Electronic Supplementary Information for PCCP article

A Computational Study of '*Al*-kanes' and '*Al*-kenes'

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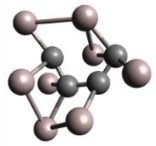
Two novel series of '*Al*-kanes' (C_nAl_{2n+2}) and `*Al*-kenes' (C_nAl_{2n}) have been studied theoretically in order to shed light on their structure, stability and properties. Density functional calculations suggest that the structures tend to be dictated by the constituent aluminium atoms, rather than the carbon backbone. This is the net effect of the aluminiums attempting to adopt preferred close-packed structures. Calculated energetics suggest a special stability of clusters with *n*(C) = 2 and 4 in both series and plausible interpretations are suggested.

Fig S1. *cis*-but-2-ene

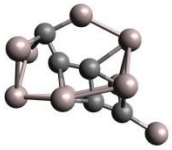


De = 23.04 eV
De' = 6.06 eV

Fig. S2 *trans*-but-2-ene

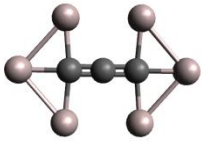
De = 23.36 eV
De' = 6.39 eV

Fig. S3 *trans*-pent-2-ene



De = 27.34 eV
De' = 4.71 eV

Fig. S4 *symmetric* C_3Al_6 structure obtained using coordinates from previous MP2 calculation.[20]



De = 17.84 eV
De' = 6.59 eV