

# Acetone Clusters Molecular Dynamics Using a Semiempirical Intermolecular Potential

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**Abstract.** A semiempirical force field for the intermolecular acetone ( $\text{CH}_3\text{-CO-CH}_3$ ) small clusters interaction has been build and applied to characterize the acetone behaviour of some small clusters by Molecular Dynamics. Preliminary theoretical calculations of the structural and dynamical properties of the dimer and the trimer acetone have been investigated at atomistic level of detail by molecular dynamics simulations considering a microcanonical ensemble (NVE). Predictions of the  $(\text{CH}_3\text{-CO-CH}_3)_{2-3}$  binding energies have been performed by extrapolating to 0K the mean potential energy values obtained at low temperatures. The probability of isomerization processes has been also analyzed. The extent to which a classical molecular simulation accurately predicts properties depends on the quality of the force field used to model the interactions in the fluid. The intermolecular interactions involved have been modelled by a recently developed approach targeted to accuracy and low computational cost adopting the Improved Lennard-Jones (ILJ) function to describe the long-range interaction of small clusters systems.

**Keywords:** Molecular dynamics · Empirical potential energy surface · Acetone clusters · DL-POLY

## 1 Introduction

Acetone (systematically named propanone) is the organic compound with the formula  $\text{CH}_3\text{-CO-CH}_3$ . It is a colorless, volatile, flammable liquid, and is the simplest ketone. Acetone is miscible with water and serves as an important solvent in its own right, typically for cleaning purposes in the laboratory. About 6.7 million tonnes were produced worldwide in 2010. It is a common building block in organic chemistry. Familiar household uses of acetone are as the active ingredient in nail polish remover and as paint thinner. Acetone is produced and disposed of in the human body through normal metabolic processes. It is normally present in blood and urine. People with diabetes produce it in larger amounts. Reproductive toxicity tests show that it has low potential to cause reproductive problems. Pregnant women, nursing mothers and children have

higher levels of acetone [1]. Ketogenic diets that increase acetone in the body are used to counter epileptic attacks in infants and children who suffer from recalcitrant refractory epilepsy.

There are two main ways of manufacturing propanone, both produced from propene. One of them is via cumene and the other one via isopropanol. By far the most important route is the cumene process [2–4]. Acetone is able to dissolve a wide range of chemical compounds, including polar, non-polar and polymeric materials [5,6] and is very soluble in water. Accordingly, most of the acetone production is used as a solvent, the properties as a solvent being known for a long time [7]. Due to the capability to dissolve different chemical compounds, acetone is often the primary component of cleaning agents, which present specific benefits because being effective and not expensive, they have a very low toxicity. Moreover, acetone is also important in the chemical industry, being widely used in the production of methyl methacrylate [8] and bisphenol A [9].

Owing to the central role of water in everyday life, water is the most investigated solvent. However, the understanding of the solvation mechanisms in solutions of organic solvents is crucial to improve the efficiency of processes of technological interest [10–13]. From an experimental point of view, to obtain detailed dynamical information on simple and complex liquids, spectroscopic methods based on a second rank molecular property, such as the polarizability anisotropy, can be suitably applied [12]. On the other hand, Molecular Dynamics (MD) simulations is a theoretical powerful tool to analyze extensively the structural rearrangement of pure solvents, solution mixtures and the combustion processes. Combustion is a complex of chemical and physical nature of the process that leads to the conversion of chemical energy into heat energy stored in fuels. From a molecular point of view, the combustion is the result of numerous elementary processes, chemical reactions including mono-, bi- and ter-molecular and energy-transfer processes (which ensure the distribution of the energy released by the exothermic reactions to everything the system). The characterization of the elementary processes (like organic compounds, acetone) is therefore essential for a detailed understanding and for the optimization of combustion systems. Given the complexity of the problem, we resort to a multidisciplinary approach based on the use of computer models that are considered all possible elementary processes. However, the accuracy of the results depends largely on the reliability of the interaction potential. In the last years some of us have formulated a potential energy function [14] to describe the non permanent charge interactions ( $V_{nel}$ ), which combined with the electrostatic contributions ( $V_{el}$ ), when present, is able to describe accurately ionic and neutral systems. In such model, the relevant parameters of  $V_{nel}$  are derived from the values of the molecular polarizability. On another hand, polarization effects are indirectly considered by increasing the value of the dipole moment of the molecules in respect with those corresponding to gas phase. Such formulation has been proved to be adequate not only to describe systems on gas phase (see for instance Refs. [15–17]) but also the liquid behavior of water, [18–21] acetonitrile, [13] and ammonia [22].

