The stepwise energies for forming any cluster can be calculated from the combination of tables T1-T6 and tables 1-6 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 8, 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 T4. | No calculation needed. |
| (SA)(DMA) + NA ⇌ (SA)(NA)(DMA) | -6.07 | Energy for forming (SA)(NA)(DMA) from monomers was extracted from Table 2 (-19.69) and the energy to form (SA)(DMA) (previous step: -13.62) was subtracted from it. | -19.69 – -13.62 = -6.07  (Table 2) – (Table T4) = (Final) |
| (SA)(NA)(DMA) + A ⇌ (SA)(NA)(A)(DMA) | -4.86 | Energy for forming (SA)(NA)(A)(DMA) from monomers was extracted from Table 5 (-24.55) and the energy to form (SA)(NA)(DMA) (Table 2: -19.69) was subtracted from it. | -24.55 – -19.69 = -4.86  (Table 3) – (Table 5) = (Final) |
| (SA)(NA)(A)(DMA) + HCl ⇌(SA)(NA)(HCl)(A)(DMA) | -7.45 | Energy for forming pentamer from monomers was extracted from Table 6 (-32.00) and the energy to form (SA)(NA)(A)(DMA) (Table 5: -24.55) was subtracted from it. | -32.00 – -24.55 = -7.45  (Table 6) – (Table 5) = (Final) |