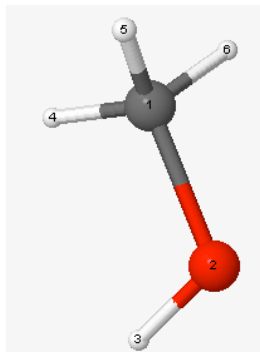
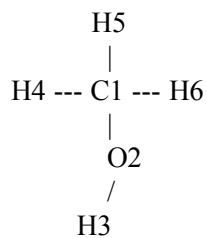


## Methanol Natural Hybrid Orbitals Data Sheet

Methanol:



Bond/Lone Pairs	Description	Occupancy (number of electrons)	Energy (in hartrees)
C1 – O2	1s p		
O2 – C1	2s p		
C1 – H4	1s p		
H4 – C1	4s		
C1 – H5	1s p		
H5 – C1	5s		
C1 – H6	1s p		
H6 – C1	6s		
O2 – H3	2s p		
H3 – O2	3s		
LP(1)	s p		
LP(2)	s p		

To convert Hartrees (a unit of energy):

1 Hartree = 2625.5 kJ/mole

1 Hartree = 627.5095 kcal/mole