Isolation of 1,4–Li_2–C_6H_4 and its reaction with [(Ph_3P)AuCl]

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Received (in XXX, XXX) 1st January 2007, Accepted 1st January 2007
First published on the web 1st January 2007
DOI: 10.1039/b000000x

Supplementary Material

Packing diagrams for **2a–d** generated using Mercury**.**

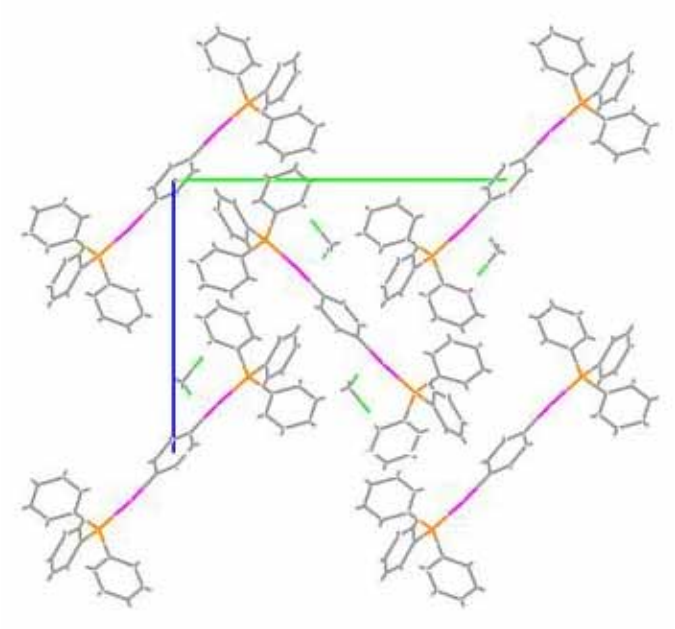

Figure S1: Packing of **2a** viewed down the a axis.

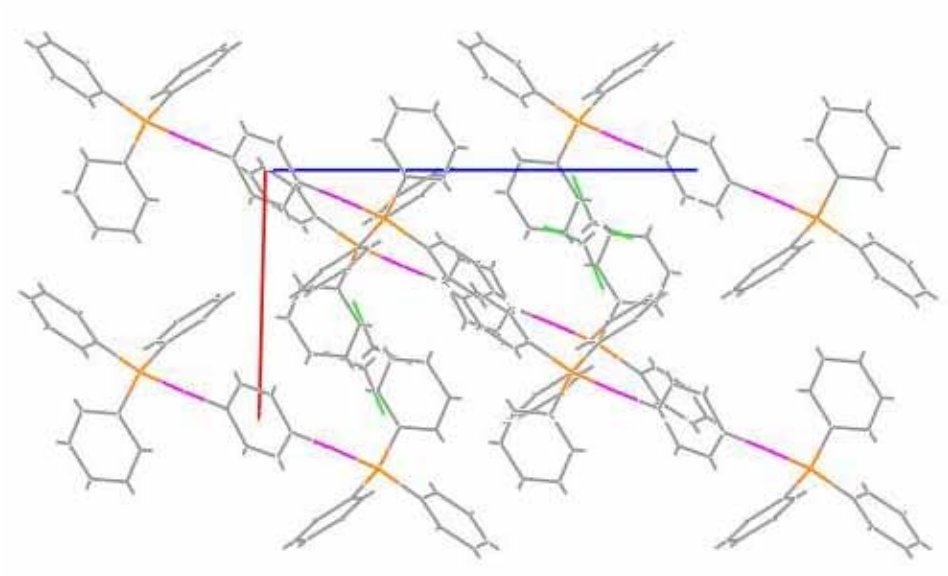

Figure S2: Packing of **2a** viewed down the b axis.

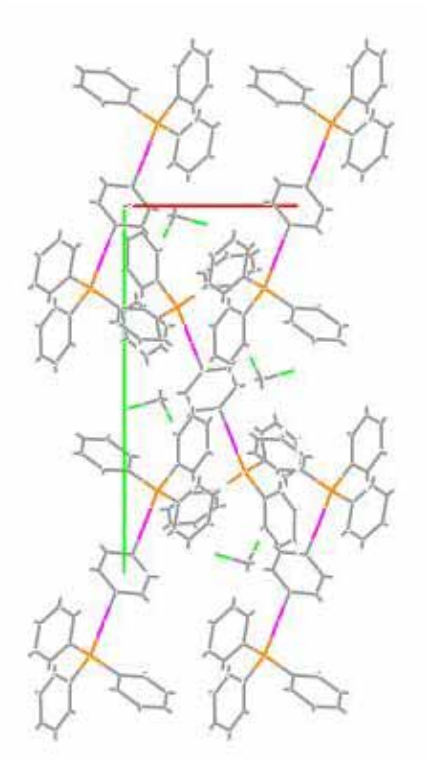

Figure S3: Packing of **2a** viewed down the c axis.

