|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Crystal Relaxation | | ONIOM:UFF | | Constrained | | ONIOM:AMBER | |
|  | SB | BB | SB | BB | SB | BB | SB | BB |
| S1 | 3.34 (0.078) | 3.25 (0.058) | 3.56 (0.028) | 3.46 (0.029) | 3.62 (0.0163) |  | 3.54  (0.046) |  |
| S2 | 3.44 (0.018) | 3.38 (2.072) | 3.59 (0.025) | 3.52 (0.001) | 3.64 (0.116) |  | 3.57 (0.019) |  |
| S3 | 3.47 (2.163) | 3.38 (0.138) | 3.69 (2.14) | 3.58  (2.11) | 3.73 (2.073) |  | 3.66 (2.169) |  |
| Coupling | 0.062 | 0.061 | 0.063 | 0.057 | 0.057 |  | 0.060 |  |
| Monomer (s1) | 3.44  (1.19) | 3.35 (1.209) | 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) |  |  |  |  |  |  |  |