All the previous results encouraged us the use of the same methodology to construct the acetone-acetone force field.

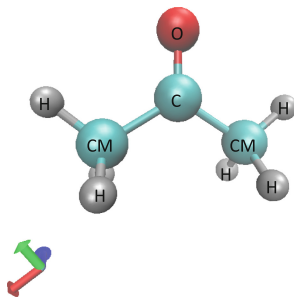
The original potential model used here is based on a formulation of the non electrostatic approach to the intermolecular interaction that exploits the decomposition of the molecular polarisability [23] into effective components associated with atoms, bonds or groups of atoms of the involved molecules. This type of contribution to the intermolecular energy was already applied in the past to the investigation of several neutral [24–32] and ionic [33–35] systems, often involving weak interactions [24,36], difficult to calculate. The adequacy of such potential energy functions to describe several intermolecular systems was proved by comparing energy and geometry predictions at several configurations with *ab initio* calculations.

In the present paper, we present the preliminary theoretical results of the potential model, based in a modification of the Lennard Jones (LJ) function which is applied to investigate the small clusters of acetone,  $(\text{CH}_3\text{-CO-CH}_3)_2$  and  $(\text{CH}_3\text{-CO-CH}_3)_3$ . The paper is organized as follows: in Sect. 2, we outline the construction of the potential energy function. We give in Sect. 3 the details of the Molecular Dynamics simulations. Results are presented in Sect. 4 and concluding remarks are given in Sect. 5.

## 2 Potential Energy Surface

As it has been indicated in the Introduction, the formulation of the potential energy interaction has been performed by assuming the separability of non permanent ( $V_{nel}$ ) and permanent ( $V_{el}$ ) charge interaction contributions.  $V_{nel}$  is described by considering four interaction centers localized on the  $\text{CH}_3\text{-CO-CH}_3$  molecule, considered as a rigid body. The representation of the acetone molecule is given in Fig. 1.

Two of the interaction centers are placed on the C atoms of the methyl groups, represented by CM, and the other two placed on the C and O atoms of the  $\text{C=O}$  group, described by C and O respectively. This means that the acetone molecule is given by a rigid set of four interaction sites, located on oxygen



**Fig. 1.** Graphical representation of the labeled atoms in the acetone molecule.

and carbon atoms. Accordingly,  $V_{nel}$  is represented as a sum of pair contributions between interaction centers on different molecules. Each pair contribution described by means of an ILJ function,  $V_{ILJ}(r)$ , depending on the distance  $r$  between the considered centers. Specifically,

$$V_{ILJ}(r) = \varepsilon \left[ \frac{m}{n(r) - m} \left( \frac{r_0}{r} \right)^{n(r)} - \frac{n(r)}{n(r) - m} \left( \frac{r_0}{r} \right)^m \right] \quad (1)$$

with,

$$n(r) = \beta + 4 \left( \frac{r}{r_0} \right)^2 \quad (2)$$

The ILJ function defined in Eq. 1, thanks to the additional parameter  $\beta$ , is more flexible than the traditional Lennard Jones (LJ) one. For the acetone-acetone interactions, independently of the involved interaction centers,  $\beta$  has been taken equal to 11, while  $m$ , as correspond to neutral-neutral interactions, is equal to 6. For neutral systems usually  $\beta$  take values between 6 and 11. Due to the relative role played by  $\beta$  and the dipole moment ( $\mu$ ), the specific value depends on the selected value of  $\mu$  [21]. Small modifications of  $\beta$  can be compensated by varying  $\mu$ . As it has been indicated in the Introduction section, the relevant parameters,  $\varepsilon$  describing for each pair the depth of the potential well and its location  $r_0$  are evaluated using the values of the polarizability associated to each interaction center [37]. The values of such parameters are given in Table 1.

