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Sixfold phenyl embraces with substituted phenyl in PPh_3 †

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Examination of the Cambridge Structural Database reveals that Ph_4P^+ cations and PPh_3 ligands in crystals associate through phenyl···phenyl non-bonded interactions which are attractive, concerted, and widespread. The strongest and most prevalent interaction is the energetically favourable sextuple phenyl embrace (6PE) in which there are six concerted edge-to-face (EF) phenyl–phenyl interactions. We have questioned the extent to which substitution on one or more phenyl rings would interfere with XPh_3 as a 6PE tecton. Substitution in the 4-position of Ph does not interfere with the formation of 6PEs. Substituents in other positions can be out of the interaction domain and not affect the 6PE, or if small like methyl they can form 6PE in which some of the EF motifs are replaced by methyl-to-face (MF). In some cases the substitution of Ph destroys the 6PE. Perfluorination, in $(C_6F_5)_3PPtCl_2PtP(C_6F_5)_3$, does not obstruct occurrence of chains of intermolecular 6PE. Hetero-molecular 6PE occur, and could be deployed for generation of acentric crystals. The cation $(o\text{-}NH_2C_6H_4)Ph_3P^+$ can form chains of embraces analogous to the ZZI6PE, which is prevalent for Ph_4P^+.

Introduction

The occurrence of multiple phenyl embraces between PPh_3 moieties is now known to be widespread. The most prevalent embrace is the six-fold phenyl embrace (6PE), where there is a concerted cycle of six edge-to-face (EF) phenyl···phenyl interactions.[1–3] The 6PE is $(EF)_6$. This embrace is attractive, even between Ph_4P^+ cations.[4,5] In fact, the formation of extended motifs incorporating the 6PE can dominate a crystal structure, to the extent that it allows trapping of unusual ions not observable in solution.[6]

The question arises as to whether substitution on the phenyl ring will disrupt the formation of the 6PE. For each ring on the PPh_3 moiety there are five possible substitution positions, numbered 2–6. Substitution in the 2-position is locally equivalent to that in the 6-position, with similar equivalence for substitution in the 3- and 5-positions. However, these pairs of substitution positions become inequivalent when two PPh_3 approach in embrace formation, and it is necessary to develop notation to describe this. We have adopted the following definitions to differentiate substitution locations for molecules and for supramolecular motifs. For molecular structures, substitution will be denoted *ortho* (*o*), *meta* (*m*), or 4 (for which there is no ambiguity). In an embrace, the numbered positions 2, 3 will correspond to *o*, *m* positions *between pairs of P atoms in the interaction domain*, while the higher numbers 6, 5 represent *o*, *m* substitution away from the interaction domain. This convention for number of ring positions in a 6PE is illustrated in Fig. 1. The hydrogen atoms in the 2- and 3-positions (H2, H3) are involved in the EF interactions of the 6PE, and are directed approximately towards C3 and C4. Substitution of H2, H3 would clearly affect 6PE formation, but as we shall see, embraces of compositions different to $(EF)_6$ are possible, and are still energetically favourable.

Results

There are various ways in which the PPh_3 group can bear substituents. (i) Mono substitution on each phenyl ring. (ii) Mono substitution on one phenyl ring only. (iii) Substitution in more than one position on one ring, or on all rings. (iv) Substitution on one participating partner, but not the other.

We will show that there are examples of most of these possibilities and that association of groups can still take place. The size of the substituent varies from a single F atom, through methyl groups to larger and bulkier groups such as $CH_2N(CH_3)_2$. In addition, the substituent can act as a link to other parts of the molecule and can participate in chelation to the metal atom of $MPPh_3$ moieties. We used the Cambridge

