|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Crystal Relaxed | | Crystal Unrelaxed | | ONIOM:UFF | | Constrained | | ONIOM:AMBER | |
|  | SB | BB | SB |  | SB | BB | SB | BB | SB | BB |
| S1 | 3.34 (0.078) | 3.25 (0.058) | 3.64 (0.016) |  | 3.56 (0.028) | 3.46 (0.029) | 3.62 (0.016) | 3.51 (0.030) | 3.54  (0.046) | 3.44 (0.045) |
| S2 | 3.44 (0.018) | 3.38 (2.072) | 3.67 (0.002) |  | 3.59 (0.025) | 3.52 (0.001) | 3.64 (0.116) | 3.55 (0.227) | 3.57 (0.019) | 3.50 (0.006) |
| S3 | 3.47 (2.163) | 3.38 (0.138) | 3.73 (1.133) |  | 3.69 (2.14) | 3.58  (2.11) | 3.73 (2.073) | 3.62 (1.888) | 3.66 (2.169) | 3.55 (2.126) |
| Coupling (TDM) | **0.062** | **0.061** | **0.044** |  | **0.063** | **0.057** | **0.057** | **0.054** | **0.060** | **0.055** |
| Coupling (ATC) | **0.063** |  | **0.045** |  | **0.063** |  | **0.057** |  | **0.059** |  |
| Monomer (s1) | 3.44  (1.19) | 3.35 (1.209) | 3.72 (0.822) |  | 3.67 (1.173) | 3.57 (1.161) | 3.72 (1.183) | 3.61 (1.147) | 3.64 (1.192) | 3.53 (0.178) |
|  |  |  |  |  |  |  |  |  |  |  |
| Monomer REF | 3.65 (1.143) |  |  |  |  |  |  |  |  |  |

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| System | Stacking | Arrangement | J |
| 2HC-1 | Edge-Face | P | 0.061 |
| AP | 0.108 |
| 2HC-2 | Edge-Face | P | 0.033 |
| AP |  |
| 2HC-3 | Edge-Face | P | 0.044 |
| AP | 0.080 |
| 2HC-4 | Edge-Face | P | 0.052 |
| AP | 0.093 |
| 2HC-5 | Face-Face | P | 0.116 |
| AP | 0.148 |
| Edge-Face | AP | 0.028 |
| 2HP-1 | Face-Face | AP | 0.048 |
| Edge-Tail | P | 0.007 |
| AP | 0.002 |
| 2HP-2 | Face-Face | P | 0.021 |
| AP | 0.157 |
| Edge-Edge | AP | 0.063 |
| P | 0.034 |
| 2HP-3 | Face-Face | AP | 0.147 |
| 2HP-4 | Edge-Tail | AP | 0.001 |
| P | 0.005 |
| Face-Face | P | 0.044 |
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