The stepwise energies for forming any cluster can be calculated from the combination of tables S3-S10 and tables 1-5 by using Hess’s Law. An example showing the calculation of the optimal pathway of the dry pentamer at 298 K, as shown in table 7, is below.

|  |  |  |  |
| --- | --- | --- | --- |
| Pathway Steps | ΔG° at 298 K | How Energy was calculated | Calculation |
| SA + DMA ⇌ (SA)(DMA) | -13.62 | Energy was extracted directly from Table S7. | No calculation needed. |
| (SA)(DMA) + FA ⇌ (SA)(FA)(DMA) | -6.86 | Energy for forming (SA)(FA)(DMA) from monomers was extracted from Table 2 (-20.48) and the energy to form (SA)(DMA) (previous step: -13.62) was subtracted from it. | -20.48 – -13.62 = -6.86 |
| (SA)(FA)(DMA)+ NA ⇌ (SA)(FA)(NA)(DMA) | -4.42 | Energy for forming (SA)(FA)(NA)(DMA) from monomers was extracted from Table 3 (-24.90) and the energy to form (SA)(FA)(DMA) (sum of previous steps: -13.62 + -6.86) was subtracted from it. | -24.90 – (-13.62 + -6.86) = -4.42  (Table 3) – (Sum of previous steps) = (Final) |
| (SA)(FA)(NA)(DMA)+ A ⇌ (SA)(FA)(NA)(A)(DMA) | -3.10 | Energy for forming pentamer from monomers was extracted from Table 5 (-28.00) and the energy to form (SA)(FA)(NA)(DMA) (sum of all previous steps: -13.62 + -6.86 + -4.42) was subtracted from it. | -28.00 – (-13.62 + -6.86 + -4.42) = -3.10 |