Supporting Material for

Reactive Molecular Dynamics Simulation of Solid Nitromethane Impact on (010) Surfaces Induced and Non-impact Thermo Decomposition

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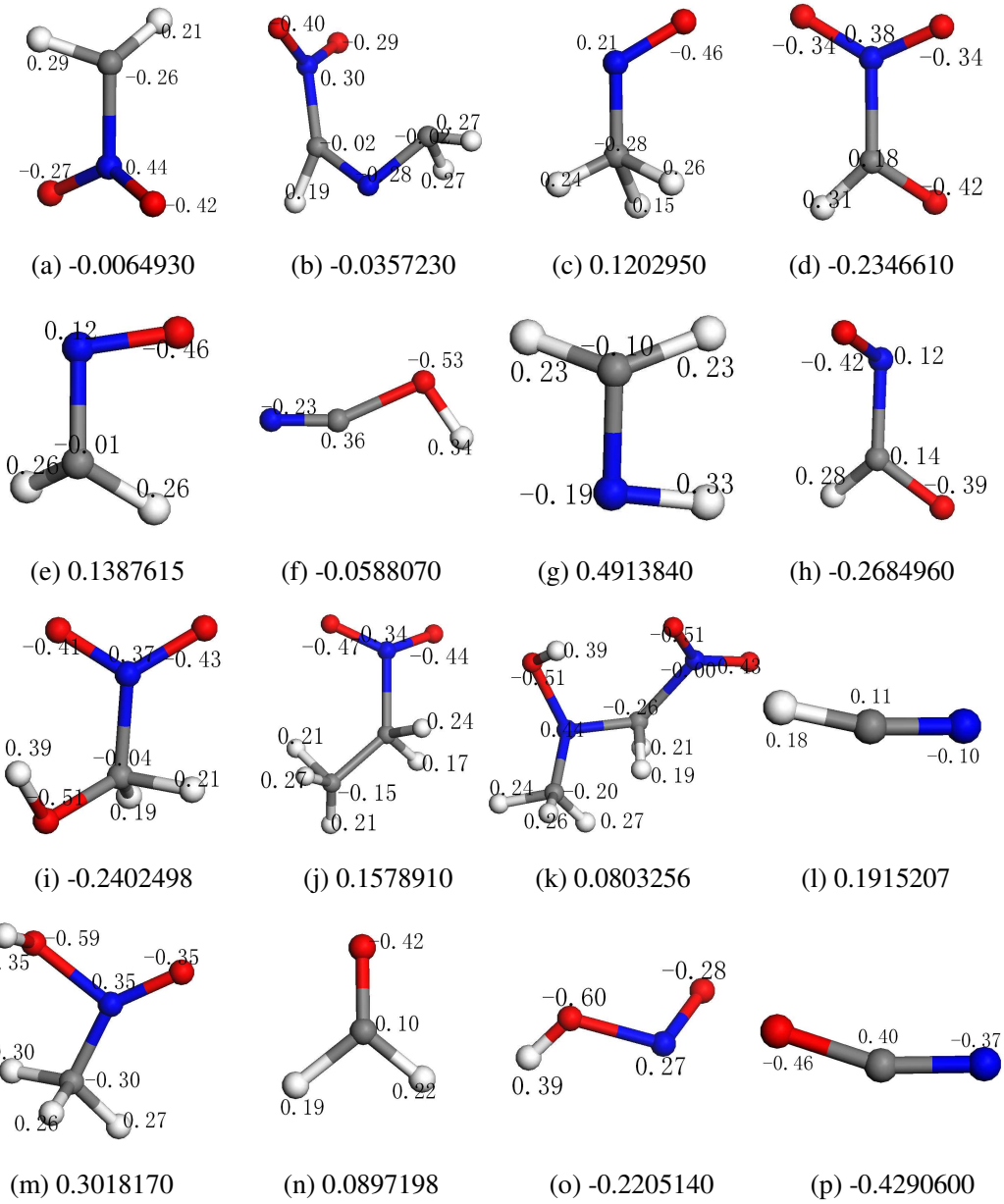

(a) -0.0064930 (b) -0.0357230 (c) 0.1202950 (d) -0.2346610

(e) 0.1387615 (f) -0.0588070 (g) 0.4913840 (h) -0.2684960

(i) -0.2402498 (j) 0.1578910 (k) 0.0803256 (l) 0.1915207

(m) 0.3018170 (n) 0.0897198 (o) -0.2205140 (p) -0.4290600

Figure 1. A part of intermediates observed in early time in simulations, the C atoms are indicated in gray, the H in white, O in red, and N in blue. Charges of every atom are labeled near the atoms, and total charge of every fragment is labeled under the intermediate.