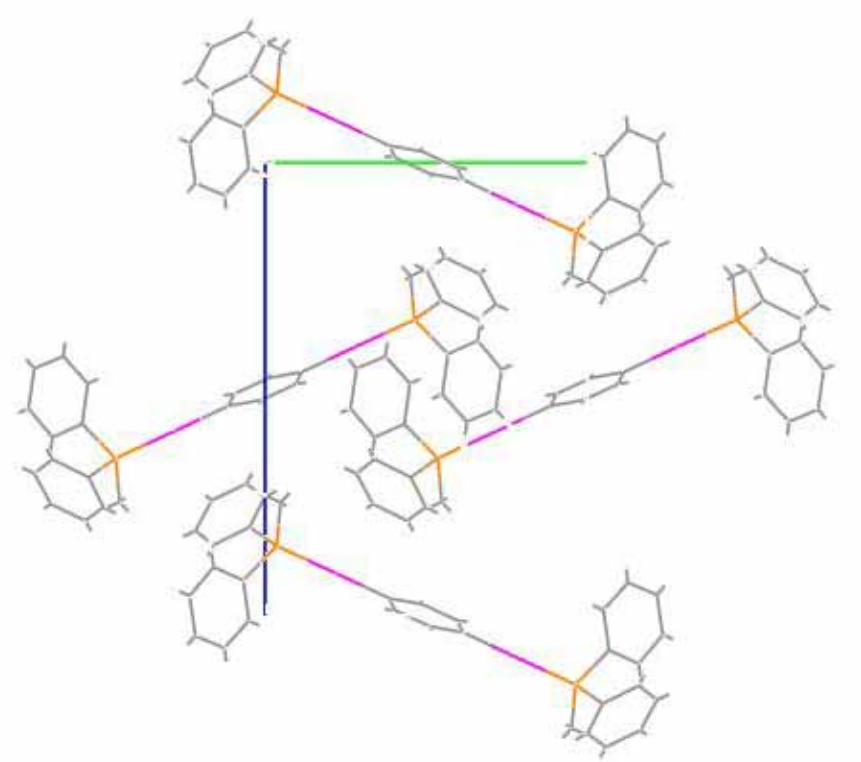

Figure S4: Packing of **2b** viewed down the a axis.

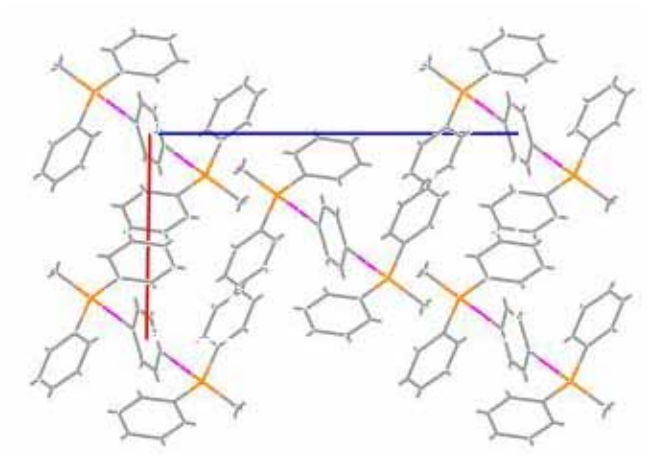

Figure S5: Packing of **2b** viewed down the b axis.

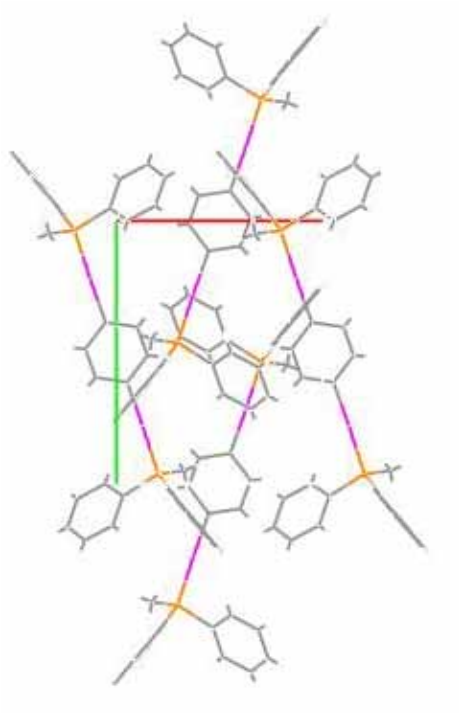

Figure S6: Packing of **2b** viewed down the c axis.

