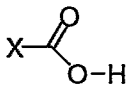
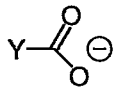
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1998, 120(13), 3159-3165, DOI:10.1021/ja972745j

Table S1. Calculated Total Energies for Substituted Formic Acids Using the 6-31+G(d,p) Basis Set.



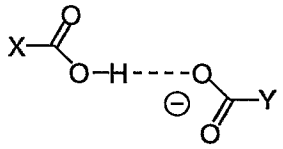
Substituent	HF	MP2	BLYP	B3LYP
H	-188.777514	-189.275334	-189.743363	-189.775493
CH_3	-227.829338	-228.469990	-229.045514	-229.105825
CH_2F	-326.673099	-327.478002	-328.274294	-328.332694
CHF_2	-425.530888	-426.502160	-427.517242	-427.573739
CF_3	-524.397764	-525.534866	-526.766503	-526.822475
F	-287.648626	-288.309390	-288.995228	-289.027188
OH	-263.669271	-264.341382	-264.982391	-265.022470
CN	-280.493996	-281.267389	-281.962267	-282.003002

Table S2. Calculated Total Energies for Substituted Formate Anions Using the 6-31+G(d,p)Basis Set.



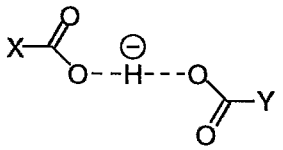
Substituent	HF	MP2	BLYP	B3LYP
H	-188.209691	-188.719219	-189.193377	-189.220751
CH_3	-227.254208	-227.906862	-228.488176	-228.543475
CH_2F	-326.115669	-326.933368	-327.735642	-327.788616
CHF_2	-424.985224	-425.969580	-426.990002	-427.041432
CF_3	-523.864283	-525.013270	-526.250023	-526.301225
F	-287.112049	-287.786268	-288.478729	-288.504343
OH	-263.110528	-263.795278	-264.441966	-264.476578
CN	-279.971834	-280.751993	-281.452858	-281.489891

Table S3. Calculated Total Energies for Substituted Formic Acid –Formate Anion Complexes Using the 6-31+G(d,p)Basis Set.



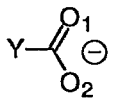
X	Y	HF	MP2	BLYP	B3LYP
H	H	-377.022622	-378.037421	-378.979663	-379.039621
CH_3	CH_3	-455.115868	-456.416930	-457.572598	-457.688965
CH_2F	CH_2F	-652.827597	-654.457914	-656.054639	-656.167251
CHF_2	CHF_2	-850.555369	-852.520556	-854.555045	-854.663461
CF_3	CF_3	-1048.303926	-1050.598324	-1053.065137	-1053.173055
F	F	-574.802671	-576.143814	-577.521632	-577.580435
OH	OH	-526.816722	-528.181496	-529.468256	-529.543814
CN	CN	-560.508656	-562.069795	-563.464343	-563.542932
H	F	-475.918533	-477.094643	-478.253856	-478.313412
H	CN	-468.775367	-470.059501	-471.226848	-471.296813
H	CH_3	-416.068334	DNC	DNC	DNC
CH_3	H	DNC	-417.227546	-418.276323	-418.364628
H	CH_2F	-514.926923	-516.248683	-517.517825	-517.604210
H	CHF_2	-613.793632	-615.281760	-616.769375	-616.853881
H	CF_3	-712.670160	-714.322425	-716.025884	-716.110293
H	OH	-451.921867	-453.110525	-454.224595	-454.292478

Table S4. Calculated Total Energies for Proton Transfer in Substituted Formic Acid –Formate Anion Complexes Using the 6-31+G(d,p) Basis Set.



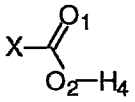
X	Y	HF	MP2	BLYP	B3LYP
H	H	-377.020321	-378.037418	-378.979645	-379.039660
CH_3	CH_3	-455.113443	-456.416931	-457.572607	-457.688940
CH_2F	CH_2F	-652.825622	-654.457915	-656.054636	-656.167248
CHF_2	CHF_2	-850.553454	-852.520556	-854.555026	-854.663450
CF_3	CF_3	-1048.302028	-1050.598324	-1053.065093	-1053.173136
F	F	-574.800693	-576.143812	-577.521571	-577.580453
OH	OH	-526.815036	-528.181496	-529.468261	-529.543796
CN	CN	-560.506639	-562.069795	-563.464681	-563.543174

Table S5. Optimized Geometry for Substituted Formate Anions (**2**) Using the 6-31+G(d,p) Basis Set. Bond Lengths in Angstroms (Å). Bond Angles in Degrees.



