

## Supplementary Information for “The Role of Electrostatic Induction in Secondary Isotope Effects on Acidity: Theory and Computational Confirmation”, by E. Amitai Halevi, New Journal of Chemistry, ....

### Cartesian Matrices of all structures computed (Standard Orientation)

(The hydrates are labeled by the Structure number)

#### Formate Ion

##### Formate ion (anhydrous):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	1	0	0.000000	0.000000	1.457755
2	6	0	0.000000	0.000000	0.308455
3	8	0	0.000000	1.141068	-0.206780
4	8	0	0.000000	-1.141068	-0.206780

##### Formate ion monohydrate (1)

1	1	0	-0.002187	2.260990	0.000000
2	6	0	0.000000	1.128460	0.000000
3	8	0	-1.139827	0.600502	0.000000
4	8	0	1.140890	0.603663	0.000000
5	1	0	-0.709044	-1.335090	0.000000
6	8	0	-0.001282	-1.998421	0.000000
7	1	0	0.712979	-1.342610	0.000000

##### Formate ion dihydrate-a (2)

1	1	0	-0.000183	0.609669	-0.000203
2	6	0	-0.000032	-0.516727	-0.000062
3	8	0	1.129414	-1.057704	0.098019
4	8	0	-1.129407	-1.057922	-0.097981
5	1	0	2.297484	0.207884	0.156221
6	1	0	-2.297282	0.208120	-0.156282
7	8	0	2.838996	1.022726	0.033779
8	8	0	-2.838924	1.022825	-0.033785
9	1	0	2.490011	1.317819	-0.807640
10	1	0	-2.490466	1.317469	0.808013

##### Formate ion dihydrate-b (3)

1	1	0	2.336714	-1.151540	-0.159666
2	6	0	1.432388	-0.495471	-0.023855
3	8	0	0.554594	-0.941996	0.760801
4	8	0	1.453863	0.578954	-0.672583
5	1	0	-0.762247	0.921522	0.985497
6	8	0	-0.848382	1.642477	0.351416
7	1	0	-0.031138	1.436793	-0.152971
8	1	0	-1.915470	0.037273	-0.459891
9	8	0	-2.039221	-0.918343	-0.442698
10	1	0	-1.189020	-1.159963	-0.045337

**Formate ion trihydrate-a (4)**

1	1	0	-0.002420	-1.266592	0.000209
2	6	0	-0.000451	-0.148555	-0.001563
3	8	0	-1.127442	0.401257	0.108291
4	8	0	1.128573	0.396780	-0.113140
5	1	0	-2.317470	-0.910174	0.180391
6	1	0	2.313381	-0.919264	-0.180230
7	8	0	-2.826727	-1.734573	0.034962
8	8	0	2.819264	-1.745269	-0.032067
9	1	0	-2.566033	-1.928225	-0.865891
10	1	0	2.560936	-1.932595	0.870812
11	1	0	-0.708905	2.414937	0.074319
12	1	0	0.719065	2.411354	-0.072813
13	8	0	0.006851	3.059540	0.002276

**Formate ion trihydrate-b (5)**

1	1	0	-3.095688	0.000561	0.005667
2	6	0	-1.974875	0.000205	0.003670
3	8	0	-1.425906	0.017549	1.136996
4	8	0	-1.430599	-0.017709	-1.132372
5	1	0	0.109519	-1.276588	0.734581
6	8	0	0.580254	-1.702161	0.003203
7	1	0	0.085971	-1.273810	-0.712344
8	1	0	0.103576	1.271864	-0.738673
9	8	0	0.581349	1.702921	-0.015155
10	1	0	0.096798	1.280333	0.709729
11	1	0	2.310609	0.735047	-0.009885
12	8	0	2.936080	-0.000972	0.005688
13	1	0	2.309044	-0.735663	0.002037

**Formate ion tetrahydrate-a (6)**

1	1	0	3.688806	-0.005911	0.002848
2	6	0	2.569954	-0.003676	0.001089
3	8	0	2.022736	0.150107	-1.123491
4	8	0	2.018810	-0.155104	1.124237
5	1	0	0.442938	-1.134394	-0.859525
6	8	0	0.004457	-1.642147	-0.161863
7	1	0	0.524204	-1.297985	0.582339
8	1	0	0.448981	1.135392	0.856320
9	8	0	0.011893	1.646891	0.160330
10	1	0	0.530479	1.302235	-0.584357
11	1	0	-1.806781	-1.562729	-0.034042
12	8	0	-2.770157	-1.452846	0.050424
13	1	0	-2.828842	-0.686702	0.626152
14	1	0	-1.798612	1.563363	0.033285
15	8	0	-2.762385	1.455301	-0.049839
16	1	0	-2.823732	0.691164	-0.627941

