**Table SI** Short Ring/[C–H∙∙∙*Cg*(π-ring)] Interactions. [*Cg*–*Cg/*(H∙∙∙*Cg*) Distances in Å and Angles *α, β,* γ in o]

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Cg(I) | | Cg(1) | Cg(2) | Cg(2) | C(I)-H(I) | C20-H20 | C20-H20 |
| Cg(J) | | Cg(2)a | Cg(3)b | Cg(4)b | Cg(J) | Cg(5)c | Cg(6)c |
| Cg-Cg | | 3.677(2) | 3.968(2) | 3.700(2) | C···Cg | 3.487(4) | 3.634(4) |
| Transformed  J-Plane | P | -0.3331 | -0.3801 | -0.3815 | P | 0.1487 | 0.1585 |
| Q | 0.1920 | -0.1808 | -0.1845 | Q | 0.9649 | 0.9575 |
| R | -0.9231 | -0.9071 | -0.9258 | R | 0.2164 | 0.2409 |
| S | 2.0825 | -2.6796 | -2.6637 | S | 12.3496 | 12.4764 |
| α | | 3.0(2) | 2.9(2) | 2.97(17) | H-Prep | -2.57 | -2.56 |
| β | | 17.7 | 25.3 | 16.8 |
| γ | | 18.6 | 28.2 | 19.2 | γ | 1.17 | 23.75 |
| CgI\_Perp | | -3.4856(16) | -3.4958(18) | -3.4943(18) | C-H···Cg | 169 | 150 |
| CgJ\_Perp | | -3.5029(18) | -33.5427(13) | -3.5427(13) | H···Cg | 2.57 | 2.80 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Slippage | 1.117 | 1.0698 | 1.067 | C-H···π | 78 | 77 |

Symmetry codes: a = -x, ½ + y, ½ - z; b = -x, -½ + y, ½ - z; c = ½ - x, ½ + y, z.

The Representations and Definitions

The Representations and Definitions:

Cg(I) = Plane number I (= ring number in () above)

Cg(J) = Center of gravity of ring J (Plane number above)

α = Dihedral Angle between Planes I and J (o)

β = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (o)

γ = Angle Cg(I)-->Cg(J) vector and normal to plane J (o)

or Angle between Cg-H vector and ring J normal

Cg-Cg = Distance between ring Centroids (Å)

CgI\_Perp = Perpendicular distance of Cg(I) on ring J (Å)

CgJ\_Perp = Perpendicular distance of Cg(J) on ring I (Å)

Slippage = Distance between Cg(I) and Perpendicular Projection of CgH-Perp = Perpendicular distance of H to ring plane J

C-H∙∙∙Cg = C-H-Cg angle (o)

C∙∙∙Cg = Distance of C to Cg (Å)

C-H, π = Angle of the C-H bond with the π-plane (i.e.' Perpendicular = 90o, Parallel = 0o)

5-Membered Ring (1) N1 --> C15 --> N2 --> C16 --> C21 -->

6-Membered Ring (2) C2 --> C3 --> C4 --> C5 --> C6 --> C7 -->

6-Membered Ring (3) C16 --> C17 --> C18 --> C19 --> C20 --> C21 -->

9-Membered Ring (4) N1 --> C15 --> N2 --> C16 --> C17 --> C18 --> C19 --> C20 --> C21

5-Membered Ring (5) N3 --> C22 --> N4 --> C23 --> C28 -->

9-Membered Ring (6) N3 --> C22 --> N4 --> C23 --> C24 --> C25 --> C26 --> C27 --> C28 -->