HCN…H_2O – ground state

H	0.000000	0.041131	0.353678
C	0.000000	0.026894	1.426831
N	0.000000	0.009461	2.593951
O	0.000000	0.044703	-1.668491
H	0.757940	-0.220542	-2.194706
H	-0.757940	-0.220542	-2.194706

HCN – (H_2O) – ($\pi \rightarrow \pi^*$) excited state
CASSCF optimized minimum

C	-1.500690	-0.567793	-0.000991
N	-2.361310	0.429167	0.000560
O	2.806910	0.030861	0.000977
H	-0.417357	-0.413768	-0.000490
H	3.274720	0.358586	0.750537
H	3.283980	0.367491	-0.761533

HCN – (H_2O) – ($\pi \rightarrow \pi^*$) excited state
From CASPT2 scan

C	0.000000	0.000000	1.305700
N	0.000000	0.000000	2.611700
O	-2.797613	0.000000	-0.504157
H	-0.931343	0.000000	0.707329
H	-3.366849	0.748886	-0.560987
H	-3.377714	-0.763194	-0.562083

HCN – (H_2O) – ($\pi \rightarrow \sigma^*$) excited state
CASSCF optimized minimum

C	1.445980	-0.020184	-0.135656
N	2.601710	0.013455	0.090789
O	-2.821230	0.001590	-0.033953
H	-1.959910	-0.111107	0.374202
H	-3.433600	-0.723122	0.287183
H	-3.209270	0.862539	0.232450

HCN…$(H_2O)_2$ – ground state

N	-1.270559	0.267602	-1.619308
C	-1.148855	-0.143958	-0.533296
H	-0.935921	-0.477263	0.466709
O	0.582377	-0.528612	1.817943
H	1.163264	-0.053897	1.201392
H	0.689408	-0.073714	2.655249
O	1.851337	0.795610	-0.349782
H	1.107983	0.956116	-0.941577
H	2.463476	0.280384	-0.881259