006000000
O3	-1.2534000000	1.0888000000	-0.3731000000
C4	-1.4938000000	-1.1584000000	0.4668000000
H5	1.2635000000	0.9249000000	-0.3479000000
O6	1.4136000000	-0.9820000000	0.3416000000
H7	-1.1964000000	-2.0270000000	-0.1225000000
H8	-2.5635000000	-0.9899000000	0.3860000000
H9	-1.2226000000	-1.3828000000	1.5001000000

(a) cluster

C1	-0.7453000000	0.0567000000	0.0011000000
C2	0.7649000000	-0.0107000000	0.0006000000
O3	-1.3057000000	1.0813000000	-0.4427000000
C4	-1.4930000000	-1.2001000000	0.3737000000
H5	1.2583000000	0.9698000000	-0.0198000000
O6	1.3790000000	-1.0831000000	-0.1895000000
I7	0.4564000000	0.7586000000	3.1088000000
H8	-1.0391000000	-2.0639000000	-0.1244000000
H9	-2.5459000000	-1.1019000000	0.0984000000
H10	-1.4030000000	-1.3546000000	1.4539000000

(b)

C1	-0.7165000000	0.2340000000	0.0711000000
C2	0.5642000000	1.0706000000	0.1203000000
O3	-1.3225000000	0.1211000000	-1.0030000000
C4	-1.1894000000	-0.3990000000	1.3547000000
H5	-1.4353000000	0.3672000000	2.1024000000
O6	0.3625000000	2.3199000000	0.8078000000

O7	1.5517000000	0.2606000000	0.7748000000
H8	0.8461000000	1.3545000000	-0.8952000000
H9	0.1438000000	2.1509000000	1.7493000000
H10	2.4340000000	0.6803000000	0.7162000000
H11	-0.3957000000	-1.0245000000	1.7758000000
H12	-2.0821000000	-0.9953000000	1.1596000000

(b) cluster

C1	-0.7165000000	0.2340000000	0.0711000000
C2	0.5715000000	1.0754000000	0.1206000000
O3	-1.2775000000	0.0512000000	-1.0256000000
C4	-1.2492000000	-0.3446000000	1.3550000000
H5	-1.3116000000	0.4209000000	2.1411000000
O6	0.2437000000	2.4678000000	0.2425000000
O7	1.4814000000	0.5959000000	1.1222000000
H8	1.0701000000	0.9655000000	-0.8437000000
H9	-0.0075000000	2.6828000000	1.1837000000
H10	1.2506000000	0.9883000000	2.0048000000
H11	-0.5543000000	-1.1090000000	1.7242000000
H12	-2.2297000000	-0.7921000000	1.1765000000
I13	-0.0457000000	2.6698000000	3.8294000000

(c)

C1	-0.6294000000	0.4713000000	-0.0359000000
C2	0.5864000000	-0.3587000000	0.1030000000
O3	-0.6806000000	1.5497000000	-0.5927000000
C4	-1.9291000000	-0.0783000000	0.5733000000
H5	-2.7905000000	0.5971000000	0.4241000000
H6	1.8308000000	0.9766000000	-0.9231000000
C7	1.7593000000	0.0307000000	-0.3994000000
H8	0.5006000000	-1.3001000000	0.6279000000
C9	2.9938000000	-0.8096000000	-0.2597000000
O10	-2.0056000000	-1.1297000000	1.1509000000
C11	4.2562000000	-0.2446000000	-0.8657000000
O12	2.9625000000	-1.8799000000	0.3097000000
H13	5.0884000000	-0.9209000000	-0.6963000000
H14	4.4768000000	0.7334000000	-0.4313000000
H15	4.1178000000	-0.0884000000	-1.9383000000

(c) cluster

C1	-0.6294000000	0.4713000000	-0.0359000000
C2	0.5718000000	-0.3487000000	0.1013000000
O3	-0.6215000000	1.6877000000	0.2712000000
C4	-1.9028000000	-0.1461000000	-0.6015000000
H5	-1.7947000000	-1.0049000000	-1.2877000000
H6	-0.2286000000	-2.2877000000	-0.3605000000
C7	0.6294000000	-1.6916000000	-0.0590000000
H8	1.4751000000	0.1883000000	0.3820000000

C9	1.9106000000	-2.4266000000	0.1316000000
O10	-3.0150000000	0.3277000000	-0.3291000000
C11	1.8733000000	-3.9153000000	-0.0848000000
O12	2.9618000000	-1.8347000000	0.4653000000
H13	2.8817000000	-4.3288000000	-0.0182000000
H14	1.4103000000	-4.1474000000	-1.0536000000
H15	1.2349000000	-4.3886000000	0.6748000000
I16	-1.1192000000	-3.6353000000	-2.7734000000