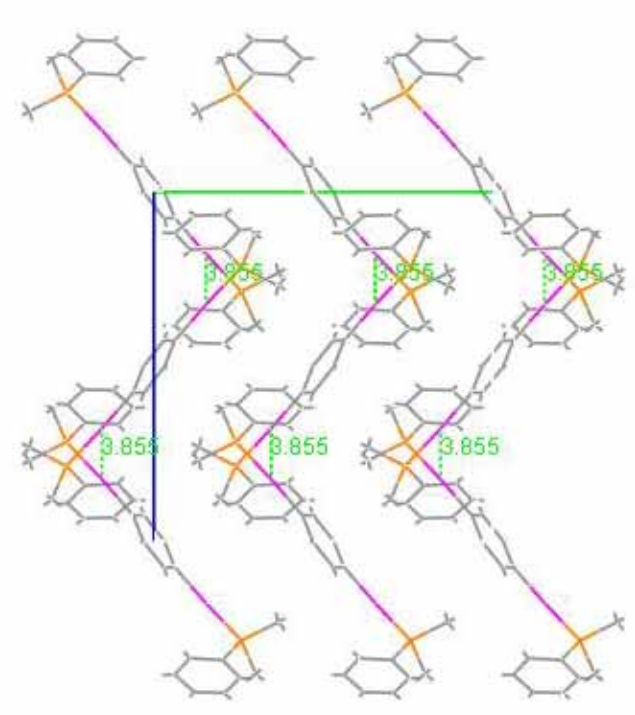

Figure S7: Packing of **2c** viewed down the a axis.

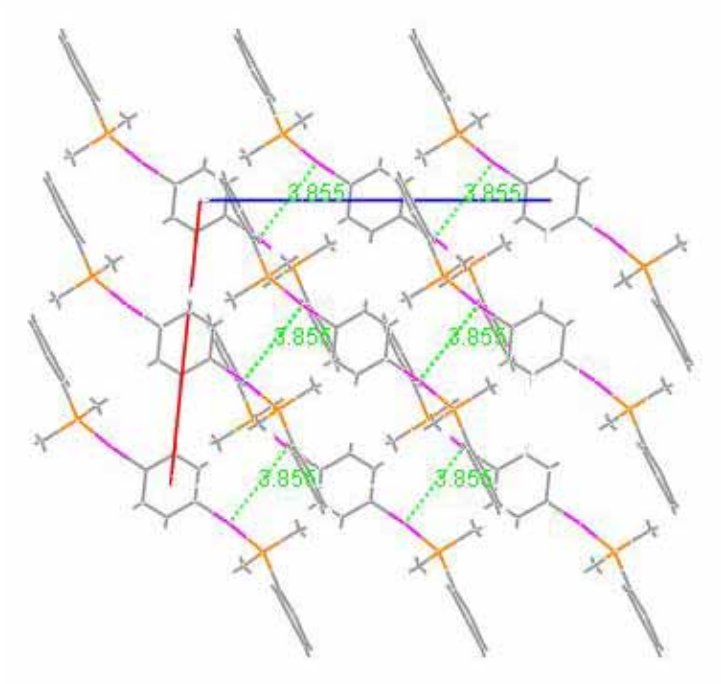

Figure S8: Packing of **2c** viewed down the b axis.

