

Energetic Data of the Cu_nH_n ($n = 3-6$) Molecules Computed at the B3LYP Level of Theory Using the 6-311+G(d,p) and LANL2DZ Basis Sets.

Compound	Basis Set	Sum of electronic and zero-point Energies (a.u.)	Sum of electronic and thermal Energies (a.u.)	Sum of electronic and thermal Enthalpies (a.u.)	Sum of electronic and thermal Free Energies(a.u.)
$\text{Cu}_3\text{H}_3(D_{3h})$, 1	6-311+G(d,p)	-4923.335962	-4923.330518	-4923.329574	-4923.367025
	LANL2DZ	-590.264083	-590.258492	-590.257548	-590.295336
$\text{Cu}_4\text{H}_4(D_{4h})$, 2	6-311+G(d,p)	-6564.493494	-6564.485709	-6564.484765	-6564.528796
	LANL2DZ	-787.060908	-787.052976	-787.052032	-787.096511
$\text{Cu}_4\text{H}_4(T_d)$, 3	6-311+G(d,p)	-6564.420233	-6564.411835	-6564.410891	-6564.454860
	LANL2DZ	-786.995235	-786.986368	-786.985424	-787.030751
$\text{Cu}_5\text{H}_5(D_{5h})$, 4	6-311+G(d,p)	-8205.631922	-8205.621339	-8205.620395	-8205.672513
	LANL2DZ	-983.840271	-983.829245	-983.828301	-983.881915s
$\text{Cu}_5\text{H}_5(C_{2v})$, 5	B6-311+G(d,p)	-8205.587898	-8205.577454	-8205.576510	-8205.626846
	LANL2DZ	-983.801320	-983.790557	-983.789612	-983.840962
$\text{Cu}_6\text{H}_6(D_{5h})$, 6	6-311+G(d,p)	-9846.761373	-9846.747716	-9846.746772	-9846.808480
	LANL2DZ	-1180.610789	-1180.596923	-1180.595979	-1180.658108
$\text{Cu}_6\text{H}_6(D_{2h})$, 7	6-311+G(d,p)	-9846.712762	-9846.700170	-9846.699226	-9846.753762
	LANL2DZ	-1180.574417	-1180.561497	-1180.560553	-1180.616272