

**Table V.** Energies (hartrees) calculated by different methods

Molecule	RHF/6d <sup>a</sup>	MP2/6d	RHF/5d <sup>b</sup>	MP2/5d <sup>c</sup>	DMol	DG/L	DG/N	DN/L	DN/N
CH <sub>3</sub> CH <sub>2</sub> OH	-154.1230350	-154.6397426	-154.1224796	-154.6344594	-153.837216	-153.777156	-155.078652	-153.7770954	-155.0834611
CH <sub>3</sub> CH <sub>2</sub> OH <sub>2</sub> <sup>+</sup>	-154.4392299	-154.9508198	-154.4386628	-154.9455746	-154.130723	-154.076033	-155.385157	-154.0754390	-155.3904492
HCOO <sup>-</sup>	-188.2371228 <sup>d</sup>	-188.7719162 <sup>e</sup>	-188.2361850	-188.7649065	-187.903715	-187.838977	-189.256199	-187.8352964	-189.2577825
HCOOH	-188.8150210 <sup>f</sup>	-189.3453762 <sup>g</sup>	-188.8143368	-189.3385059	-188.449596	-188.393595	-189.819241	-188.3897471	-189.8212464
HCOOH <sub>2</sub> <sup>+</sup>	-189.1195374	-189.6398706	-189.1189471	-189.6330064	-188.727812	-188.679666	-190.112747	-188.6764299	-190.1147460
CH <sub>3</sub> OH	-115.0744354	-115.4357648	-115.0740581	-115.4318878	-114.862138	-114.820143	-115.753584	-114.8193904	-115.7563149
CH <sub>3</sub> OH <sub>2</sub> <sup>+</sup>	-115.3826246	-115.7396017	-115.3822221	-115.7357520	-115.145634	-115.110564	-116.050971	-115.1093237	-116.0542486
CH <sub>3</sub> NH <sub>2</sub>	-95.2405075	-95.5936421	-95.2402897	-95.5902318	-95.068884	-95.029013	-95.881481	-95.0283120	-95.8846917
CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup>	-95.6053542	-95.9564758	-95.6050615	-95.9531765	-95.410276	-95.377146	-96.237388	-95.3760231	-96.2405465

<sup>a</sup>For methods see footnotes to Table I.

<sup>b</sup>RHF using DH5D basis set

<sup>c</sup>MP2 using DH5D basis set

<sup>d</sup>-188.2481335 with DH6D<sup>(+)</sup>.

<sup>e</sup>-188.7940720 with DH6D<sup>(+)</sup>.

<sup>f</sup>-188.8182181 with DH6D<sup>(+)</sup>.

<sup>g</sup>-189.3543538 with DH6D<sup>(+)</sup>.