## Appendix A. Particles Data

Table 1. Properties of elementary birth and death events in generation of A–B heteromers [[1](#_ENREF_1)].

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ID** | A–B**-1** | A–B**-2** | A–B**-3** | A–B**-4** | A–B**-5** | A–B**-6** | A–B**-7** | A–B**-8** | A–B**-9** |
| ***bb*** | -18.932 | -5.355 | -3.170 | 1.068 | -6.192 | 1.776 | 0.408 | -4.765 | -3.997 |
| ***be*** | -14.760 | -22.007 | -7.976 | -16.593 | -20.840 | 1.270 | -16.827 | -18.715 | -14.425 |
| ***db*** | -4.172 | 16.652 | 4.806 | 17.661 | 14.648 | 0.506 | 17.235 | 13.95 | 10.428 |
| ***de*** | 14.76 | 22.007 | 7.976 | 16.593 | 20.84 | -1.27 | 16.827 | 18.715 | 14.425 |
| *bb*: birth barrier/resistance, *be*: birth energy release, *db*: death barrier/resistance and *de*: death energy release. All energies are in kcal/mol. | | | | | | | | | |

Table 2. Properties of elementary birth and death events in generation of A–A homomers [[1](#_ENREF_1)].

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **ID** | A–A**-1** | A–A**-2** | A–A**-3** | A–A**-4** | A–A**-5** | A–A**-6** | A–A**-7** | A–A**-8** | A–A**-9** |
| ***bb*** | 0.371 | -2.107 | -2.369 | -1.975 | 0.205 | 0.161 | 0.166 | 0.261 | -2.385 |
| ***be*** | -11.810 | -8.447 | -10.789 | -2.930 | -3.627 | -15.878 | -11.738 | -12.011 | -2.267 |
| ***db*** | 12.181 | 6.34 | 8.42 | 0.955 | 3.832 | 16.039 | 11.904 | 12.272 | -0.118 |
| ***de*** | 11.81 | 8.447 | 10.789 | 2.93 | 3.627 | 15.878 | 11.738 | 12.011 | 2.267 |
| *bb*: birth barrier/resistance, *be*: birth energy release, *db*: death barrier/resistance and *de*: death energy release. All energies are in kcal/mol. | | | | | | | | | |

Table 3. Properties of elementary birth and death events in generation of B–B homomers [[1](#_ENREF_1)].

|  |  |  |  |
| --- | --- | --- | --- |
| **ID** | B–B**-1** | B–B**-2** | B–B**-3** |
| ***bb*** | -5.051 | -5.038 | -4.933 |
| ***be*** | -12.653 | -2.208 | -2.737 |
| ***db*** | 7.602 | -2.83 | -2.196 |
| ***de*** | 12.653 | 2.208 | 2.737 |
| *bb*: birth barrier/resistance, *be*: birth energy release, *db*: death barrier/resistance and *de*: death energy release. All energies are in kcal/mol. | | | |

Table 4. The details of particles defined in dynamics.

|  |  |  |  |
| --- | --- | --- | --- |
| **ID** | **Occupied Volume (Å3)** | **Effective Radius (Å)** | **Net Mass (gr/mol)** |
| A–B-**1** | 336.42 | 4.314505885 | 328.412 |
| A–B-**2** | 331.3 | 4.292506309 | 328.412 |
| A–B-**3** | 337.42 | 4.318776577 | 328.412 |
| A–B-**4** | 337.81 | 4.320439859 | 328.412 |
| A–B-**5** | 335.8 | 4.311853805 | 328.412 |
| A–B-**6** | 339.75 | 4.328694657 | 328.412 |
| A–B-**7** | 341.56 | 4.336368010 | 328.412 |
| A–B-**8** | 338.38 | 4.322868509 | 328.412 |
| A–B-**9** | 339.74 | 4.328652187 | 328.412 |
| B–B-**1** | 452.53 | 4.762696663 | 412.570 |
| B–B-**2** | 455.1 | 4.771695722 | 412.570 |
| B–B-**3** | 456.4 | 4.776234876 | 412.570 |
| A–A-**1** | 225.83 | 3.777730812 | 244.254 |
| A–A-**2** | 226.07 | 3.779068595 | 244.254 |
| A–A-**3** | 227.78 | 3.788572999 | 244.254 |
| A–A-**4** | 226.22 | 3.779904228 | 244.254 |
| A–A-**5** | 226.18 | 3.779681429 | 244.254 |
| A–A-**6** | 220.58 | 3.748226623 | 244.254 |
| A–A-**7** | 224.05 | 3.767779218 | 244.254 |
| A–A-**8** | 226.44 | 3.781129156 | 244.254 |
| A–A-**9** | 225.57 | 3.776280478 | 244.254 |
| B | 223.3 | 3.763570346 | 206.285 |
| A | 111.83 | 2.988752175 | 122.127 |