**Formate ion tetrahydrate-b (7)**

1	1	0	-1.757105	0.000066	0.000003
2	6	0	-0.642986	0.000023	0.000004
3	8	0	-0.097584	-1.133057	-0.047920
4	8	0	-0.097496	1.133061	0.047922
5	1	0	-1.462341	-2.318612	-0.078665
6	1	0	-1.462160	2.318708	0.078669
7	8	0	-2.306935	-2.775935	0.097512
8	8	0	-2.306725	2.776085	-0.097515
9	1	0	-2.452612	-2.507233	1.005110
10	1	0	-2.452430	2.507359	-1.005103
11	1	0	1.709709	-1.380510	-0.185735
12	8	0	2.677415	-1.413887	-0.298601
13	1	0	2.827719	-0.580050	-0.750548
14	1	0	1.709814	1.380383	0.185707
15	8	0	2.677522	1.413706	0.298576
16	1	0	2.827749	0.579975	0.750745

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**Formic Acid****Formic Acid (anhydrous)**

1	1	0	-0.387510	1.447337	0.000000
2	6	0	0.000000	0.420846	0.000000
3	8	0	-1.034452	-0.442361	0.000000
4	8	0	1.162518	0.111394	0.000000
5	1	0	-0.637018	-1.324681	0.000000

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**Formic Acid monhydrate (8)**

1	1	0	2.282243	0.134535	0.041253
2	6	0	1.197474	-0.027219	0.014457
3	8	0	0.555365	1.135314	0.001485
4	8	0	0.686537	-1.129100	-0.000127
5	1	0	-0.408337	0.929851	-0.022999
6	8	0	-1.899205	-0.005239	-0.088506
7	1	0	-2.453927	-0.110297	0.686870
8	1	0	-1.346393	-0.798576	-0.094691

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**Formic Acid dihydrate (9)**

1	1	0	-1.065089	1.284288	-0.000876
2	6	0	-0.174052	0.648823	-0.005771
3	8	0	-0.238559	-0.570837	-0.030560
4	8	0	0.938989	1.359550	0.018559
5	1	0	1.692663	0.721918	0.004550
6	8	0	2.584758	-0.767309	-0.071506
7	1	0	1.749614	-1.252396	-0.093091
8	1	0	3.053056	-1.128593	0.683593
9	1	0	-2.271557	-0.731216	-0.169247
10	8	0	-3.132560	-0.310012	-0.071484
11	1	0	-3.335397	-0.478067	0.849624

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**Formic Acid dihydrate (10)**

1	1	0	-2.704011	-0.695740	-0.003486
2	6	0	-1.639665	-0.427056	0.004331
3	8	0	-0.758984	-1.265765	0.067831
4	8	0	-1.492909	0.879785	-0.063859
5	1	0	-0.523935	1.120599	-0.056551
6	8	0	1.052794	1.569972	-0.054924
7	1	0	1.585582	0.750600	-0.076467
8	1	0	1.373967	2.040010	0.716474
9	1	0	1.103931	-1.221394	0.115690
10	8	0	2.028643	-0.935610	0.049086
11	1	0	2.366103	-1.418795	-0.706719

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**Formic Acid trihydrate (11)**

1	1	0	-1.642580	-1.345652	0.065025
2	6	0	-0.664516	-0.852651	0.070662
3	8	0	0.389426	-1.457030	0.116374
4	8	0	-0.816677	0.464195	0.019280
5	1	0	0.072373	0.924852	0.010427
6	8	0	1.484999	1.715785	-0.031657
7	1	0	2.190851	1.041962	-0.105496
8	1	0	1.732896	2.234168	0.735910
9	1	0	2.202356	-0.990379	0.071480
10	8	0	3.021870	-0.483658	-0.038119
11	1	0	3.434499	-0.872259	-0.811059
12	8	0	-3.729534	0.154772	-0.169035
13	1	0	-2.910875	0.634749	-0.322770
14	1	0	-3.893086	0.335955	0.757771

