

1. Carbamate solvated by 1 water molecule

M06-2X/6-311++G(d,p) $E_{\text{SCF}} = -321.040701$ hartree.

N	7.0	2.05740905	0.00013275	0.02071070
H	1.0	2.43982768	0.84543186	-0.37467769
C	6.0	0.62324739	-0.00023693	0.01313861
H	1.0	2.44012332	-0.84532505	-0.37409377
O	8.0	0.08235429	1.12871850	0.02304819
O	8.0	0.08299372	-1.12947249	0.02323774
O	8.0	-2.50663280	0.00070147	-0.02642109
H	1.0	-1.86438811	-0.72841096	-0.00693690
H	1.0	-1.86493504	0.73011392	-0.00376190

2. Carbamate solvated by 2 water molecules

M06-2X/6-311++G(d,p) $E_{\text{SCF}} = -397.493309$ hartree.

N	7.0	2.39887857	-0.33499125	-0.10765085
H	1.0	2.84273791	0.02610544	-0.93715084
C	6.0	1.04841220	0.08632393	0.02521560
H	1.0	2.51669979	-1.32554471	0.03527818
O	8.0	0.74276429	1.15102983	-0.55547094
O	8.0	0.31421304	-0.64516854	0.73831016
O	8.0	-2.08339500	-1.49127018	-0.52402526
H	1.0	-1.20293355	-1.43219876	-0.11339898
H	1.0	-2.36168051	-0.56679547	-0.49726605
O	8.0	-1.81874788	1.28813255	0.44922239
H	1.0	-1.44115245	0.65134877	1.07115424
H	1.0	-1.01295495	1.46928346	-0.07773089

3. Carbamate solvated by 3 water molecules

M06-2X/6-311++G(d,p) $E_{\text{SCF}} = -473.943374$ hartree.

N	7.0	-1.57681036	1.36602604	-0.18390667
H	1.0	-2.31980371	0.87646204	-0.66114289
C	6.0	-0.44568011	0.59855449	0.13496609
H	1.0	-1.36297607	2.29199457	-0.51347154
O	8.0	-0.61719203	-0.65627873	0.19064246
O	8.0	0.61539000	1.21462762	0.37246665
O	8.0	2.96241331	0.42387420	-1.05773580
H	1.0	2.18249941	0.89433479	-0.72020489
H	1.0	2.90491366	-0.40930495	-0.57273513
O	8.0	1.91802287	-1.26587725	1.12767196
H	1.0	1.87625432	-0.32716334	1.35353589
H	1.0	1.02569377	-1.36712515	0.74346733
O	8.0	-3.08107424	-1.32549548	-0.54832971

H	1.0	-2.11899066	-1.19786656	-0.33945414
H	1.0	-3.50077868	-1.32989085	0.31375363