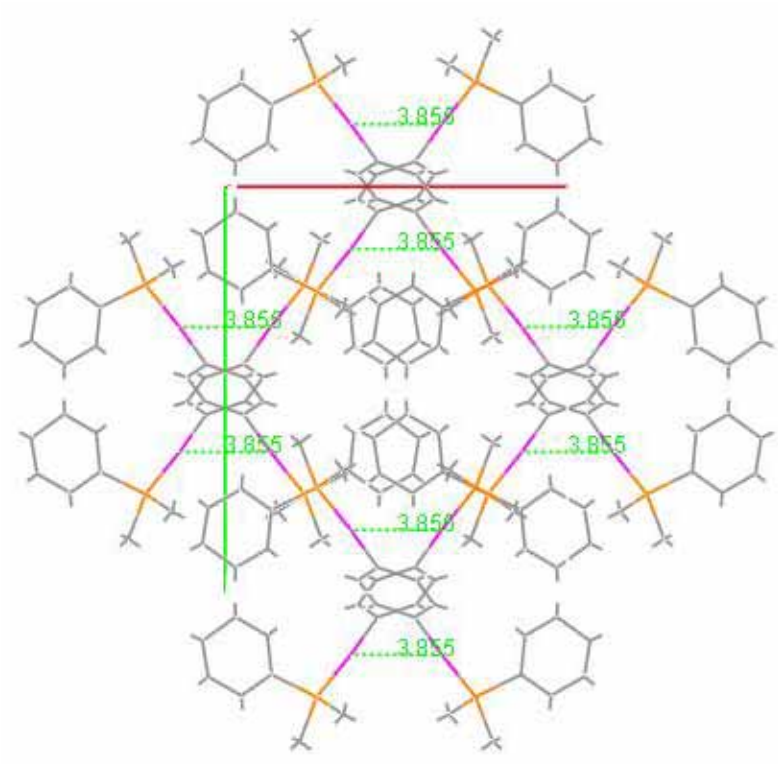

Figure S9: Packing of **2c** viewed down the c axis.

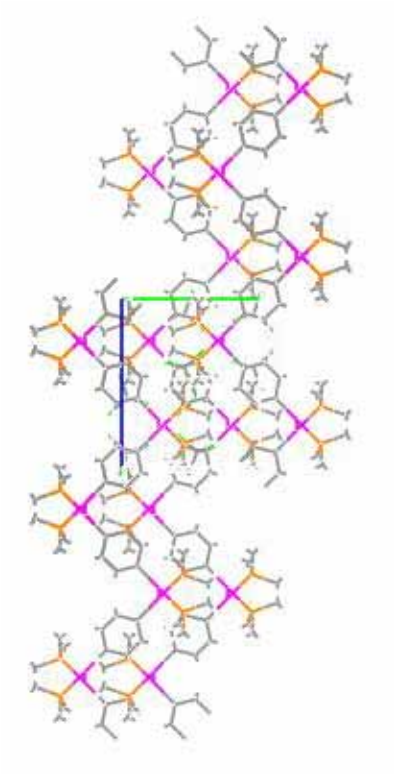

Figure S10: Packing of **2d** viewed down the a axis.

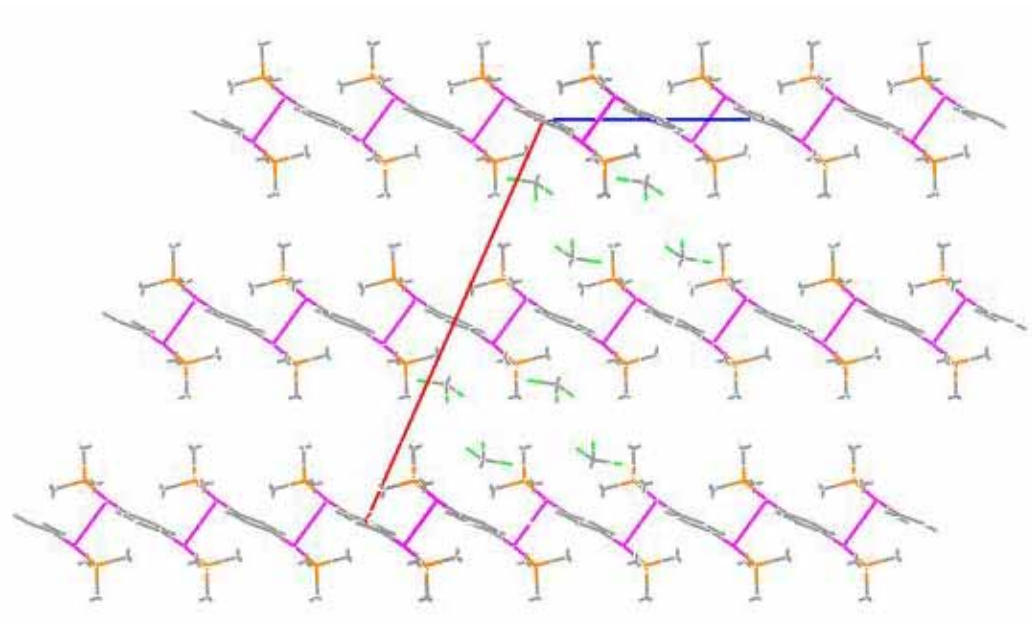

Figure S11: Packing of **2d** viewed down the b axis.