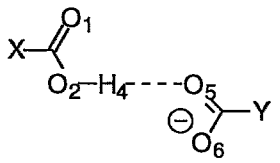
	Substituent (X)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
HF								
C-O_1	1.235	1.237	1.226	1.225	1.222	1.212	1.221	1.219
C-Y	1.119	1.547	1.542	1.551	1.568	1.411	1.395	1.557
O_1-C-O_2	130.4	128.7	130.6	131.5	132.9	135.2	131.5	134.0
O_1-C-Y	114.8	116.3	118.4	115.8	114.8	112.4	114.7	113.0
MP2								
C-O_1	1.268	1.271	1.258	1.259	1.257	1.235	1.248	1.257
C-Y	1.125	1.552	1.546	1.548	1.547	1.519	1.453	1.534
O_1-C-O_2	130.2	128.8	130.9	131.7	133.0	138.0	132.7	133.0
O_1-C-Y	114.9	116.4	118.8	115.9	115.0	111.0	113.9	113.5
BLYP								
C-O_1	1.272	1.276	1.263	1.263	1.260	1.238	1.253	1.262
C-Y	1.147	1.582	1.568	1.578	1.610	1.579	1.487	1.548
O_1-C-O_2	130.3	128.8	130.5	131.4	133.1	138.8	133.0	132.8
O_1-C-Y	114.8	116.3	119.3	116.5	114.7	110.6	114.0	113.6
B3LYP								
C-O_1	1.259	1.262	1.250	1.249	1.247	1.228	1.241	1.247
C-Y	1.136	1.564	1.554	1.564	1.588	1.507	1.448	1.543
O_1-C-O_2	130.3	128.7	130.6	131.4	132.9	137.4	132.4	133.1
O_1-C-Y	114.8	116.3	118.8	116.2	114.8	111.3	114.1	113.5

Table S6. Optimized Geometry for Substituted Formic Acids (**1**) Using the 6-31+G(d,p) Basis Set. Bond Lengths in Angstroms (Å). Bond Angles in Degrees.



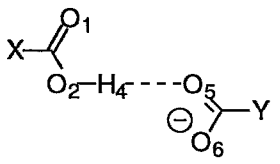
	Substituent (X)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
HF								
$C\text{-}O_1$	1.184	1.189	1.182	1.185	1.178	1.172	1.190	1.178
$C\text{-}O_2$	1.321	1.331	1.329	1.313	1.313	1.307	1.314	1.312
C-X	1.084	1.501	1.510	1.525	1.536	1.300	1.314	1.476
$O_2\text{-}H_4$	0.949	0.948	0.949	0.949	0.949	0.948	0.947	0.950
$O_1\text{-}C\text{-}O_2$	124.7	122.2	124.1	125.4	126.4	127.9	125.1	126.4
$O_1\text{-}C\text{-}X$	124.5	125.7	126.3	121.9	123.1	123.4	125.1	122.7
$H_4\text{-}O_2\text{-}C$	109.5	109.0	109.5	109.9	110.0	109.3	108.6	109.7
MP2								
$C\text{-}O_1$	1.216	1.221	1.214	1.219	1.213	1.201	1.219	1.216
$C\text{-}O_2$	1.353	1.365	1.362	1.344	1.344	1.338	1.346	1.347
C-X	1.092	1.501	1.514	1.525	1.539	1.344	1.346	1.467
$O_2\text{-}H_4$	0.971	0.973	0.972	0.973	0.973	0.971	0.970	0.975
$O_1\text{-}C\text{-}O_2$	125.1	122.5	124.6	126.0	126.9	129.0	125.9	126.3
$O_1\text{-}C\text{-}X$	125.2	126.3	126.6	122.5	123.7	123.8	125.9	123.5
$H_4\text{-}O_2\text{-}C$	106.9	106.4	106.9	107.3	107.4	106.8	106.1	107.1
BLYP								
$C\text{-}O_1$	1.220	1.226	1.226	1.223	1.216	1.206	1.225	1.221
$C\text{-}O_2$	1.367	1.380	1.361	1.357	1.358	1.352	1.361	1.362
C-X	1.106	1.517	1.530	1.547	1.564	1.362	1.361	1.471
$O_2\text{-}H_4$	0.986	0.984	0.984	0.984	0.984	0.981	0.980	0.985
$O_1\text{-}C\text{-}O_2$	125.2	122.2	124.5	125.6	126.5	129.1	125.9	126.0
$O_1\text{-}C\text{-}X$	125.4	126.3	121.5	122.3	123.8	123.7	125.9	123.5
$H_4\text{-}O_2\text{-}C$	107.1	106.3	106.5	107.2	107.4	106.9	106.0	107.1
B3LYP								
$C\text{-}O_1$	1.207	1.213	1.213	1.209	1.203	1.194	1.212	1.207
$C\text{-}O_2$	1.348	1.360	1.342	1.339	1.339	1.333	1.342	1.341
C-X	1.098	1.505	1.518	1.536	1.551	1.338	1.342	1.468
$O_2\text{-}H_4$	0.974	0.972	0.973	0.973	0.973	0.971	0.970	0.974
$O_1\text{-}C\text{-}O_2$	125.0	122.2	124.4	125.6	126.5	128.6	125.6	126.1
$O_1\text{-}C\text{-}X$	125.2	126.1	121.5	122.2	123.6	123.6	125.6	123.3
$H_4\text{-}O_2\text{-}C$	107.9	107.0	107.2	108.1	108.2	107.6	106.8	107.8