Table . The calculated Flory-Hugging’s interaction parameter.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | **A** | **B** | **A-A-1** | **A-A-2** | **A-A-3** | **A-A-4** | **A-A-5** | **A-A-6** | **A-A-7** | **A-A-8** | **A-A-9** | **B-B-1** | **B-B-2** | **B-B-3** | **A-B-1** | **A-B-2** | **A-B-3** | **A-B-4** | **A-B-5** | **A-B-6** | **A-B-7** | **A-B-8** | **A-B-9** |
| **A** | 0.00 | 1.59 | 4.95 | 9.07 | 6.00 | 8.96 | 4.23 | 7.94 | 6.68 | 2.80 | 7.61 | 20.75 | 8.78 | 16.05 | 9.89 | 10.76 | 15.58 | 8.46 | 11.62 | 7.77 | 4.21 | 19.98 | 4.52 |
| **B** | 1.55 | 0.00 | 4.82 | 12.38 | 6.12 | 9.55 | 3.98 | 8.62 | 10.13 | 4.16 | 7.05 | 17.25 | 3.27 | 7.30 | 5.55 | 6.74 | 10.81 | -1.59 | 7.65 | 4.47 | 2.53 | 15.69 | 2.73 |
| **A-A-1** | 4.94 | 5.23 | 0.00 | 5.20 | 3.84 | 4.25 | 0.67 | 0.60 | 1.54 | 2.20 | 4.04 | 16.50 | 10.01 | 14.53 | 3.79 | 6.10 | 13.81 | 8.01 | 12.42 | 0.01 | 2.01 | 18.84 | 4.31 |
| **A-A-2** | 9.16 | 12.38 | 5.05 | 0.00 | 2.82 | 1.16 | 2.34 | 1.35 | 1.62 | 5.90 | 3.90 | 20.60 | 19.69 | 23.91 | 14.16 | 12.59 | 20.25 | 17.86 | 16.09 | 3.10 | 2.77 | 26.37 | 12.55 |
| **A-A-3** | 6.16 | 6.22 | 3.68 | 2.87 | 0.00 | 2.65 | -1.70 | 2.41 | 1.75 | 1.87 | 3.62 | 17.12 | 12.38 | 14.95 | 8.40 | 6.25 | 15.10 | 7.06 | 12.28 | 3.78 | 0.79 | 18.46 | 7.51 |
| **A-A-4** | 9.03 | 9.59 | 4.55 | 1.57 | 1.97 | 0.00 | 2.92 | 1.90 | 3.51 | 5.87 | 2.38 | 21.84 | 15.70 | 18.35 | 13.42 | 12.88 | 17.85 | 14.22 | 15.01 | -0.11 | 1.50 | 20.73 | 10.41 |
| **A-A-5** | 4.19 | 3.98 | 0.14 | 2.43 | -1.81 | 2.47 | 0.00 | 2.68 | 2.81 | 0.34 | 2.44 | 16.77 | 6.20 | 10.53 | 7.69 | 5.74 | 9.74 | 7.05 | 6.17 | 2.10 | -0.65 | 11.58 | 2.84 |
| **A-A-6** | 8.01 | 8.58 | 0.19 | 1.37 | 2.14 | 1.83 | 2.70 | 0.00 | 2.83 | 5.85 | 3.36 | 20.72 | 12.02 | 15.29 | 10.53 | 10.39 | 14.71 | 12.10 | 9.75 | 5.99 | 1.41 | 17.45 | 7.41 |
| **A-A-7** | 6.63 | 10.28 | 1.15 | 1.26 | 1.64 | 3.84 | 2.45 | 2.67 | 0.00 | 3.48 | 4.65 | 21.19 | 16.05 | 19.18 | 11.82 | 10.03 | 17.88 | 14.69 | 13.54 | 3.34 | 3.21 | 22.83 | 8.75 |
| **A-A-8** | 2.83 | 3.99 | 2.00 | 5.76 | 1.70 | 5.76 | -0.04 | 5.78 | 3.38 | 0.00 | 4.94 | 16.55 | 7.68 | 12.53 | 7.07 | 6.80 | 12.81 | 6.53 | 11.67 | 4.15 | 2.16 | 18.62 | 4.22 |
| **A-A-9** | 7.83 | 7.08 | 4.27 | 4.62 | 3.92 | 2.22 | 2.35 | 3.40 | 4.69 | 4.56 | 0.00 | 19.73 | 12.35 | 17.23 | 11.38 | 12.12 | 16.88 | 13.00 | 14.07 | -3.68 | 2.88 | 21.14 | 7.85 |
| **B-B-1** | 20.93 | 13.30 | 22.28 | 22.82 | 18.99 | 24.52 | 16.55 | 20.59 | 18.12 | 16.12 | 15.54 | 0.00 | 9.33 | 16.44 | 17.93 | 16.78 | 8.75 | 13.90 | 18.01 | 14.47 | 13.43 | 29.34 | 9.63 |