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**Formic Acid trihydrate (12)**

1	1	0	1.695789	-1.395711	-0.116320
2	6	0	0.721113	-0.899684	-0.061059
3	8	0	0.630966	0.320272	0.013583
4	8	0	-0.267116	-1.758108	-0.086221
5	1	0	-1.149755	-1.287439	-0.037492
6	8	0	-2.605995	-0.585149	0.025004
7	1	0	-2.472113	0.382353	-0.020937
8	1	0	-3.134513	-0.717329	0.813905
9	1	0	-0.796036	1.541902	0.064272
10	8	0	-1.680679	1.936132	0.024640
11	1	0	-1.649630	2.502454	-0.748127
12	8	0	3.530534	0.473089	-0.029633
13	1	0	2.609207	0.750945	-0.077872
14	1	0	3.708689	0.531041	0.909944

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**Formic Acid trihydrate (13)**

1	1	0	3.109864	0.355079	0.766667
2	6	0	2.091497	0.232043	0.375992
3	8	0	1.311138	1.168246	0.308772
4	8	0	1.874594	-1.011808	0.019375
5	1	0	0.938911	-1.116965	-0.333433
6	8	0	-0.543535	-1.345506	-0.892034
7	1	0	-1.212365	-1.335101	-0.183812
8	1	0	-0.818436	-0.580953	-1.410776
9	1	0	-0.356388	1.393392	-0.321794
10	8	0	-1.266113	1.401678	-0.667441
11	1	0	-1.405017	2.299934	-0.969881
12	1	0	-2.189076	-0.352393	1.872572
13	8	0	-2.422980	-0.511392	0.956917
14	1	0	-2.241303	0.335002	0.519782

**Formic Acid tetrahydrate (14)**

1	1	0	-1.626898	0.147998	0.019949
2	6	0	-0.539933	0.033643	-0.002588
3	8	0	0.218539	0.988312	-0.099309
4	8	0	-0.187619	-1.233445	0.086538
5	1	0	0.811063	-1.337141	0.059255
6	8	0	2.394376	-1.564979	0.040250
7	1	0	2.821550	-0.685196	0.072914
8	1	0	2.775594	-1.988461	-0.731026
9	1	0	2.094624	1.214855	-0.107037
10	8	0	3.043581	1.034195	-0.032186
11	1	0	3.324912	1.560310	0.718064
12	8	0	-2.151625	2.690482	0.101364
13	1	0	-1.222850	2.446337	0.029982
14	1	0	-2.427587	2.711842	-0.816038
15	1	0	-2.126912	-2.178327	-0.090652
16	8	0	-3.057149	-1.937254	-0.094292
17	1	0	-3.264720	-1.912567	0.841193

**Acetate Ion****Acetate ion (anhydrous):**

1	6	0	0.048356	-1.349651	0.000000
2	6	0	0.000000	0.220978	0.000000
3	8	0	1.112474	0.798929	0.000000
4	8	0	-1.161880	0.695623	0.000000
5	1	0	1.075410	-1.728403	0.000000
6	1	0	-0.485148	-1.727987	0.880472
7	1	0	-0.485148	-1.727987	-0.880472

**Acetate ion monohydrate (15)**

1	6	0	0.038359	2.127610	0.000000
2	6	0	0.000000	0.574666	0.000000
3	8	0	-1.142299	0.047744	0.000000
4	8	0	1.131871	0.022214	0.000000
5	1	0	-0.967600	2.555159	0.000000
6	1	0	0.589763	2.473428	0.880989
7	1	0	0.589763	2.473428	-0.880989
8	1	0	-0.740161	-1.890577	0.000000
9	8	0	-0.037635	-2.559375	0.000000
10	1	0	0.682586	-1.909756	0.000000

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**Acetate ion dihydrate-a (16)**

1	6	0	0.054856	-1.023097	0.314399
2	6	0	-0.005462	0.511743	0.105940
3	8	0	-1.143403	1.049120	0.154777
4	8	0	1.099138	1.094862	-0.056396
5	1	0	-0.924061	-1.481446	0.168984
6	1	0	0.803821	-1.467446	-0.344659
7	1	0	0.374742	-1.212440	1.346433
8	1	0	-2.548503	0.060835	0.068167
9	1	0	2.498626	0.126788	-0.276914
10	8	0	-3.280705	-0.551065	-0.184364
11	8	0	3.253521	-0.509969	-0.282910
12	1	0	-3.046370	-0.696290	-1.101975
13	1	0	3.116966	-0.925465	0.569072

