Table V. Geometries of formate anion, formic acid and its protonated form by different methods.

	$HCOO^-$							
Variable[a]	RHF/6d[b]	RHF/+6d[c]	MP2/6d	MP2/+6d[d]	DMol	DG/L	DN/L	DN/N
C1–O2	1.236	1.236	1.266	1.267	1.261	1.261	1.260	1.273
C1–O3	1.236	1.236	1.266	1.267	1.261	1.261	1.261	1.273
C1–H4	1.122	1.119	1.130	1.125	1.155	1.154	1.154	1.152
H4–C1–O3	114.639	114.821	114.674	114.979	114.770	114.842	114.934	114.954
H4–C1–O2	114.641	114.821	114.674	114.979	114.768	114.726	114.699	114.609
O3–C1–O2	130.720	130.358	130.651	130.042	130.461	130.432	130.367	130.437

	HCOOH									$HCOOH_2^+$					
Variable[a]	RHF/6d[b]	RHF/+6d[c]	MP2/6d	MP2/+6d[d]	DMol	DG/L	DN/L	DN/N	Exp.[e]	RHF/6d	MP2/6d	DMol	DG/L	DN/L	DN
C1–O2	1.323	1.322	1.352	1.352	1.343	1.342	1.342	1.365	1.340	1.247	1.270	1.268	1.267	1.267	1
C1–O3	1.184	1.184	1.215	1.214	1.211	1.212	1.211	1.219	1.202	1.256	1.280	1.277	1.277	1.276	1
C1–H4	1.086	1.086	1.094	1.094	1.111	1.114	1.113	1.109	1.091	1.080	1.088	1.104	1.107	1.106	1
O2–H5	0.950	0.950	0.972	0.973	0.998	0.987	0.988	0.985	0.969	0.960	0.982	1.009	0.997	0.997	0
O3–H6										0.956	0.977	1.003	0.991	0.991	0
H4–C1–O3	124.604	124.478	125.561	125.292	125.001	125.694	125.585	125.721	123.26	122.640	123.296	123.163	123.284	123.484	123
H4–C1–O2	110.475	110.750	109.232	109.749	109.981	109.451	109.613	109.187	111.94	116.612	116.132	116.324	116.511	116.176	116
O3–C1–O2	124.921	124.772	125.206	124.959	125.018	124.856	124.801	125.092	124.80	120.748	120.572	120.513	120.205	120.340	120
H5–O2–C1	109.202	109.224	106.531	106.460	105.555	106.416	106.140	106.160	106.61	115.909	113.633	113.677	114.148	114.629	114
H6–O3–C1										116.255	113.867	113.664	114.716	115.010	113
H4–C1–O2–H5	−179.949	−179.94	180.000	180.000	180.000	180.000	180.000	180.000	*planar*	180.000	180.000	180.000	179.816	180.000	180
O3–C1–O2–H5	0.033	0.033	0.000	0.000	0.000	0.000	0.000	0.000		0.000	0.000	0.000	−0.095	0.000	−0
H4–C1–O3–H6										0.000	0.000	0.000	0.168	0.000	−0
O2–C1–O3–H6										180.000	180.000	180.000	−179.927	180.000	180

[a] I–J bond length in Å; I–J–K bond angle in deg; I–J–K–L torsional angle in deg. Atom numbering in Fig 1.
[b] Methods as in Table I or otherwise noted.
[c] RHF geometry optimization with $DH6D^{(+)}$ basis set.
[d] MP2 geometry optimization with $DH6D^{(+)}$ basis set.
[e] Formic acid gas phase geometry taken from ref [Davies].