Table S7. Optimized Geometry for Substituted Formate Anion Hydrogen Bonded to Substituted Formic Acid Using 6-31+G(d,p) Basis Set. Bond Lengths in Å, Angles in Degrees.



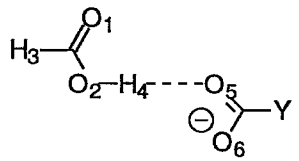
	Substituent (X_1=X_2)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
HF								
C-O_1	1.197	1.201	1.193	1.191	1.188	1.181	1.191	1.187
C-O_2	1.287	1.295	1.292	1.286	1.273	1.271	1.291	1.278
C-X	1.084	1.516	1.519	1.534	1.543	1.334	1.344	1.500
O_2-H_4	1.017	1.015	1.020	1.021	1.021	1.018	1.022	1.018
O_5-H_4	1.504	1.509	1.483	1.478	1.476	1.475	1.465	1.485
C-O_5	1.252	1.256	1.257	1.252	1.244	1.234	1.257	1.241
C-O_6	1.222	1.225	1.214	1.212	1.209	1.201	1.210	1.207
C-Y	1.107	1.532	1.530	1.542	1.554	1.369	1.368	1.526
O_1-C-O_2	128.9	126.8	128.5	129.4	130.4	132.0	129.0	130.5
O_1-C-X	120.6	121.7	122.9	120.5	119.6	119.0	120.3	118.8
H_4-O_2-C	117.9	117.8	118.0	117.5	116.8	115.7	117.4	116.0
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	125.3	125.2	124.6	123.7	123.8	123.0	123.1	123.2
O_6-C-O_5	129.4	127.6	129.3	130.1	131.3	133.1	129.8	131.9
O_6-C-Y	116.9	118.2	120.2	117.8	116.8	115.2	117.1	115.5
MP2								
C-O_1	1.240	1.246	1.235	1.235	1.234	1.216	1.228	1.235
C-O_2	1.303	1.305	1.305	1.301	1.292	1.282	1.303	1.294
C-X	1.106	1.526	1.529	1.536	1.550	1.408	1.397	1.498
O_2-H_4	1.169	1.205	1.195	1.205	1.205	1.167	1.202	1.198
O_5-H_4	1.258	1.216	1.220	1.211	1.208	1.243	1.205	1.218
C-O_5	1.296	1.304	1.303	1.301	1.292	1.275	1.303	1.292
C-O_6	1.245	1.246	1.237	1.236	1.234	1.220	1.228	1.236
C-Y	1.108	1.527	1.529	1.536	1.550	1.417	1.397	1.499
O_1-C-O_2	129.1	127.3	129.2	130.1	131.1	133.7	130.3	130.7
O_1-C-X	119.6	120.4	122.1	119.4	118.7	117.2	118.4	118.0
H_4-O_2-C	117.4	117.8	117.8	117.0	116.3	114.3	116.6	115.8
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	118.6	118.0	118.1	117.1	116.3	115.3	116.7	116.1
O_6-C-O_5	129.1	127.3	129.3	130.1	131.1	133.9	130.4	130.7
O_6-C-Y	118.8	120.3	121.9	119.4	118.7	116.4	118.4	117.8

Table S7 (cont'd). Optimized Geometry for Substituted Formate Anion Hydrogen Bonded to Substituted Formic AcidUsing 6-31+G(d,p) Basis Set. Bond Lengths in Å, Angles in Degrees.