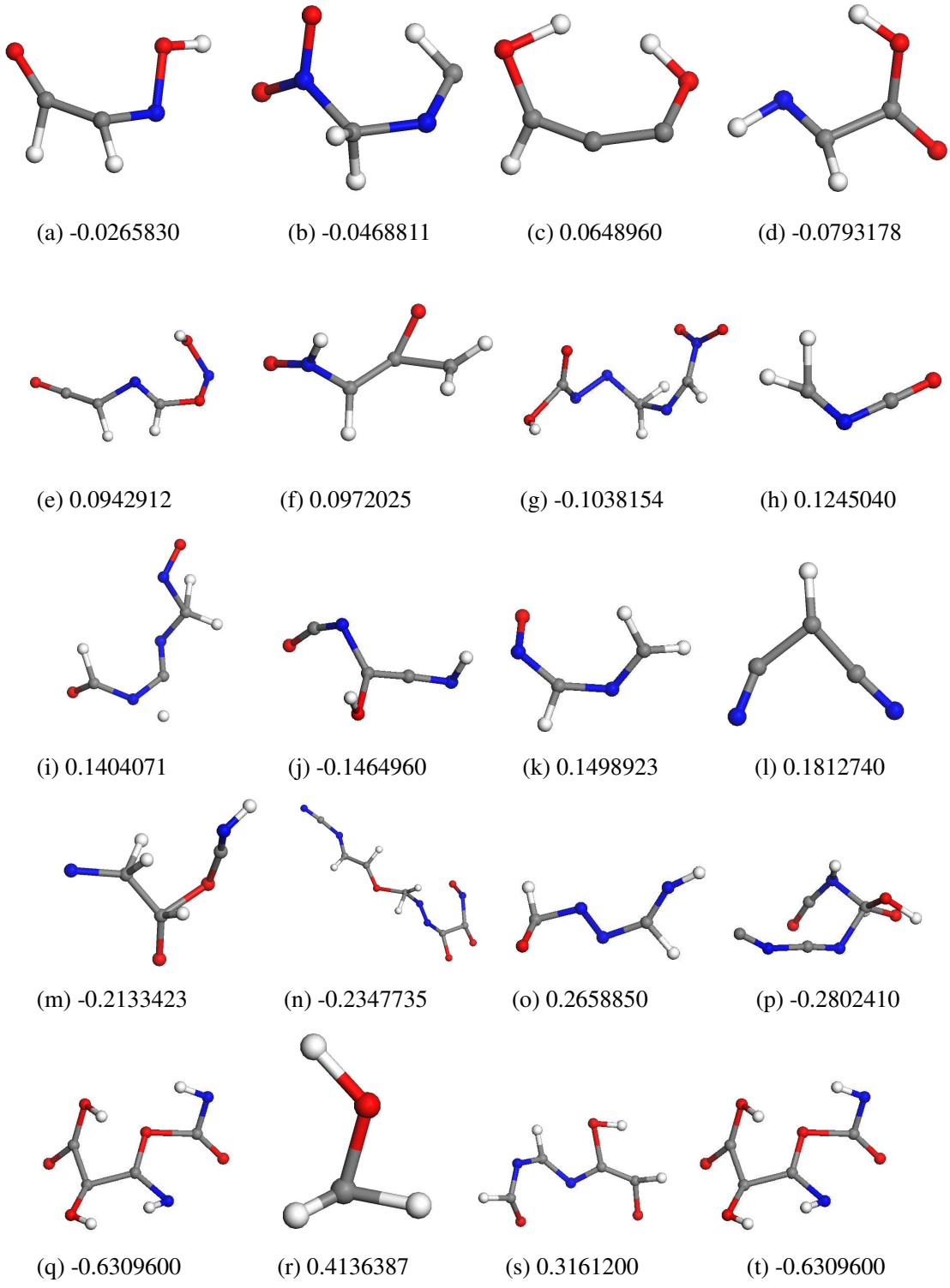

Figure 2. A part of C-N-O chain structures observed in simulation times about 20.0 ps. Total charges is labeled under each molecular fragment. As simulation increase, these fragments formed larger clusters step by step.