Erratum Notes for 2011 J. Phys. Chem. A article– RQT Sept 2014 - Based on contributions from John Biswakarma and also on my own discovery

(1) The 2011 article by Topper et al. states that the original MFT potential was used in the simulated annealing calculations. Instead, a modified version of the original 1996 Matro/Freeman/Topper potential was used. The modified parameters were developed by Feldman and Topper in an independent study at MU during 2008, and were used subsequently by both Feldman and Markus. The new potential is identical to the old in the normal interaction region. However, unlike the original MFT potential, the modified potential is free of computational singularities at very small interparticle distances. These singularities were not encountered in previous work; probably Matro's code simply kept any two atoms from getting too close together with a hard sphere radius. In addition, the magwalking algorithm occasionally puts particles very close together in trial moves at very high temperatures. The modified MFT potential introduced new Dij parameters as follows:

Modified MFT Potential

	Aij	αij	Cij	Dij
H-H	1.0162	1.9950	2.9973	100.0
N-N	104.74	1.5611	25.393	40.0
Cl-Cl	124.55	1.7489	113.68	800.0
H-N	10.318	1.7780	8.7229	80.0
H-Cl	0	0	10.033	43884.0
N-Cl	114.22	1.6550	53.736	200.0

Original MFT Potential

	A	α	C	D
H-H	1.0162	1.9950	2.9973	2021.01
N-N	104.74	1.5611	25.393	0
Cl-Cl	124.55	1.7489	113.68	0
H-N	10.318	1.7780	8.7229	0
H-Cl	0	0	10.033	43884.0
N-Cl	114.22	1.6550	53.736	0

Both models assume the same atomic charges, q_i (H=0.35, N=-0.40, Cl=-1.00). The pairwise interaction energies, lattice energies, and cell parameters predicted by the two models are very similar, as shown below (calculations by Katherine Russamano):

	Cell Parameter (A)	Lattice Energy (kJ/mol)
MFT	3.777	-724.6
Modified MFT	3.782	-724.7
GG (low barrier)	3.849	-739.5
FEMD/LDA	3.891	N/A
Experimental	3.868	-697

(2) The article states that 25,000 single particle moves were made at each temperature. However, between 100,000 and 250,000 particle moves were used for each cluster in Feldman's 2008 calculations. In addition, the radial parameter for the C-potential ranged from 10 to 40 in Feldmann's work.

Traditionally the number of Monte Carlo "cycles" is defined as the number of particle moves divided by the number of particles. Using this definition, the number of cycles used ranged from about 5600 to 80,000 with the average number of cycles around 10,000 for the neutrals and cations and about 26,000 for the anions (which were sampled more thoroughly than the rest for no obvious reason). It is unclear where the number 25,000 came from but I currently believe that it came from Markus, who may have re-run the calculations using the values cited in the paper and found the same structures that Feldman found.
The numbers below are from Feldman's documentation:

Neutral Run Parameters (starting at 10,000K; 10 Teeth; 20 Runs/Tooth)

Cluster Size	C-Potential	Iterations
1		100000
2		100000
3		100000
4		100000
5		100000
6		100000
7	25	100000
8	30	100000
9	30	100000
10	30	200000
11	35	200000
12	35	200000
13	40	200000

Cation Run Parameters (starting at 10,000K; 10 Teeth; 20 Runs/Tooth)

Cluster Size	C-Potential	Iterations
1+	15	100000
2+	15	100000
3+	20	100000
4+	20	100000
5+	25	100000
6+	25	100000
7+	30	100000
8+	30	100000
9+	30	200000
10+	35	200000
11+	35	200000
12+	40	200000
13+	40	200000

Anion Run Parameters (starting at 10,000K; 10 Teeth; 20 Runs/Tooth)

Cluster Size	C-Potential	Iterations
1-	10	250000
2-	10	250000
3-	15	250000
4-	15	250000
5-	15	250000
6-	20	250000
8-	20	250000
9-	30	250000
10-	30	250000
11-	30	250000
12-	30	250000
13-	35	250000

(3) In Figure 5, the squares are the M06-2X calculated values and the circles are from Ref. 14. The caption is reversed, i.e., it should have the "circle" symbol where it has the "square" symbol and vice versa.

(4) Figure 8 should not has the phrase …" by monomer addition…" within the caption.

(5) This last correction is tentative as of 9/11/14….reactions R1-R3 should, I believe, all have n-1 on the reactant side and n on the product side. Table 5 needs to be rechecked…