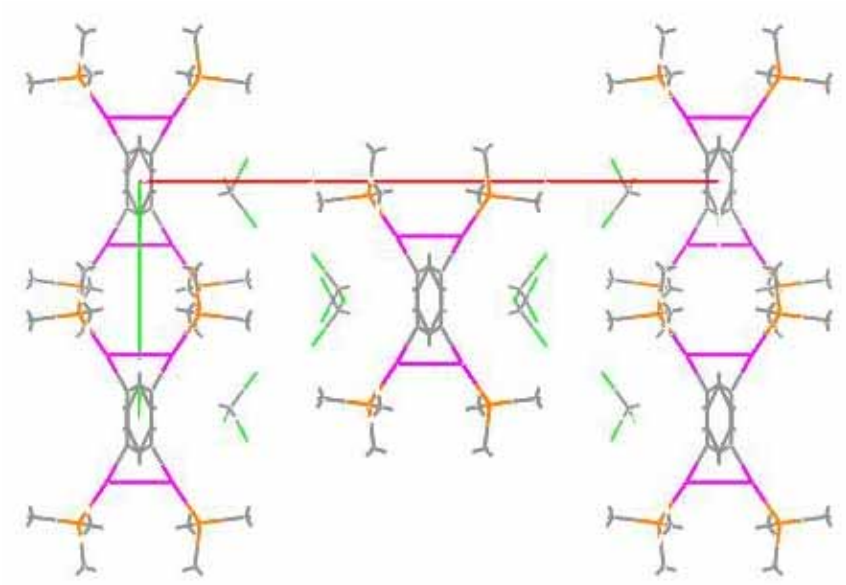

Figure S12: Packing of **2d** viewed down the c axis.

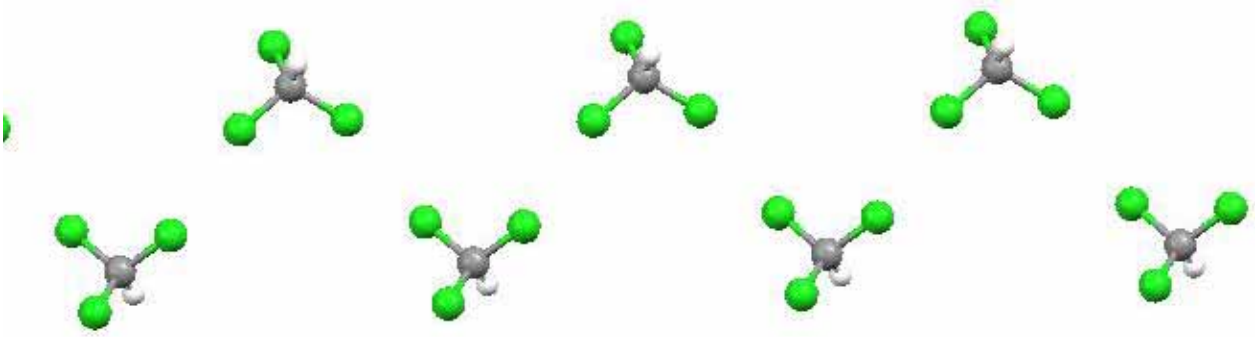

Figure S13: Representation of the infinite $CHCl_3$ chain linked by Cl···Cl interactions in **2d**: Lengths (Å); angles (°) C(7)–Cl(2) 1.748, Cl(2)···Cl(1) 3.316; C(7)–Cl(2)–Cl(1) 153.2, Cl(2)–Cl(1)–C(7) 156.8, Cl(1)–C(7) 1.737, Cl(2)–C(7)–Cl(1) 110.3 .

Mercury generated diagrams illustrating the aryl interactions with the diaurated rings in **2a – 2d**