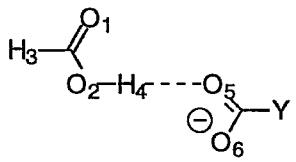
	Substituent (X_1=X_2)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
BLYP								
C-O_1	1.247	1.251	1.240	1.239	1.237	1.222	1.234	1.240
C-O_2	1.309	1.314	1.315	1.310	1.300	1.286	1.313	1.303
C-X	1.125	1.550	1.551	1.562	1.581	1.445	1.419	1.507
O_2-H_4	1.230	1.223	1.211	1.222	1.223	1.218	1.220	1.215
O_5-H_4	1.230	1.234	1.239	1.229	1.226	1.223	1.223	1.236
C-O_5	1.308	1.313	1.313	1.310	1.300	1.285	1.313	1.302
C-O_6	1.247	1.251	1.242	1.240	1.237	1.223	1.234	1.241
C-Y	1.125	1.551	1.552	1.562	1.581	1.446	1.419	1.508
O_1-C-O_2	129.3	127.3	129.1	130.0	131.0	134.4	130.7	130.6
O_1-C-X	119.3	120.2	122.1	119.9	118.5	116.6	118.2	117.8
H_4-O_2-C	119.4	119.5	119.4	118.6	117.9	116.4	118.2	117.1
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	119.5	119.4	119.8	118.7	117.7	116.6	118.2	117.5
O_6-C-O_5	129.4	127.3	129.2	129.9	131.0	137.4	130.7	130.7
O_6-C-Y	119.2	120.1	121.9	119.9	118.5	116.5	118.1	117.7
B3LYP								
C-O_1	1.231	1.237	1.227	1.226	1.224	1.211	1.222	1.225
C-O_2	1.296	1.298	1.299	1.294	1.284	1.273	1.297	1.286
C-X	1.115	1.535	1.537	1.548	1.565	1.407	1.384	1.503
O_2-H_4	1.172	1.208	1.197	1.207	1.208	1.204	1.205	1.200
O_5-H_4	1.262	1.218	1.223	1.213	1.211	1.208	1.208	1.221
C-O_5	1.289	1.297	1.296	1.293	1.284	1.272	1.297	1.284
C-O_6	1.236	1.238	1.226	1.226	1.224	1.212	1.222	1.226
C-Y	1.117	1.536	1.537	1.550	1.565	1.407	1.394	1.504
O_1-C-O_2	129.2	127.2	129.1	129.9	130.9	133.6	130.2	130.7
O_1-C-X	119.4	120.1	121.8	119.6	118.4	116.8	118.4	117.7
H_4-O_2-C	119.4	119.8	119.8	119.1	118.5	117.1	118.6	117.6
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	120.3	120.1	120.2	119.1	118.4	117.4	118.6	117.9
O_6-C-O_5	129.2	127.3	129.1	129.9	130.9	133.6	130.2	130.8
O_6-C-Y	118.7	120.0	121.7	119.5	118.4	116.7	118.3	117.5

Table S8. Optimized Geometry for Substituted Formate Anion Hydrogen Bonded to Formic Acid Using 6-31+G(d,p) Basis Set. Bond Lengths in Angstroms (Å). Bond Angles in Degrees.