**Table 1.**  $\varepsilon$  (well depth),  $r_0$  (equilibrium distance) parameters used to define  $V_{nel}$  for the acetone-acetone intermolecular interactions using ILJ functions. The atoms are named as in Fig. 1.

Interaction partners	$\varepsilon/\text{meV}$	$r_0/\text{\AA}$
CM-CM	11.362	4.053
C-C	6.520	3.628
O-O	5.160	3.398
CM-C	8.819	3.866
CM-O	6.688	3.789
C-O	5.640	3.521

The electrostatic contribution,  $V_{el}$ , is calculated from a ten point charge distribution by applying the Coulomb law. Such distribution is compatible with the value of the experimental dipole moment of acetone, equal to 2.88 D [38] and charges of  $-0.4290$  a.u. and  $0.4290$  a.u. placed on the C and O atoms, while on the methyl groups charges of  $0.406$  a.u.,  $-0.406$  and  $0.0702$  are placed on the CM and H centers, respectively.

It is interesting to note that using the ILJ function, the consideration of different charge distributions can be compensated by variations of the  $\beta$  parameter. The modulation of  $\beta$  can also partially compensate the case of different representations of the charge distributions and indirectly include in the contribution of other less important components, at intermediate and short distances [13, 18, 19, 21, 22, 39].

### 3 The Simulation Protocol of the Molecular Dynamics

Classical molecular dynamics simulations were performed using the DL-POLY [40] molecular dynamics simulation package. We performed classical MD simulations of  $(\text{CH}_3\text{-CO-CH}_3)_n$ ,  $n = 2 - 3$ . For each optimized structure, we performed simulations with increasing temperature. A microcanonical ensemble (NVE) of particles, where the number of particles,  $N$ , volume,  $V$ , and total energy,  $E$ , are conserved, has been considered. The total energy,  $E$ , is expressed as a sum of potential and kinetic energies. The first one is decomposed in non electrostatic and electrostatic contributions and its mean value at the end of the trajectory is represented by the average configuration energy  $E_{cfg}$  ( $E_{cfg} = E_{nel} + E_{el}$ ). The kinetic energy at each step,  $E_{kin}$ , allows to determine the instantaneous temperature,  $T$ , whose mean values can be calculated at the end of the simulation. The total time interval for each simulation trajectory was set equal to 5 ns after equilibration (1 ns) at each temperature. We implemented the Improved Lennard-Jones potential function and used it to treat all the intermolecular interactions in  $(\text{CH}_3\text{-CO-CH}_3)_2$  and  $(\text{CH}_3\text{-CO-CH}_3)_3$ .

### 4 The $(\text{CH}_3\text{-CO-CH}_3)_2$ and $(\text{CH}_3\text{-CO-CH}_3)_3$ Small Aggregates

The binding energies for  $(\text{CH}_3\text{-CO-CH}_3)_2$  and  $(\text{CH}_3\text{-CO-CH}_3)_3$  have been estimated by performing MD calculations at low temperatures  $T$ . As it has been explained in previous papers [16, 22, 41], when no isomerization occurs, the extrapolation of the configuration (potential) energy values,  $E_{cfg}$ , to 0 K provides a good estimation of the binding energy (as  $E$  is conserved along the trajectory, at very low temperatures, the configuration energy, tends to become almost constant).