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**Acetate ion dihydrate-b (17)**

1	6	0	-2.651310	-0.023502	-0.015598
2	6	0	-1.105892	0.013254	0.011715
3	8	0	-0.554743	-1.090001	0.264470
4	8	0	-0.574116	1.126449	-0.235325
5	1	0	-2.975452	-0.611768	-0.880914
6	1	0	-3.021464	-0.532471	0.879357
7	1	0	-3.071702	0.982410	-0.082296
8	1	0	1.160360	-1.369822	0.014796
9	8	0	2.122832	-1.446453	-0.164817
10	1	0	1.140893	1.370373	-0.019826
11	1	0	2.261222	-0.641904	-0.670610
12	8	0	2.107643	1.436191	0.147189
13	1	0	2.236422	0.655191	0.690660

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**Acetic Acid****Acetic acid (anhydrous):**

1	6	0	0.959736	-0.979743	0.000000
2	6	0	0.000000	0.194076	0.000000
3	8	0	0.328184	1.349718	0.000000
4	8	0	-1.321072	-0.146306	0.000000
5	1	0	1.982081	-0.607251	0.000000
6	1	0	0.796814	-1.600409	0.885958
7	1	0	0.796814	-1.600409	-0.885958
8	1	0	-1.391022	-1.105231	0.000000

**Acetic acid monohydrate (18)**

1	6	0	2.157442	-0.032456	0.018312
2	6	0	0.657485	0.094326	0.001691
3	8	0	0.060617	1.157735	-0.008975
4	8	0	0.056811	-1.100508	-0.007528
5	1	0	2.608391	0.956201	0.077885
6	1	0	2.463761	-0.644409	0.869195
7	1	0	2.484424	-0.540864	-0.891663
8	1	0	-0.912595	-0.933847	-0.029261
9	8	0	-2.450852	-0.055227	-0.080108
10	1	0	-1.893500	0.736559	-0.092365
11	1	0	-2.972648	0.039142	0.719077

**Acetic acid dihydrate-a (19)**

1	6	0	-1.025576	1.613743	0.003905
2	6	0	0.093262	0.609625	-0.000229
3	8	0	-0.073419	-0.605343	-0.020634
4	8	0	1.294357	1.179790	0.018694
5	1	0	1.962874	0.455149	0.001118
6	8	0	2.681675	-1.130649	-0.080748
7	1	0	1.780417	-1.480435	-0.102978
8	1	0	3.077572	-1.541840	0.690121
9	1	0	-1.982257	-1.171991	-0.159134
10	8	0	-2.943875	-1.182066	-0.082325
11	1	0	-3.067019	-1.295126	0.861283
12	1	0	-1.982328	1.096177	-0.006752
13	1	0	-0.930008	2.256059	-0.874338
14	1	0	-0.935271	2.247942	0.888726

**Acetic acid dihydrate-b (20)**

1	6	0	2.683509	-0.245458	0.002888
2	6	0	1.182499	-0.105915	-0.008407
3	8	0	0.424675	-1.062477	-0.077424
4	8	0	0.803093	1.161744	0.067847
5	1	0	2.956983	-1.295615	-0.079364
6	1	0	3.107517	0.323836	-0.827115
7	1	0	3.078047	0.177027	0.929744
8	1	0	-0.190349	1.226712	0.063783
9	8	0	-1.833632	1.419387	0.052777
10	1	0	-2.216781	0.520555	0.080637
11	1	0	-2.216162	1.811528	-0.734002
12	1	0	-1.397062	-1.320248	-0.117430
13	8	0	-2.360109	-1.217129	-0.043652
14	1	0	-2.590455	-1.747755	0.720485

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**Methylammonium ion****Methylammonium ion (anhydrous)**

1	7	0	0.000000	0.000000	0.710080
2	6	0	0.000000	0.000000	-0.794371
3	1	0	0.000000	0.955613	1.073744
4	1	0	0.000000	-1.032681	-1.141855
5	1	0	0.827585	-0.477806	1.073744
6	1	0	-0.894328	0.516341	-1.141855
7	1	0	-0.827585	-0.477806	1.073744
8	1	0	0.894328	0.516341	-1.141855