| **B-B-2** | 8.51 | 4.02 | 9.63 | 19.74 | 12.56 | 15.24 | 7.50 | 12.25 | 15.98 | 7.63 | 13.12 | 6.65 | 0.00 | 2.58 | -5.07 | 4.66 | 4.27 | 2.11 | 7.03 | 5.03 | 4.12 | 14.54 | 2.26 |
| **B-B-3** | 17.94 | 6.02 | 13.12 | 26.10 | 14.56 | 19.06 | 10.19 | 18.30 | 18.70 | 12.58 | 18.68 | 14.09 | 2.36 | 0.00 | 4.34 | -0.03 | 5.73 | 4.07 | 2.39 | 11.04 | 4.17 | 5.71 | 5.79 |
| **A-B-1** | 9.18 | 5.09 | 3.57 | 15.67 | 9.29 | 13.45 | 8.25 | 10.55 | 12.51 | 6.95 | 11.40 | 18.59 | -6.36 | 8.14 | 0.00 | 6.70 | 12.49 | 3.55 | 5.36 | 6.65 | 4.95 | 13.01 | 3.66 |
| **A-B-2** | 10.35 | 6.03 | 5.89 | 12.18 | 6.21 | 12.84 | 5.41 | 10.10 | 10.50 | 6.78 | 12.05 | 16.10 | 3.37 | -2.62 | 6.77 | 0.00 | 2.53 | 2.46 | -0.01 | 9.93 | 3.80 | -3.06 | 5.80 |
| **A-B-3** | 15.72 | 14.35 | 18.77 | 22.63 | 15.62 | 19.20 | 13.16 | 20.76 | 21.31 | 14.68 | 19.18 | 11.92 | 4.84 | 5.44 | 13.03 | 6.86 | 0.00 | 8.75 | -0.44 | 16.72 | 8.81 | 17.79 | 11.79 |
| **A-B-4** | 8.31 | -2.09 | 7.69 | 17.45 | 6.83 | 14.47 | 6.62 | 11.64 | 14.62 | 6.48 | 13.00 | 16.24 | 0.81 | -0.84 | 4.20 | 1.79 | 5.54 | 0.00 | 0.13 | 6.95 | 1.94 | 5.29 | 0.17 |
| **A-B-5** | 11.57 | 6.72 | 12.60 | 14.23 | 13.31 | 14.10 | 5.77 | 9.31 | 13.44 | 11.73 | 14.07 | 15.93 | 3.38 | 0.55 | 4.33 | -1.39 | -0.93 | 0.47 | 0.00 | 9.36 | -1.09 | 3.97 | 6.86 |
| **A-B-6** | 7.93 | 4.36 | -0.42 | 3.41 | 3.91 | -1.08 | 2.21 | 6.26 | 3.72 | 4.47 | -2.99 | 16.88 | 5.34 | 9.97 | 6.26 | 9.85 | 13.17 | 7.62 | 8.89 | 0.00 | -1.44 | 15.53 | 3.06 |
| **A-B-7** | 4.29 | 2.55 | 2.30 | 3.06 | 1.23 | 1.84 | -0.66 | 1.55 | 3.52 | 2.34 | 2.99 | 12.43 | 3.28 | 4.39 | 4.39 | 3.85 | 7.11 | 1.51 | 0.12 | -1.32 | 0.00 | 13.19 | 1.18 |
| **A-B-8** | 20.84 | 14.03 | 19.20 | 30.46 | 15.93 | 20.57 | 10.38 | 18.28 | 21.98 | 18.32 | 20.38 | 28.02 | 12.10 | 12.15 | 11.50 | -4.51 | 13.78 | 1.68 | 3.02 | 12.53 | 13.91 | 0.00 | 11.15 |
| **A-B-9** | 3.94 | 2.74 | 3.64 | 12.24 | 7.31 | 10.15 | 2.92 | 7.50 | 9.09 | 5.17 | 7.99 | 11.84 | 0.20 | 5.59 | 3.37 | 5.03 | 10.70 | -0.07 | 6.79 | 2.75 | -1.40 | 16.24 | 0.00 |

## Appendix B. System Energies and Concentration Profiles

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|  |
| Fig. . Normalized energies (ZPVE included) of system in kcal/mol. |

|  |
| --- |
|  |
|  |
| Fig. . Concentrations versus IBF (top) and NCTA (bottom) |

## References

1. Asgarpour Khansary, M., S. Shirazian, and G. Walker, *Molecular Engineering of Cocrystallization Process in Holt Melt Extrusion based on Kinetics of Elementary Molecular Processes.* International Journal of Pharmaceutics, 2021.