

Nitrate-TAZ weak sigma complex, C_1 symmetry

Energy = -559.426975817 hartree

No negative frequencies.

13

N	0.05536	0.77043	-1.40106
C	1.15115	0.88866	-0.62926
N	1.20826	1.51793	0.55966
C	0.02798	2.00007	0.97906
N	-1.14499	1.92294	0.32635
C	-1.05861	1.28193	-0.85308
H	2.07788	0.46571	-1.01574
H	0.02063	2.51528	1.94385
H	-1.98220	1.18110	-1.42862
O	-0.59152	-2.95705	-0.19955
N	-0.05599	-1.89847	0.23069
O	1.19138	-1.70570	0.08636
O	-0.75960	-1.00923	0.80203

Nitrate-TAZ anion-pi complex, C_{3v} symmetry

Energy = -559.425710928 hartree

No negative frequencies.

13

C	-0.73238	1.07554	-1.22281
N	-1.38067	-0.10267	-1.23716
H	-1.34688	1.97810	-1.21139
N	0.00000	0.00000	1.67040
O	-0.70925	1.05182	1.66386
C	1.29764	0.09649	-1.22281
C	-0.56526	-1.17203	-1.22281
N	0.60142	1.24704	-1.23716
N	0.77926	-1.14436	-1.23716
H	2.38653	0.17738	-1.21139
H	-1.03965	-2.15548	-1.21139
O	1.26553	0.08832	1.66386
O	-0.55628	-1.14014	1.66386