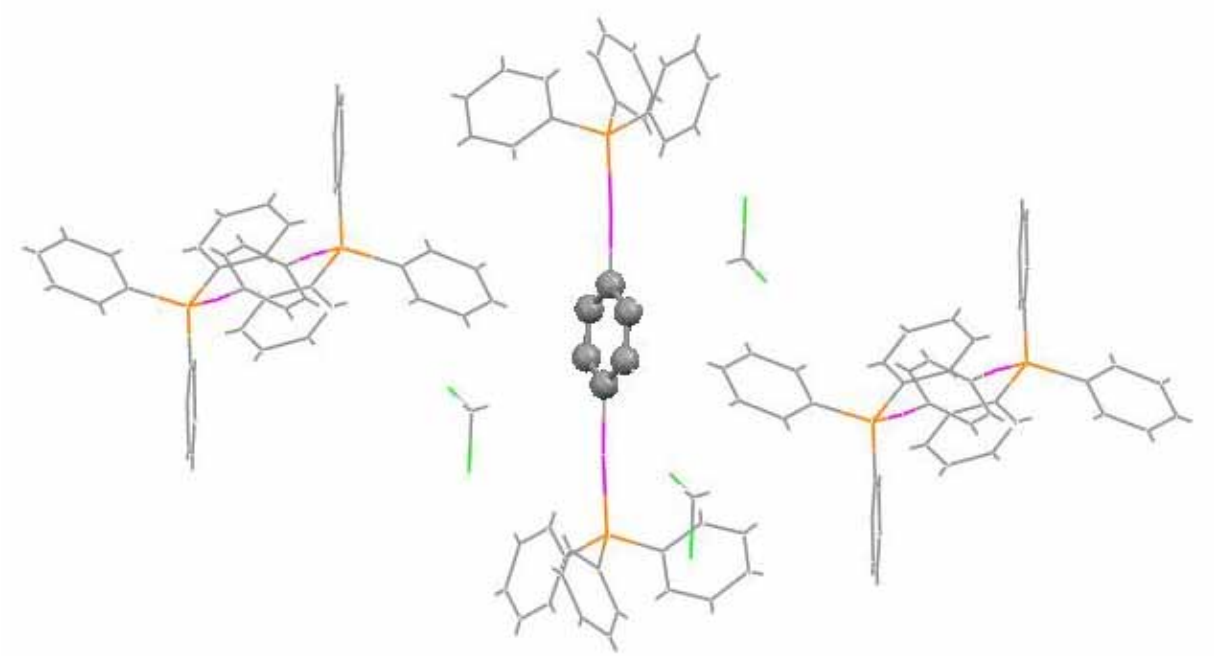

Figure S14: Diaurated ring packing interactions in **2a**.

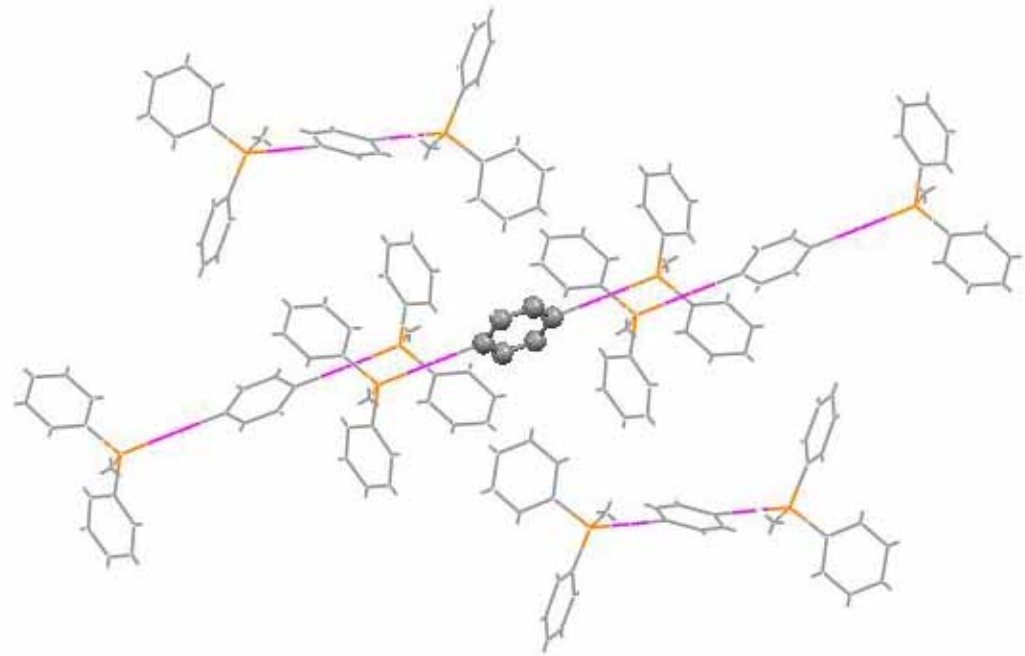

Figure S15: Diaurated ring packing interactions in **2b**.

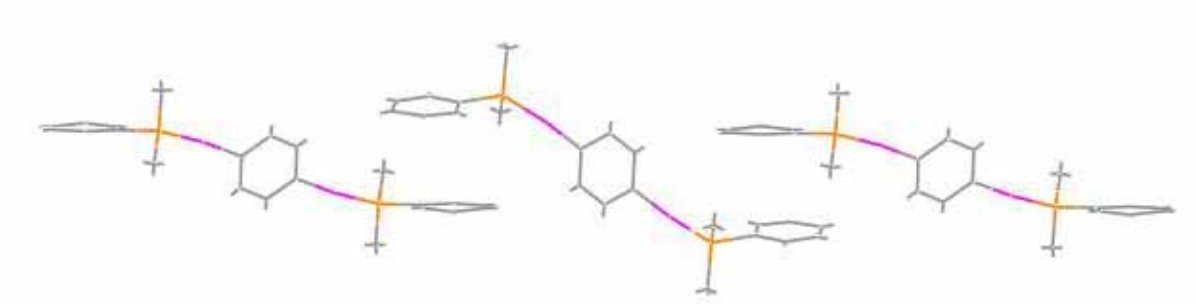

Figure S16: Diaurated ring packing interactions in **2c**.