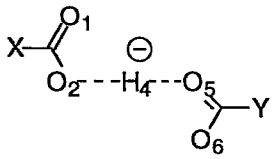
	Substituent (X_2)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
HF								
C-O_1	1.197	1.198	1.196	1.195	1.193	1.194	1.196	1.192
C-O_2	1.287	1.185	1.189	1.193	1.294	1.293	1.289	1.296
C-H_3	1.094	1.094	1.093	1.092	1.092	1.092	1.093	1.091
O_2-H_4	1.017	1.023	1.008	0.998	0.991	0.993	1.007	0.985
O_5-H_4	1.502	1.480	1.531	1.578	1.615	1.600	1.531	1.652
C-O_5	1.252	1.257	1.255	1.248	1.238	1.228	1.254	1.233
C-O_6	1.222	1.224	1.215	1.215	1.212	1.204	1.216	1.211
C-Y	1.107	1.532	1.531	1.544	1.557	1.378	1.372	1.535
O_1-C-O_2	128.9	129.0	128.7	128.5	128.5	128.6	128.7	128.3
O_1-C-H_3	120.6	120.4	120.8	121.1	121.3	121.2	120.8	121.5
H_4-O_2-C	117.9	118.1	117.3	116.8	116.7	116.9	117.2	116.3
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	125.3	124.7	126.3	126.2	125.1	124.0	125.3	124.5
O_6-C-O_5	129.4	127.5	129.5	130.5	131.7	133.5	130.2	132.5
O_6-C-Y	116.8	118.4	120.0	117.3	116.3	114.7	116.7	114.6
MP2								
C-O_1	1.240		1.234	1.232	1.229	1.230	1.234	1.228
C-O_2	1.303		1.311	1.316	1.319	1.318	1.311	1.321
C-H_3	1.106		1.103	1.101	1.101	1.101	1.103	1.100
O_2-H_4	1.169		1.089	1.062	1.046	1.047	1.087	1.038
O_5-H_4	1.258		1.379	1.439	1.485	1.476	1.376	1.512
C-O_5	1.296		1.294	1.287	1.275	1.259	1.291	1.274
C-O_6	1.245		1.243	1.245	1.245	1.227	1.235	1.247
C-Y	1.108		1.533	1.540	1.557	1.447	1.410	1.522
O_1-C-O_2	129.1		128.9	128.7	128.6	128.7	128.9	128.5
O_1-C-H_3	119.6		120.6	121.1	121.4	121.4	120.6	121.6
H_4-O_2-C	117.4		115.6	114.9	114.6	114.7	115.4	114.3
O_5-H_4-O_2	180.0		180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	118.6		120.6	120.3	119.3	117.6	119.4	118.9
O_6-C-O_5	129.1		129.6	130.6	131.8	135.1	130.9	131.6
O_6-C-Y	118.8		121.1	118.0	117.0	114.3	117.0	115.7

Table S8 (cont'd). Optimized Geometry for Substituted Formate Anion Hydrogen Bonded to Formic Acid Using 6-31+G(d,p) Basis Set. Bond Lengths in Å. Bond Angles in Degrees.



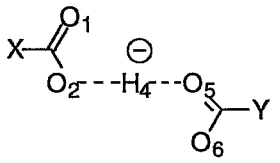
	Substituent (X_2)							
Parameter	H	CH_3	CH_2F	CHF_2	CF_3	F	OH	CN
BLYP								
C-O_1	1.247		1.241	1.237	1.235	1.235	1.241	1.234
C-O_2	1.308		1.319	1.324	1.328	1.327	1.318	1.330
C-H_3	1.125		1.121	1.119	1.118	1.118	1.121	1.117
O_2-H_4	1.230		1.130	1.095	1.075	1.078	1.131	1.064
O_5-H_4	1.230		1.353	1.419	1.467	1.452	1.346	1.500
C-O_5	1.309		1.304	1.297	1.283	1.267	1.302	1.283
C-O_6	1.247		1.246	1.248	1.248	1.231	1.239	1.251
C-Y	1.125		1.555	1.566	1.591	1.481	1.432	1.523
O_1-C-O_2	129.4		129.1	128.9	128.9	129.0	129.1	128.8
O_1-C-H_3	119.2		120.4	121.0	121.3	121.3	120.4	121.6
H_4-O_2-C	119.5		117.4	116.4	116.2	116.5	117.4	115.6
O_5-H_4-O_2	180.0		180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	119.4		121.7	122.0	120.9	119.2	120.4	121.1
O_6-C-O_5	129.3		129.5	130.5	131.8	135.5	131.1	131.5
O_6-C-Y	119.3		121.3	118.6	116.8	114.3	117.1	115.8
B3LYP								
C-O_1	1.231		1.226	1.224	1.221	1.222	1.227	1.220
C-O_2	1.296		1.303	1.308	1.311	1.310	1.302	1.313
C-H_3	1.115		1.112	1.110	1.109	1.109	1.112	1.108
O_2-H_4	1.172		1.104	1.077	1.057	1.060	1.108	1.047
O_5-H_4	1.262		1.356	1.412	1.460	1.449	1.346	1.494
C-O_5	1.289		1.287	1.280	1.268	1.254	1.287	1.266
C-O_6	1.236		1.234	1.235	1.234	1.220	1.227	1.236
C-Y	1.117		1.541	1.554	1.573	1.437	1.405	1.518
O_1-C-O_2	129.2		129.0	128.8	128.8	128.8	129.0	128.6
O_1-C-H_3	119.4		120.3	120.7	121.1	121.1	120.2	121.4
H_4-O_2-C	119.4		117.7	116.8	116.7	116.9	117.8	116.0
O_5-H_4-O_2	180.0		180.0	180.0	180.0	180.0	180.0	180.0
C-O_5-H_4	120.3		122.5	122.7	121.4	120.1	121.2	121.4
O_6-C-O_5	129.2		129.4	130.4	131.6	134.7	130.6	131.6
O_6-C-Y	118.7		120.9	118.3	116.8	114.6	117.4	115.7

