Table II. Zero point energies (ZPE) and vibrational heat contents, at 298.15 K (E'^{vib}) in kcal/mol

Molecule	RHF/6d[a]		MP2/6d		RHF/5d		MP2/5d		DMol		DG/L		DN/L		DN/N	
	ZPE[b]	E'^{vib}[c]	ZPE	E'^{vib}	ZPE	E'^{vib}	ZPE	E'^{vib}	ZPE	E'^{vib}	ZPE	E'^{vib}	ZPE	E'^{vib}	ZPE	E'^{vib}
CH_3CH_2OH	53.854	0.814	51.763	0.851	53.880	0.814	51.785	0.853	48.558	0.941	48.704	0.938	48.797	0.936	48.949	0.925
$CH_3CH_2OH_2^+$	62.002	1.114	59.773	1.094	62.021	1.114	59.776	1.097	56.234	1.318	56.341	1.158	56.389	1.162	56.526	1.228
$HCOO^-$	14.022	0.062[d]	13.038	0.088[e]	14.034	0.061	13.043	0.088	12.130	0.106	12.565	0.096	12.310	0.101	12.133	0.106
HCOOH	23.260	0.170[f]	21.642	0.206[g]	23.285	0.169	21.650	0.205	20.387	0.239	20.596	0.225	20.602	0.226	20.511	0.232
$HCOOH_2^+$	31.882	0.234	30.025	0.269	31.916	0.233	30.034	0.269	28.181	0.326	28.451	0.310	28.437	0.313	28.437	0.313
CH_3OH	34.631	0.278	33.161	0.295	34.651	0.278	33.180	0.294	30.963	0.342	31.192	0.312	31.234	0.329	31.274	0.340
$CH_3OH_2^+$	43.066	0.489	41.522	0.452	43.079	0.489	41.513	0.455	39.248	0.475	39.272	0.458	39.285	0.482	39.418	0.506
CH_3NH_2	43.034	0.325	41.456	0.342	43.053	0.324	41.470	0.343	38.845	0.393	39.025	0.391	39.094	0.391	39.299	0.375
$CH_3NH_3^+$	53.280	0.351	51.169	0.368	53.304	0.350	51.195	0.367	48.433	0.370	48.390	0.382	48.453	0.396	48.789	0.406

[a] See footnotes *a*–*h* in Table I for method description.
[b] Zero Point Energy.
[c] Temperature dependent vibrational enthalpy at 298.15 K.
[d] 13.959 and 0.063 for DHD6$^{(+)}$.
[e] 12.904 and 0.093 for DHD6$^{(+)}$.
[f] 23.219 and 0.171 for DHD6$^{(+)}$.
[g] 21.547 and 0.209 for DHD6$^{(+)}$.