Note: There are no aromatic π-interactions in **2d**. The diaurated ring interacts instead with two chloroform C–H bonds Figure 10 main text.

CCDC database searches.

Search parameters for the CCDC database search relating to CAuL and XAuL (X = halogen) with scatter plots that combine all data. Note how the combined scatter plots mirror that presented for the [ClAuL] system in the main text and further tighten the clusters.

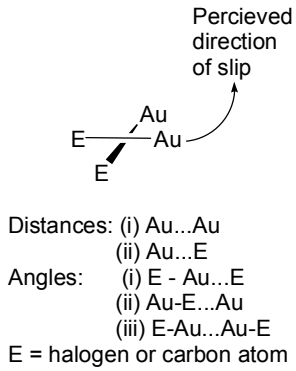

Figure S17: Illustration of the search parameters.

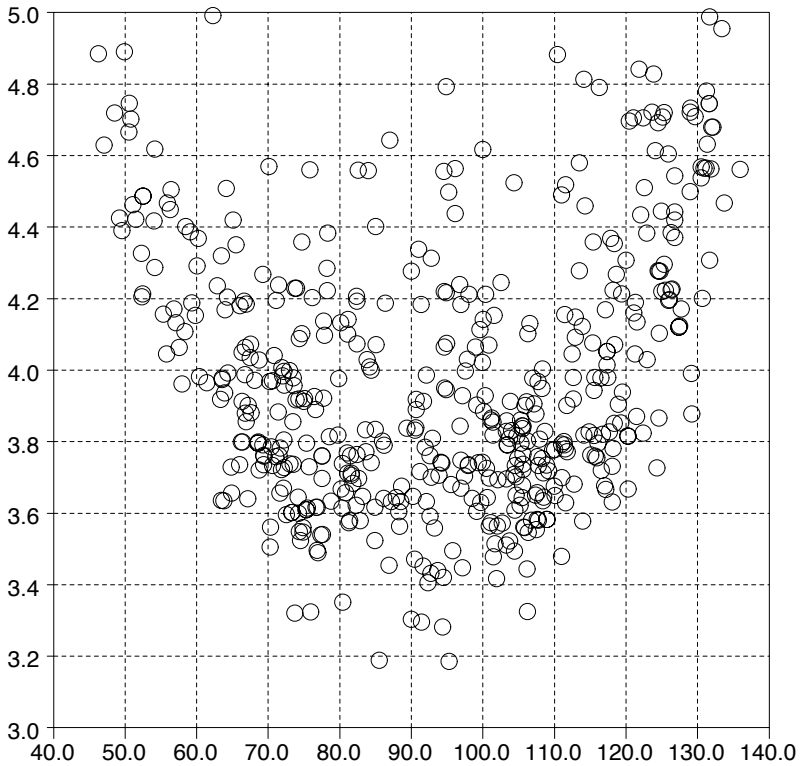

Figure S18 Scatter plot of E–Au···E angle versus Au···E distance.

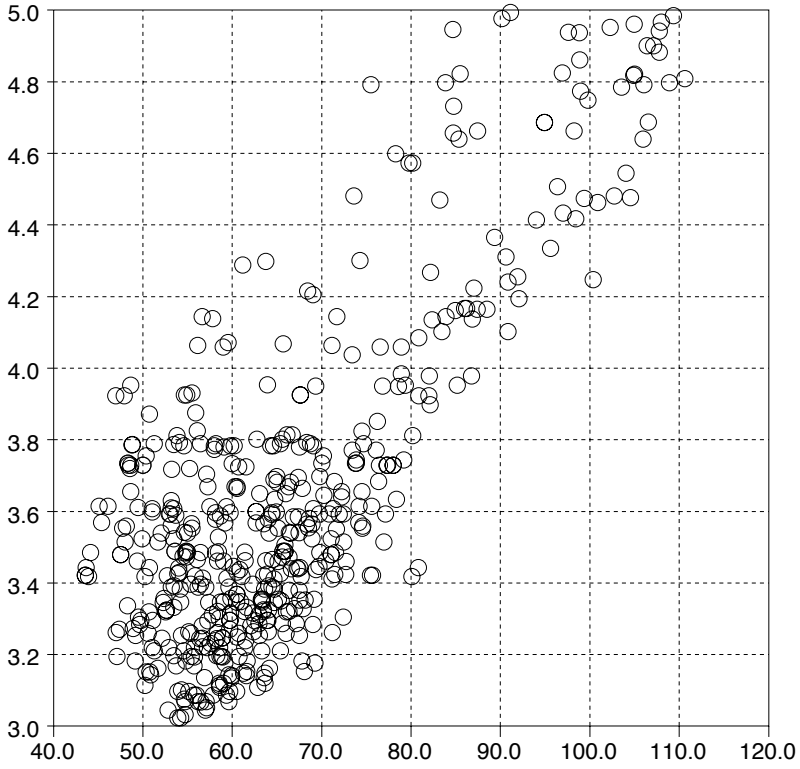

Figure S19 Scatter plot of Au–E···Au angle versus Au···Au distance.

