

To assess the influence of imaginary modes on the models they were compared against the newly generated models to calculate the RMSD values (**Table 1**) and compare the Fukui functions (**Table 2**).

Table 1 shows that there is a considerable correlation between the models, as all of the calculated values are below 0.2 Å, while it is commonly accepted that values below 1.5 Å show significant correlation.

Table 2 shows that for the majority of models that the presence of imaginary modes did not influence the number of electrophilic or nucleophilic attack sites and that in the instance where a difference was observed it was very small and likely to be associated with the isovalue used to visually explore the models. The observed differences also did not alter the initial rankings produced within this body of work.

Table 1 – Breakdown of the determined RMSD values

Model name	RMSD Value (Å)
CHDA	0.004
HMMM CHDA	0.197
HHPA	0
HMMM HHPA	0.002
TMA	0.002
TMA NPG	0.607
HMMM TMA	1.099
DDSA	0.708

Table 2 – Comparing the number of attack sites between models with imaginary modes and without

Model designation	Before removal of imaginary modes		After removal of imaginary modes		Difference in number of sites
	Electrophilic attack site	Nucleophilic attack site	Electrophilic attack site	Nucleophilic attack site	
CHDA	8	12	8	12	0
HMMM CHDA	6	6	6	6	0
HHPA	8	8	8	8	0
HMMMM HHPA	12	10	9	10	-3 electrophilic
TMA	10	18	10	18	0
TMA NPG	8	8	8	8	0
HMMMM TMA	16	16	16	16	0
DDSA	3	8	5	8	+2 electrophilic

Table 3 – Weighted attack sites as a function of the polyester-melamine ratio

Monomer base	Number of electrophilic sites	Number of nucleophilic sites	Total
HHPA	17.8	14.8	32.6
CHDA	22.8	23.6	46.4
TMA	24.8	35.2	60
DDSA	13.2	19.6	32.8