(d)

C1	-0.6294000000	0.4713000000	-0.0359000000
C2	0.6051000000	-0.3715000000	0.1051000000
O3	-0.6538000000	1.5776000000	-0.6125000000
C4	-1.9330000000	-0.0270000000	0.5633000000
H5	-2.7806000000	0.6632000000	0.4304000000
O6	2.1810000000	1.4494000000	-0.4612000000
C7	1.7497000000	0.1088000000	-0.7974000000
H8	1.4073000000	0.0802000000	-1.8469000000
C9	2.9601000000	-0.8236000000	-0.7096000000
O10	-2.0303000000	-1.1097000000	1.1464000000
C11	4.3276000000	-0.2096000000	-0.8171000000
O12	2.7744000000	-2.0455000000	-0.5810000000
H13	5.0846000000	-0.9950000000	-0.7911000000
H14	4.4809000000	0.5006000000	0.0025000000
H15	4.4178000000	0.3732000000	-1.7413000000
H16	0.3785000000	-1.4258000000	-0.0891000000
H17	0.9282000000	-0.3342000000	1.1569000000
H18	1.4401000000	2.0634000000	-0.6512000000

(d) cluster

C1	-0.6294000000	0.4713000000	-0.0359000000
C2	0.6081000000	-0.3735000000	0.1055000000
O3	-1.1364000000	0.7540000000	-1.1357000000
C4	-1.2639000000	0.9912000000	1.2552000000
H5	-0.9494000000	0.4970000000	2.1864000000
O6	1.6488000000	1.2099000000	1.7188000000
C7	1.8351000000	0.5072000000	0.4751000000
H8	1.9371000000	1.2952000000	-0.2833000000
C9	3.1343000000	-0.3134000000	0.4134000000
O10	-2.1003000000	1.9028000000	1.2407000000
C11	4.0713000000	-0.2381000000	1.5858000000
O12	3.3774000000	-0.9954000000	-0.6001000000
H13	5.0129000000	-0.7316000000	1.3362000000
H14	3.6047000000	-0.7386000000	2.4491000000
H15	4.2374000000	0.8016000000	1.8863000000
H16	0.8130000000	-0.8834000000	-0.8386000000
H17	0.4765000000	-1.1124000000	0.9099000000
H18	1.4923000000	0.5614000000	2.4669000000

I19	0.9724000000	-1.4476000000	4.0041000000
-----	--------------	---------------	--------------

(e)

C1	-0.4148000000	0.6649000000	-0.0252000000
C2	0.4457000000	-0.5213000000	0.0478000000
O3	-0.0136000000	1.7597000000	0.4709000000
C4	-1.7522000000	0.5460000000	-0.6902000000
O5	2.2153000000	0.6566000000	1.2054000000
C6	1.6910000000	-0.4800000000	0.6425000000
O7	-0.0788000000	-1.6580000000	-0.5147000000
C8	2.5509000000	-1.6666000000	0.7141000000
H9	0.5818000000	-2.4039000000	-0.4117000000
H10	-2.2639000000	1.5083000000	-0.6525000000
H11	-2.3567000000	-0.2246000000	-0.1984000000
H12	-1.6331000000	0.2220000000	-1.7306000000
C13	3.8911000000	-1.5503000000	1.3742000000
O14	2.1459000000	-2.7607000000	0.2196000000
H15	4.4000000000	-2.5141000000	1.3361000000
H16	3.7772000000	-1.2243000000	2.4145000000
H17	4.4963000000	-0.7826000000	0.8787000000
H18	1.5531000000	1.4010000000	1.1049000000

(e) cluster

C1	-0.4148000000	0.6649000000	-0.0252000000
C2	0.4438000000	-0.5187000000	0.0476000000
O3	-0.0741000000	1.7640000000	0.5345000000
C4	-1.7208000000	0.5493000000	-0.7582000000
O5	2.0791000000	0.6568000000	1.3326000000
C6	1.6341000000	-0.4880000000	0.7391000000
O7	0.0603000000	-1.6381000000	-0.6767000000
C8	2.5651000000	-1.6485000000	0.9120000000
H9	-0.7348000000	-2.1237000000	-0.2715000000
H10	-2.2220000000	1.5181000000	-0.7655000000
H11	-2.3566000000	-0.2050000000	-0.2733000000
H12	-1.5581000000	0.1901000000	-1.7792000000
C13	2.0813000000	-3.0517000000	0.6483000000
O14	3.7293000000	-1.4385000000	1.3172000000
H15	2.8615000000	-3.7450000000	0.9762000000
H16	1.8632000000	-3.1900000000	-0.4143000000
H17	1.1392000000	-3.2585000000	1.1723000000
H18	1.3790000000	1.3657000000	1.1725000000
I19	-2.6061000000	-3.1588000000	0.9142000000

