Table I. Energies (hartrees) calculated by different methods

Molecule	RHF/6d[a]	MP2/6d[b]	RHF/5d[c]	MP2/5d[d]	DMol[e]	DG/L[f]	DG/N[g]	DN/L[h]	DN/N[i]
CH_3CH_2OH	−154.1230350	−154.6397426	−154.1224796	−154.6344594	−153.837216	−153.777156	−155.078652	−153.7770954	−155.0834611
$CH_3CH_2OH_2^+$	−154.4392299	−154.9508198	−154.4386628	−154.9455746	−154.130723	−154.076033	−155.385157	−154.0754390	−155.3904492
$HCOO^-$	−188.2371228[j]	−188.7719162[k]	−188.2361850	−188.7649065	−187.903715	−187.838977	−189.256199	−187.8352964	−189.2577825
HCOOH	−188.8150210[l]	−189.3453762[m]	−188.8143368	−189.3385059	−188.449596	−188.393595	−189.819241	−188.3897471	−189.8212464
$HCOOH_2^+$	−189.1195374	−189.6398706	−189.1189471	−189.6330064	−188.727812	−188.679666	−190.112747	−188.6764299	−190.1147460
CH_3OH	−115.0744354	−115.4357648	−115.0740581	−115.4318878	−114.862138	−114.820143	−115.753584	−114.8193904	−115.7563149
$CH_3OH_2^+$	−115.3826246	−115.7396017	−115.3822221	−115.7357520	−115.145634	−115.110564	−116.050971	−115.1093237	−116.0542486
CH_3NH_2	−95.2405075	−95.5936421	−95.2402897	−95.5902318	−95.068884	−95.029013	−95.881481	−95.0283120	−95.8846917
$CH_3NH_3^+$	−95.6053542	−95.9564758	−95.6050615	−95.9531765	−95.410276	−95.377146	−96.237388	−95.3760231	−96.2405465

[a] Full geometry optimization at RHF level with Gaussian 90 (ref [GAUSSIAN]) using DH6D basis set.
[b] Full geometry optimization at the 2nd order Møller-Plesset level with Gaussian 90 (ref [GAUSSIAN]) using DH6D basis set.
[c] As footnote *a* but with DH5D basis set.
[d] As footnote *b* but with DH5D basis set.
[e] Full geometry optimization with DMol (ref. [DMOL]) using DNP basis set at LSD level.
[f] Full geometry optimization with DGauss (ref [DGAUSS)]) using DZVPP basis set at LSD level.
[g] Gradient correction added to energy calculated at LSD optimized geometry.
[h] Full geometry optimization at the local spin denisty level with deMon (ref [deMon]).
[i] Full geometry optimization with nonlocal Becke-Perdew gradient corrections with deMon (ref [deMon]).
[j] −188.2481335 with DH6D$^{(+)}$.
[k] −188.7940720 with DH6D$^{(+)}$.
[l] −188.8182181 with DH6D$^{(+)}$.
[m] −189.3543538 with DH6D$^{(+)}$.