Table S9. Optimized Geometry of Transition State (**4**) for Proton Transfer from Substituted Formic Acid to Substituted Formate Anion Using the 6-31+G(d,P) Basis Sete. Bond Lengths in Angstroms (Å). Bond Angles in Degrees.



	Substituent (X_1=X_2)							
Parameter	**H**	**CH_3**	**CH_2F**	**CHF_2**	**CF_3**	**F**	**OH**	**CN**
HF								
C-O_1	1.210	1.213	1.204	1.201	1.199	1.191	1.201	1.197
C-O_2	1.268	1.273	1.273	1.268	1.260	1.252	1.273	1.258
C-X	1.100	1.524	1.524	1.538	1.548	1.350	1.356	1.512
O_2-H_4	1.193	1.192	1.190	1.189	1.189	1.186	1.187	1.189
O_1-C-O_2	129.2	127.2	128.9	129.7	130.9	132.5	129.4	131.2
O_1-C-X	118.6	119.9	121.5	119.1	118.1	117.0	118.6	117.0
H_4-O_2-C	121.8	121.5	121.5	120.9	120.4	119.3	120.5	119.8
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
MP2								
C-O_1	1.243	1.246	1.236	1.235	1.234	1.218	1.228	1.243
C-O_2	1.299	1.304	1.305	1.301	1.292	1.279	1.303	1.310
C-X	1.107	1.527	1.530	1.536	1.550	1.413	1.397	1.511
O_2-H_4	1.212	1.210	1.208	1.208	1.207	1.203	1.204	1.225
O_1-C-O_2	129.1	127.3	129.3	130.1	131.1	133.8	130.3	130.8
O_1-C-X	119.2	120.3	122.0	119.4	118.7	116.8	118.4	117.3
H_4-O_2-C	118.0	117.9	117.9	117.1	116.3	114.8	116.6	117.5
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0

Table S9 (cont'd). Optimized Geometry of Transition State (**4**) for Proton Transfer from Substituted Formic Acid to Substituted Formate Anion Using the 6-31+G(d,P) Basis Set. Bond Lengths in Angstroms (Å). Bond Angles in Degrees.



	Substituent (X_1=X_2)							
Parameter	**H**	**CH_3**	**CH_2F**	**CHF_2**	**CF_3**	**F**	**OH**	**CN**
BLYP								
C-O_1	1.247	1.251	1.241	1.240	1.237	1.223	1.234	1.241
C-O_2	1.308	1.314	1.314	1.310	1.300	1.286	1.313	1.302
C-X	1.125	1.551	1.552	1.562	1.582	1.445	1.420	1.507
O_2-H_4	1.230	1.228	1.225	1.225	1.224	1.221	1.221	1.225
O_1-C-O_2	129.4	127.3	129.2	130.0	131.0	134.4	130.6	130.6
O_1-C-X	119.2	120.2	122.0	119.8	118.5	116.6	118.1	117.4
H_4-O_2-C	119.5	119.3	119.6	118.7	117.9	116.3	118.0	117.4
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
B3LYP								
C-O_1	1.234	1.238	1.228	1.226	1.224	1.211	1.220	1.226
C-O_2	1.292	1.298	1.297	1.293	1.284	1.273	1.297	1.285
C-X	1.116	1.536	1.537	1.549	1.565	1.407	1.393	1.503
O_2-H_4	1.214	1.213	1.210	1.210	1.209	1.206	1.207	1.210
O_1-C-O_2	129.2	127.2	129.1	129.9	131.0	133.6	130.2	130.7
O_1-C-X	119.0	120.1	121.7	119.5	118.4	116.8	118.4	117.3
H_4-O_2-C	120.1	119.8	120.0	119.2	118.5	117.1	118.7	118.0
O_5-H_4-O_2	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0