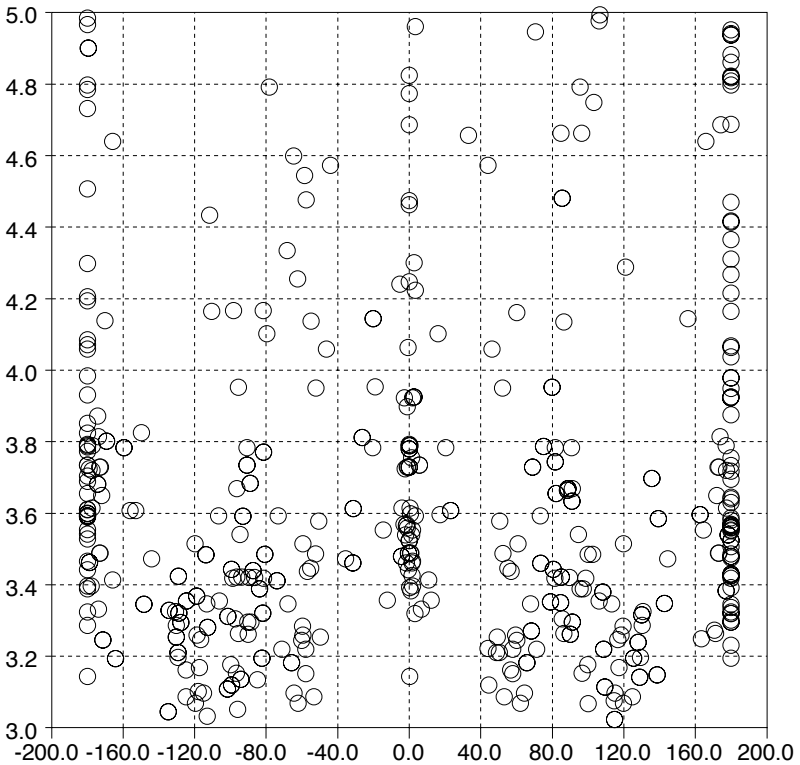

Figure S20 Scatter plot of E–Au···Au–E torsion angle versus Au···Au distance.

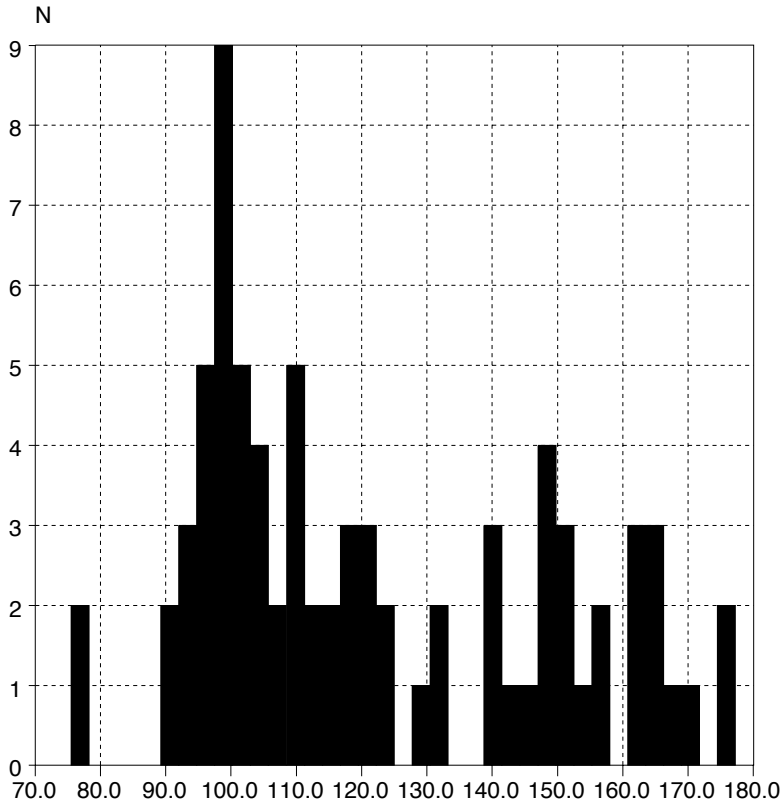

Figure S21 Histogram representation of the angles observed for the C–Cl–M search.