(f)

C1	-0.7354000000	0.1968000000	0.0092000000
C2	0.7274000000	-0.1653000000	-0.0344000000
H3	-0.8949000000	1.0911000000	-0.5946000000
H4	-1.0607000000	0.3741000000	1.0401000000

H5	-1.3502000000	-0.6276000000	-0.3683000000
O6	1.5487000000	0.5078000000	-0.6859000000
C7	1.1566000000	-1.3755000000	0.7423000000
C8	2.8040000000	-3.0315000000	1.5803000000
O9	0.0820000000	-1.9400000000	1.3773000000
C10	2.4486000000	-1.8413000000	0.7993000000
O11	3.9268000000	-3.5313000000	1.7012000000
O12	1.7157000000	-3.6390000000	2.2492000000
H13	2.0237000000	-4.4234000000	2.7488000000
H14	0.3573000000	-2.7413000000	1.8938000000
C15	3.6116000000	-1.1908000000	0.0816000000
H16	4.5194000000	-1.7631000000	0.2787000000
H17	3.7601000000	-0.1578000000	0.4102000000
H18	3.4426000000	-1.1424000000	-0.9980000000

(f) cluster

C1	-0.7354000000	0.1968000000	0.0092000000
C2	0.7314000000	-0.1663000000	-0.0345000000
H3	-0.8949000000	1.0992000000	-0.5841000000
H4	-1.0607000000	0.3572000000	1.0429000000
H5	-1.3462000000	-0.6265000000	-0.3769000000
O6	1.5461000000	0.5280000000	-0.6813000000
C7	1.1432000000	-1.3767000000	0.7232000000
C8	2.6518000000	-3.0786000000	1.6048000000
O9	0.0744000000	-1.9724000000	1.3475000000
C10	2.4292000000	-1.8533000000	0.8003000000
O11	3.9111000000	-3.4974000000	1.6446000000
O12	1.6976000000	-3.6688000000	2.2028000000
H13	4.1255000000	-4.3537000000	2.1954000000
H14	0.4307000000	-2.7883000000	1.8427000000
C15	3.6135000000	-1.2117000000	0.1228000000
H16	4.5106000000	-1.7852000000	0.3538000000
H17	3.7504000000	-0.1745000000	0.4477000000
H18	3.4807000000	-1.1673000000	-0.9638000000
I19	5.1555000000	-6.1645000000	3.2471000000

(g)

C1	-0.4148000000	0.6649000000	-0.0252000000
C2	0.4444000000	-0.5194000000	0.0477000000
O3	-0.0417000000	1.7853000000	0.4491000000
C4	-1.7725000000	0.5609000000	-0.6747000000
H5	3.0516000000	-3.4076000000	0.4564000000
O6	2.1636000000	0.7642000000	1.1816000000
C7	1.7003000000	-0.4196000000	0.6488000000
N8	-0.0075000000	-1.7107000000	-0.4797000000
C9	2.6468000000	-1.5241000000	0.7810000000
H10	0.6296000000	-2.5060000000	-0.4036000000
H11	-0.9068000000	-1.7816000000	-0.9189000000

H12	-2.2559000000	1.5377000000	-0.6351000000
H13	-2.4042000000	-0.1716000000	-0.1554000000
H14	-1.6878000000	0.2463000000	-1.7230000000
C15	3.9606000000	-1.2149000000	1.4605000000
N16	2.3214000000	-2.7010000000	0.3159000000
H17	4.5874000000	-2.1108000000	1.5057000000
H18	3.7932000000	-0.8393000000	2.4752000000
H19	4.4975000000	-0.4252000000	0.9246000000
H20	1.4634000000	1.4716000000	1.0528000000

