SUPPORTING INFORMATION

The force match to construct the sub-molecular resolution nitromethane involved six short range potentials, two bonds, and one angle. The raw potentials that resulted from the force match are presented here, as well as a comparison to the smoothed potentials, and the harmonic approximations.

The six short range potentials are presented across the three figures below. Three interactions are associated with two dimers interacting (f_{++}, f_{--}, and f_{+-} in Figure 1), one interaction describes two methyl groups interacting (f_{Me-Me} in Figure 2), and the remaining interactions are the cross interactions between a methyl group and a dimer (f_{Me-N_+}, and f_{Me-N_-} in Figure 3).

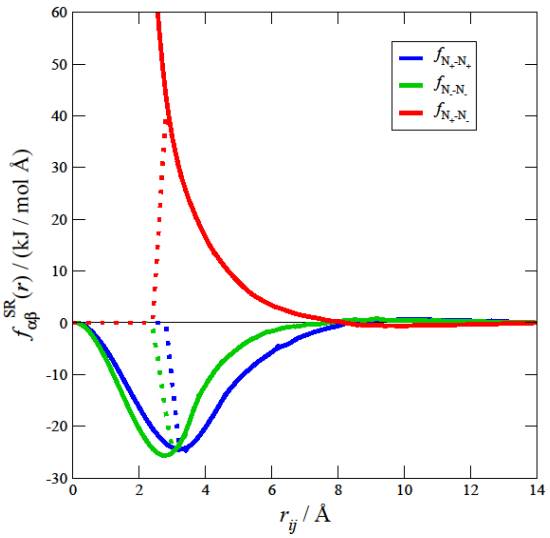

Figure 1 – Short range forces associated with two nitro groups interacting. The dashed lines represent the raw splines from the force match, and the solid lines are the smoothed potentials.

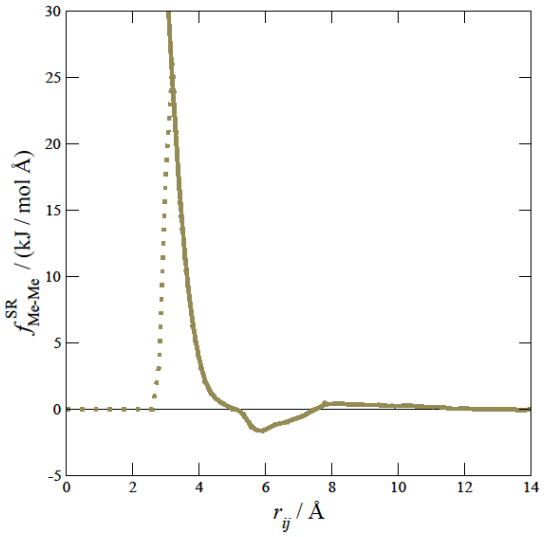

Figure 2 – The short range force from two methyl groups interacting. The dashed line is the raw spline, and the solid line has included a repulsive potential to correct short separations.

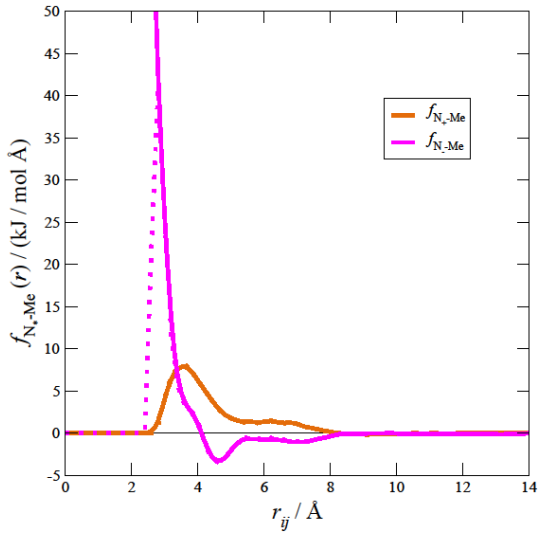

Figure 3 – The short range forces arising from a nitro dimer interacting with a methyl group. The dotted lines are the raw force match, and the solid lines are the smoothed potentials.

The topology of the sub-molecular resolution nitromethane has two bonds, and one angle, all of which were approximated using harmonic potentials in the final model. One bond describe the effective polarizability of the nitro group, and the other connects the nitro group to the methyl group. Both bonds are shown in Figure 4 with a comparison to the harmonic approximation.

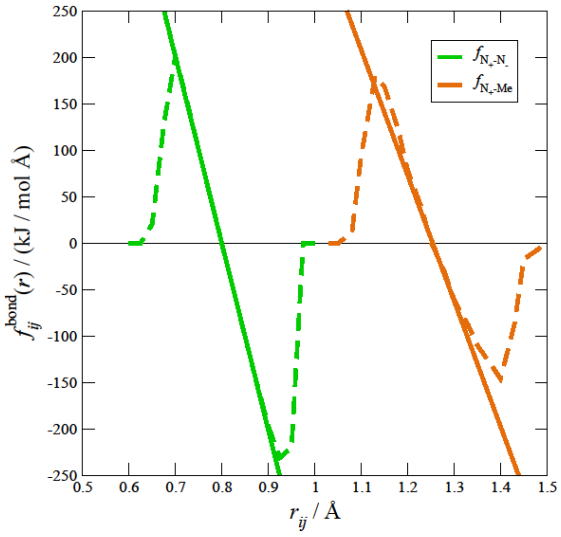

Figure 4 – The two bonds present in the sub-molecular resolution nitromethane. The dashed lines are the splines from the fit, and the solid lines are the harmonic approximations to the splines.

The angular interaction keeps the molecule linear, resulting in an anisotropy in the effective polarizability. The angle interaction is shown in Figure 5 accompanied by the harmonic approximation used in this work.

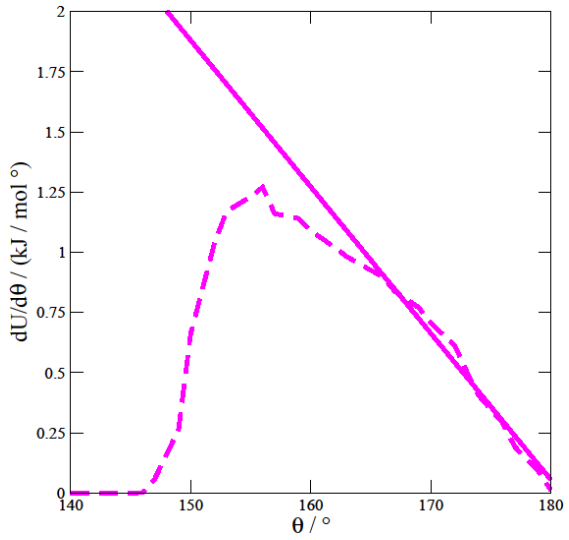

Figure 5 – Angle in the sub-molecular resolution nitromethane. The dashed line is the spline, and the solid line is the harmonic approximation to the potential gradient.