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**Methylammonium ion monohydrate (21)**

1	7	0	-0.957724	0.150626	0.000000
2	6	0	-0.845742	-1.343914	0.000000
3	1	0	0.000000	0.582801	0.000000
4	1	0	-1.843446	-1.778300	0.000000
5	1	0	-1.464475	0.485066	0.821917
6	1	0	-0.297792	-1.641764	-0.891477
7	1	0	-1.464475	0.485066	-0.821917
8	1	0	-0.297792	-1.641764	0.891477
9	8	0	1.611059	0.996250	0.000000
10	1	0	2.129014	1.274000	-0.760688
11	1	0	2.129014	1.274000	0.760688

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**Methylammonium ion dihydrate (22)**

1	7	0	-0.000592	0.398277	0.555005
2	6	0	0.001080	1.590485	-0.343308
3	1	0	0.002017	0.677221	1.536357
4	1	0	-0.005878	1.237013	-1.372225
5	1	0	0.850144	-0.175131	0.381121
6	1	0	-0.889586	2.184480	-0.148088
7	1	0	-0.854428	-0.171497	0.384013
8	1	0	0.899665	2.175181	-0.156604
9	8	0	2.368157	-0.848042	-0.107014
10	1	0	2.511019	-1.557093	-0.739104
11	1	0	3.199826	-0.783901	0.369699
12	8	0	-2.368224	-0.849010	-0.108312
13	1	0	-3.212254	-0.743979	0.338473
14	1	0	-2.502327	-1.596733	-0.696220

**Methylammonium ion trihydrate (23)**

1	7	0	0.000000	0.000000	0.117636
2	6	0	0.000000	0.000000	1.605809
3	1	0	0.038743	0.972816	-0.231403
4	1	0	-0.111829	-1.023590	1.958646
5	1	0	0.823112	-0.519960	-0.231403
6	1	0	-0.830540	0.608642	1.958646
7	1	0	-0.861854	-0.452856	-0.231403
8	1	0	0.942369	0.414948	1.958646
9	8	0	2.368534	-1.367474	-0.484859
10	1	0	3.093235	-1.080576	-1.045577
11	1	0	2.571915	-2.285125	-0.288892
12	8	0	-2.368534	-1.367474	-0.484859
13	1	0	-2.482424	-2.138532	-1.045577
14	1	0	-3.264934	-1.084782	-0.288892
15	8	0	0.000000	2.734948	-0.484859
16	1	0	-0.610811	3.219108	-1.045577
17	1	0	0.693018	3.369906	-0.288892

**Methylamine****Methylamine (anhydrous)**

1	7	0	-0.052349	-0.761653	0.000000
2	6	0	-0.052349	0.704340	0.000000
3	1	0	0.942747	1.172070	0.000000
4	1	0	0.461895	-1.094394	0.808436
5	1	0	0.461895	-1.094394	-0.808436
6	1	0	-0.592997	1.061125	-0.879756
7	1	0	-0.592997	1.061125	0.879756

**Methylamine monohydrate (24)**

1	7	0	0.785564	0.745208	0.043541
2	6	0	1.199501	-0.662942	-0.026306
3	1	0	2.258148	-0.813913	-0.270037
4	1	0	1.008029	1.211694	-0.829930
5	1	0	1.310614	1.227096	0.765279
6	1	0	0.996955	-1.135693	0.937319
7	1	0	0.584852	-1.168670	-0.772083
8	1	0	-1.119758	0.413415	0.039173
9	8	0	-1.958736	-0.056930	-0.094388
10	1	0	-2.064909	-0.517295	0.738439

**Methylamine dihydrate (25)**

1	7	0	-1.076687	0.150396	0.707604
2	6	0	-1.757804	-0.198052	-0.546422
3	1	0	-2.470069	-1.026929	-0.452608
4	1	0	-0.530851	-0.652905	1.009123
5	1	0	-1.757736	0.355011	1.430367
6	1	0	-2.288789	0.676164	-0.929773
7	1	0	-0.997172	-0.480940	-1.275587
8	1	0	0.334646	1.194658	0.172481
9	8	0	1.195126	1.403039	-0.252310
10	1	0	1.622653	1.995209	0.367982
11	8	0	1.425974	-1.368159	0.103813
12	1	0	1.555244	-0.423449	-0.077058
13	1	0	1.646909	-1.780312	-0.731656

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