(g) cluster

C1	-0.4148000000	0.6649000000	-0.0252000000
C2	0.4630000000	-0.5451000000	0.0493000000
O3	0.1521000000	1.7810000000	-0.1627000000
C4	-1.9160000000	0.5824000000	0.0142000000
H5	2.6538000000	-3.7805000000	0.0344000000
O6	-1.3336000000	-2.0622000000	0.5834000000
C7	0.0050000000	-1.8364000000	0.2558000000
N8	1.7890000000	-0.2617000000	-0.1224000000
C9	0.8729000000	-3.0072000000	0.2295000000
H10	2.4321000000	-1.0551000000	-0.1303000000
H11	2.0301000000	0.7022000000	-0.2942000000
H12	-2.3146000000	1.5942000000	-0.0943000000
H13	-2.2617000000	0.1231000000	0.9442000000
H14	-2.2984000000	-0.0627000000	-0.7864000000
C15	0.1888000000	-4.3466000000	0.3972000000
N16	2.1692000000	-2.8752000000	0.0531000000
H17	0.9258000000	-5.1575000000	0.3889000000
H18	-0.5397000000	-4.5106000000	-0.4085000000
H19	-0.3762000000	-4.3750000000	1.3349000000
H20	-1.8756000000	-2.4545000000	-0.1767000000
I21	-3.1232000000	-3.2939000000	-2.1400000000

(h)

C1	-0.4529000000	0.5947000000	-0.0104000000
C2	0.4627000000	-0.6327000000	0.0002000000
H3	-0.2235000000	1.3153000000	-0.8118000000
O4	-1.3926000000	0.7626000000	0.7654000000
O5	2.9887000000	-2.0723000000	-0.3858000000
C6	-0.2312000000	-1.8218000000	0.6687000000
C7	1.8206000000	-0.2583000000	0.7232000000
O8	0.7021000000	-0.8611000000	-1.4165000000
C9	2.7070000000	-1.4927000000	0.8326000000
O10	1.4975000000	0.1742000000	2.0618000000
C11	2.5860000000	0.8704000000	0.0060000000
O12	3.1488000000	-1.9436000000	1.8918000000
H13	3.5804000000	-2.8499000000	-0.2798000000
H14	3.5657000000	1.0117000000	0.4729000000

H15	2.0256000000	1.8011000000	0.1213000000
H16	2.7112000000	0.6503000000	-1.0552000000
H17	1.9601000000	-0.3885000000	2.7210000000
H18	1.3843000000	-1.5576000000	-1.5262000000
H19	0.3934000000	-2.7216000000	0.6296000000
H20	-1.1682000000	-2.0347000000	0.1488000000
H21	-0.4602000000	-1.5853000000	1.7098000000

(h) cluster

C1	-0.4529000000	0.5947000000	-0.0104000000
C2	0.4572000000	-0.6254000000	0.0001000000
O3	-1.3852000000	0.7912000000	0.7731000000
O4	2.9181000000	-2.1147000000	-0.5088000000
C5	-0.1990000000	-1.8017000000	0.7263000000
C6	1.8490000000	-0.2483000000	0.6400000000
O7	0.6449000000	-0.9073000000	-1.4179000000
C8	2.7762000000	-1.4727000000	0.5532000000
O9	1.6151000000	0.1159000000	2.0180000000
C10	2.5379000000	0.9290000000	-0.0781000000
O11	3.3913000000	-1.7076000000	1.7106000000
H12	-0.2331000000	1.3032000000	-0.8276000000
H13	4.0825000000	-2.5018000000	1.7903000000
H14	0.4316000000	-2.6938000000	0.6590000000
H15	-1.1635000000	-2.0248000000	0.2620000000
H16	-0.3611000000	-1.5504000000	1.7763000000
H17	1.4162000000	-1.5244000000	-1.4910000000
H18	2.2550000000	-0.3890000000	2.5703000000
H19	3.5509000000	1.0546000000	0.3179000000
H20	1.9814000000	1.8491000000	0.1205000000
H21	2.5890000000	0.7552000000	-1.1552000000
I22	5.6107000000	-4.0521000000	2.4217000000

(i)

O1	-0.5132000000	-0.3931000000	0.0000000000
C2	0.6410000000	0.4910000000	0.0000000000
O3	1.4735000000	0.2531000000	1.1458000000
C4	2.0923000000	-1.0804000000	1.1770000000
O5	1.1607000000	-2.0875000000	1.5461000000
H6	-1.0953000000	-0.1907000000	0.7635000000
C7	0.2229000000	1.9649000000	0.0226000000
H8	1.1563000000	0.2647000000	-0.9364000000
C9	2.7077000000	-0.9791000000	3.6795000000
C10	3.1751000000	-1.0111000000	2.2539000000
H11	2.5486000000	-1.2703000000	0.1978000000
H12	0.6413000000	2.5223000000	2.0447000000
H13	-1.0179000000	1.9897000000	1.7959000000
H14	-0.5186000000	3.5898000000	1.1895000000
H15	3.5651000000	-0.8998000000	4.3492000000