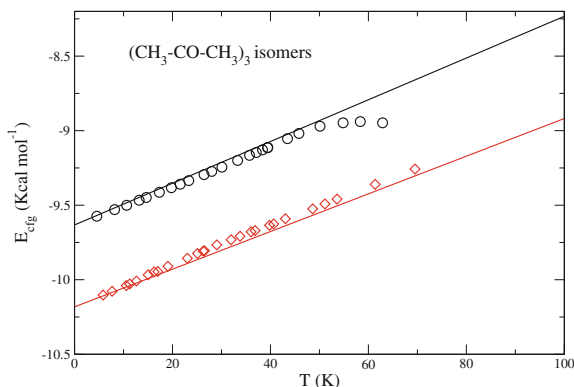
The  $E_{cfg}$  values at different (low) temperatures for  $(\text{CH}_3\text{-CO-CH}_3)_2$  and  $(\text{CH}_3\text{-CO-CH}_3)_3$  are given in the Table 2 and represented on the Fig. 2, respectively. As it can be seen, the results at temperatures lower than 40 K (values reported in Table 2) shown a linear trend, indicating the absence of isomerization processes. In the chosen temperature conditions, the linear dependence is easily reached for  $T$  in the range of 5 K–40 K which gives a value of  $-4.943 \text{ kcal mol}^{-1}$  when it was extrapolated to 0 K. At higher temperatures, when isomerization processes are likely to occur, the different steps of the simulation probe several configurations with different potential energy values, and, according with

**Table 2.**  $E_{c_{fg}}$  (Kcal mol<sup>-1</sup>) at different (low) temperatures (K) for the acetone-acetone dimer.

Temp. (K)	$E_{c_{fg}}$ (Kcal mol <sup>-1</sup> )
5.1400	-4.911
8.4487	-4.891
10.523	-4.877
13.310	-4.861
18.024	-4.831
21.041	-4.811
22.574	-4.802
24.162	-4.791
26.358	-4.778
28.464	-4.762
29.089	-4.760
32.543	-4.733
35.283	-4.722
36.149	-4.712
38.143	-4.698
41.766	-4.671
42.045	-4.671
43.120	-4.661
43.889	-4.655
48.273	-4.625
50.697	-4.609
51.025	-4.604
51.434	-4.601
51.717	-4.598
54.285	-4.581
59.947	-4.535
60.117	-4.536
68.913	-4.466

the fact that total energy must be conserved, the kinetic energy (and T) also varies. For this reason, the difficulty to achieve a chosen value of T increases.

The same range of temperatures have been used to analyze the acetone trimer. In this case, results suggest the presence of more than one isomer. As a matter of fact, the simulations, beginning from a random configuration for the trimer, show that the increase of T causes an initial linear decrease of the absolute value of  $E_{c_{fg}}$ , as it was observed for the dimer. However, for T approaching to

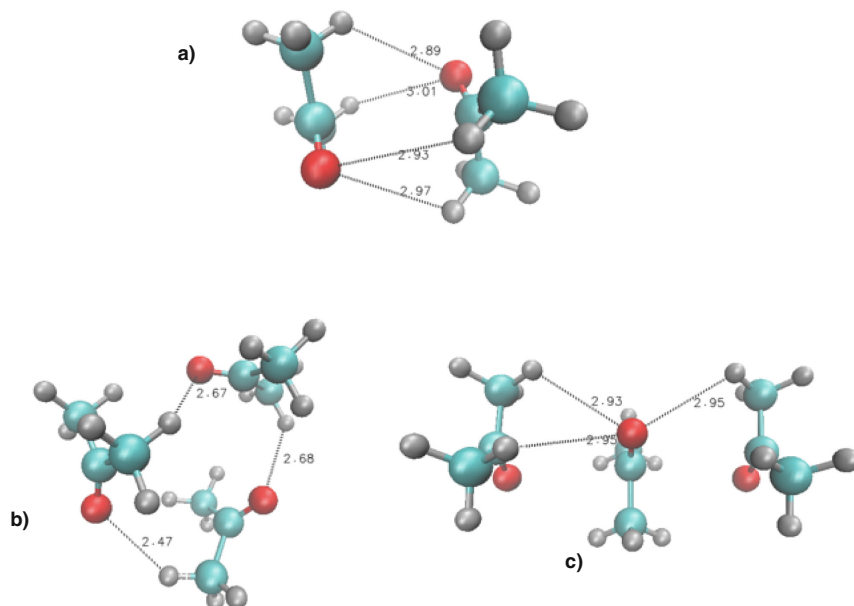


**Fig. 2.** Configuration (potential) energy values,  $E_{cfg}$ , for the acetone trimer as a function of  $T$ . The markers correspond to the MD results.

