

Table 60. Variation of atomic electronic energies (a.u.) for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	-75.963	-75.966	-75.885	-75.671
O2	-75.956	-75.960	-75.878	-75.668
N1	-55.422	-55.499	-55.324	-55.361
N3	-55.386	-55.457	-55.294	-55.315
C2	-37.036	-36.828	-37.154	-36.355
C4	-37.827	-37.756	-37.844	-37.455
C4'	-38.028	-37.993	-38.020	-37.731
C5	-38.102	-38.073	-38.092	-37.815
C6	-37.852	-37.806	-37.864	-37.586
C6'	-38.025	-37.989	-38.015	-37.724
C5'	-37.479	-37.388	-37.525	-37.086
C5''	-38.053	-38.021	-38.041	-37.761
H1	-0.466	-0.457	-0.474	-0.443
H3	-0.470	-0.461	-0.477	-0.449
H4	-0.622	-0.630	-0.618	-0.642
H41	-0.623	-0.631	-0.620	-0.642
H42	-0.612	-0.618	-0.610	-0.627
H43	-0.623	-0.631	-0.621	-0.641
H61	-0.618	-0.623	-0.617	-0.630
H62	-0.618	-0.625	-0.616	-0.635
H63	-0.608	-0.613	-0.606	-0.620
H51''	-0.606	-0.610	-0.605	-0.616
H52''	-0.621	-0.627	-0.618	-0.636
H53''	-0.615	-0.621	-0.614	-0.628
Σ	-572.232	-571.883	-572.032	-568.739