H16	2.1349000000	-1.8859000000	3.9008000000
O17	0.2284000000	2.6016000000	-1.0385000000
H18	2.0321000000	-0.1293000000	3.8309000000
C19	-0.1967000000	2.5584000000	1.3410000000
O20	4.3647000000	-0.9745000000	1.9132000000
H21	0.4458000000	-2.1316000000	0.8731000000

(i) cluster

O1	-0.5132000000	-0.3931000000	0.0000000000
C2	0.6127000000	0.4693000000	0.0000000000
O3	1.4612000000	0.3370000000	1.1703000000
C4	2.2209000000	-0.8877000000	1.3558000000
O5	1.4449000000	-2.0040000000	1.7519000000
H6	-0.9364000000	-0.4558000000	0.9037000000
I7	-1.6080000000	-0.8965000000	3.4049000000
C8	0.1778000000	1.9390000000	-0.0131000000
H9	1.1719000000	0.2499000000	-0.9150000000
C10	2.7266000000	-0.3386000000	3.8291000000
C11	3.2477000000	-0.5041000000	2.4267000000
H12	2.7437000000	-1.1628000000	0.4337000000
H13	0.4900000000	2.6496000000	1.9707000000
H14	-1.0508000000	1.8465000000	1.7637000000
H15	-0.8085000000	3.4921000000	1.0718000000
H16	3.4760000000	0.1599000000	4.4473000000
H17	2.5038000000	-1.3239000000	4.2559000000
O18	0.2422000000	2.5820000000	-1.0755000000
H19	1.7833000000	0.2178000000	3.8307000000
C20	-0.3436000000	2.5240000000	1.2703000000
O21	4.4444000000	-0.3629000000	2.1220000000
H22	0.6590000000	-1.7384000000	2.3084000000

(j)

C1	0.6935000000	0.2567000000	0.0580000000
C2	-0.7081000000	-0.2775000000	0.0000000000
O3	0.9673000000	1.4517000000	-0.1430000000
O4	2.6021000000	3.5983000000	1.3287000000
C5	1.8055000000	-0.7535000000	0.3556000000
H6	-0.7797000000	-1.0108000000	-0.8106000000
H7	-1.4101000000	0.5412000000	-0.1635000000
H8	-0.9601000000	-0.8075000000	0.9267000000
C9	3.1989000000	-0.1482000000	0.1180000000
O10	1.5712000000	-1.8731000000	-0.5311000000
H11	1.7323000000	-1.0597000000	1.4113000000
C12	4.3611000000	-1.1496000000	0.2275000000
O13	3.4480000000	0.8625000000	1.1599000000
H14	3.2347000000	0.3249000000	-0.8743000000
C15	5.7462000000	-0.5888000000	0.3560000000
S16	3.5889000000	2.5792000000	0.5650000000

O17	4.1336000000	-2.3740000000	0.1923000000
H18	6.4759000000	-1.3967000000	0.2883000000
H19	5.8555000000	-0.0641000000	1.3114000000
H20	5.9353000000	0.1556000000	-0.4274000000
H21	2.2715000000	-2.5441000000	-0.3567000000
O22	5.1983000000	2.8045000000	1.3437000000
O23	3.8231000000	2.5637000000	-1.0279000000
H24	5.1140000000	3.5995000000	1.9288000000

Ionized (j)

C1	0.6935000000	0.2567000000	0.0580000000
C2	-0.7231000000	-0.2832000000	-0.0006000000
O3	1.6677000000	-0.4931000000	0.2055000000
O4	-1.3096000000	5.3227000000	-2.6723000000
C5	0.8234000000	1.7725000000	0.0026000000
H6	-1.0037000000	-0.3941000000	-1.0538000000
H7	-1.4444000000	0.3898000000	0.4757000000
H8	-0.7556000000	-1.2656000000	0.4773000000
C9	0.1570000000	2.4570000000	-1.2194000000
O10	2.2079000000	2.1650000000	0.0681000000
H11	0.2754000000	2.1633000000	0.8781000000
C12	0.6306000000	1.9188000000	-2.5697000000
O13	0.4701000000	3.8617000000	-1.0888000000
H14	-0.9333000000	2.3160000000	-1.1549000000
C15	1.1519000000	2.9043000000	-3.5762000000
S16	-1.0970000000	4.9860000000	-1.0859000000
O17	0.5379000000	0.6982000000	-2.8055000000
H18	0.4312000000	3.7196000000	-3.7137000000
H19	1.3593000000	2.3928000000	-4.5185000000
H20	2.0660000000	3.3710000000	-3.1896000000
H21	2.2082000000	3.1386000000	-0.0770000000
O22	-0.5920000000	6.2102000000	-0.1439000000
O23	-2.2195000000	3.9754000000	-0.4419000000