70 K, more negative values of  $E_{cfg}$  can be obtained, pointing out the presence of a stabler isomer. In order to characterize both isomers, we have performed additional MD simulations at decreasing temperatures, starting from the last configuration computed at 70 K (see red markers in Fig. 2). This procedure allows to obtain two sets of independent  $E_{cfg}$  data (black and red markers) as a function of  $T$  that, by their extrapolation to 0 K, provide binding energy predictions for both isomers. For acetone the linear extrapolation has been performed in the 5–20 K temperature range. However, MD simulations have been performed from 5 K to 70 K. These results point out that, in spite of the fact that only low temperatures are used in the linear extrapolation, a study including a wider range of  $T$  is mandatory to check the presence of more isomers. The process of running consecutive MD simulations at decreasing temperatures in the low  $T$  range can be seen as a simulated annealing minimization. [42] The extrapolated values of  $E_{cfg}$  to 0 K, are equal to  $-10.182$  and  $-9.632$  kcal mol $^{-1}$ .

The analysis of the configuration energy at each step of the trajectory calculated at the lowest temperature investigated shows that, for the dimer, the lowest energy value attained along the trajectory is equal to  $-4.931$  kcal mol $^{-1}$ , very similar to the extrapolated value, representing the binding energy. For the trimer, the same analysis has been performed at the lowest temperature associated to each data set. Results indicate that the lowest energy values attained for the two data sets amount to  $-9.628$  and  $-10.177$  kcal mol $^{-1}$ , which are also very similar to the extrapolated values. Accordingly, the geometries associated to the energies of  $-4.931$ ,  $-9.628$  and  $-10.177$  kcal mol $^{-1}$  should be very similar to the actual, for dimer and trimer respectively minima. Such equilibrium-like configurations are shown in Fig. 3.

On the panel (a) of Fig. 3 is shown the equilibrium-like geometry for the dimer, which corresponds to an antiparallel structure in which the C=O bond of one molecule points toward the other one in such a way that the O of each molecule participates in the formation of two hydrogen(H)-bonds. This means that,



**Fig. 3.** Equilibrium-like structures for the acetone dimer (panel a) and for the trimer (panels b and c).

in agreement with other theoretical results, [43,44] four H-bonds are involved in the most stable configuration predicted by the potential model. All four O-H distances are very similar around to 2.9 Å. This value is in very good agreement with that of 3.0 Å reported by Frurip et al. [45]. Moreover, the same authors give a C-C distance equal to 3.84 Å similar to the value of 3.78 Å predicted by own potential model.

The equilibrium-like structures for the two isomers of the trimer are shown in panels (b) and (c) of Fig. 3. In agreement with the results of Tamenori et al. [43] the cyclic structure shown in panel (b) is the most stable one and the O-H distances are about a 15% shorter than those found for the dimer, while values of about 2.95 Å are found for the O-H distances of structure (c). The existence of two isomers and its relative stability is in agreement with the experimental results of Guan et al. [46]. The authors use size-selected IR-VUV spectroscopy to detect vibrational characteristics of neutral acetone and some of its clusters. In spite of the presence of two isomers, in the range of temperatures investigated, isomerization between them is quite unlikely. In particular, the less stable isomer can transform into the most stable one only at the high T.

## 5 Conclusions

In this paper we have done the preliminary theoretical calculation to study the properties of acetone small clusters by classical MD simulations by using



a semiempirical intermolecular potential energy surface based on the ILJ pair interaction function. The underlying interaction model is targeted to an accurate description of the weak interactions, whose reliability has been validated here by comparison of our results with those available in the literature from theory and experiments. The predicted binding energies for the acetone dimer has been found in good agreement with both experimental and *ab initio* results. No isomerization processes have been observed for the dimer at temperatures lower than 40 K, instead for the trimer system some evidence of the presence of more than one isomer has been observed. Perspectives regard the application to extensive studies of clusters with more acetone molecules and the liquid acetone at several conditions of pressure and temperature.

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