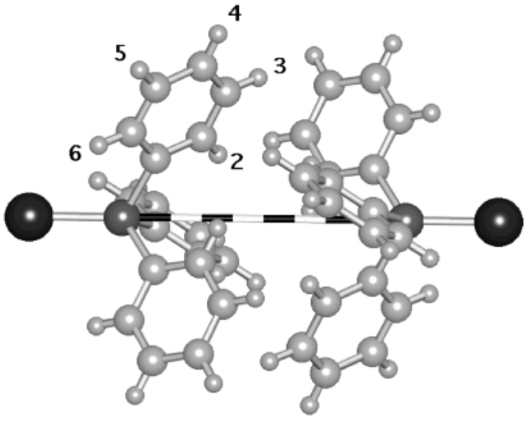

Fig. 1 A typical 6PE, showing the convention for numbering positions on the phenyl rings. Positions 2 and 3 correspond to *o*, *m* positions *between pairs of P atoms in the interaction domain*, while 6 and 5 represent *o*, *m* substitution away from the interaction domain. The 4-, 5- and 6-positions do not interfere with the 6PE. In this and all subsequent figures, black and white rods link the P atoms involved in the embrace.

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† Electronic supplementary information (ESI) available: the 6PE formed in [ZUFJAL]. See http://www.rsc.org/suppdata/dt/b0/b003559i/

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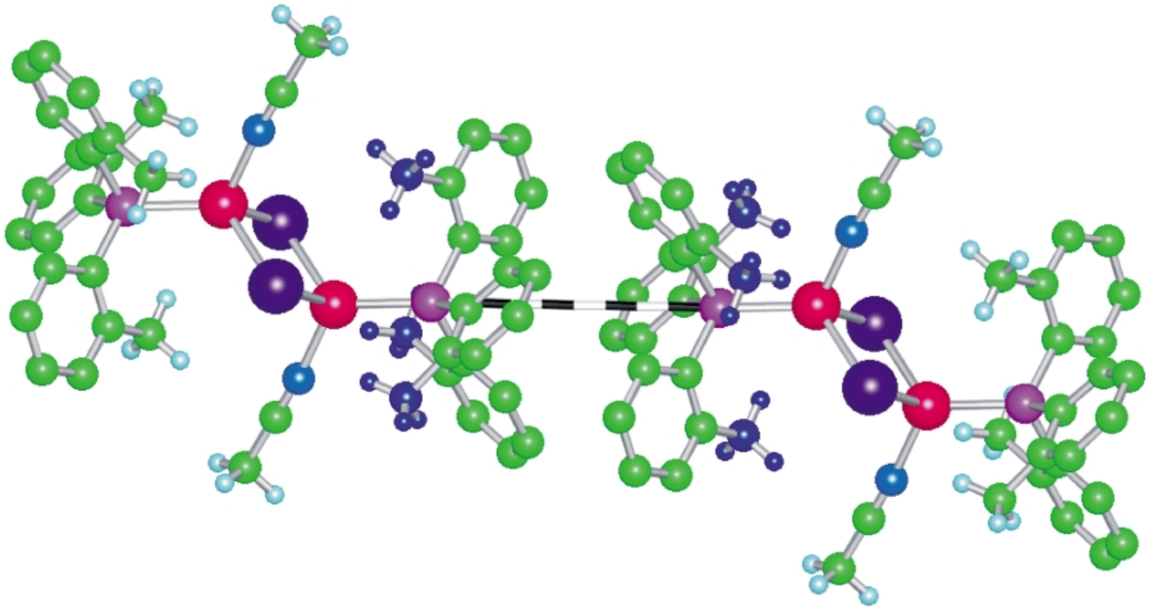

Fig. 2 The structure, $(o\text{-}CH_3C_6H_4)_3P[(CH_3CN)Cu(\mu\text{-}I)_2Cu(NCCH_3)]P(o\text{-}CH_3C_6H_4)_3$ [LEJYII], illustrating a 6-substituted 6PE. The methyl substituents on the phenyl rings taking part in the 6PE have been coloured blue and are clearly oriented away from the 6PE zone. All but the methyl hydrogen atoms have been omitted for clarity.

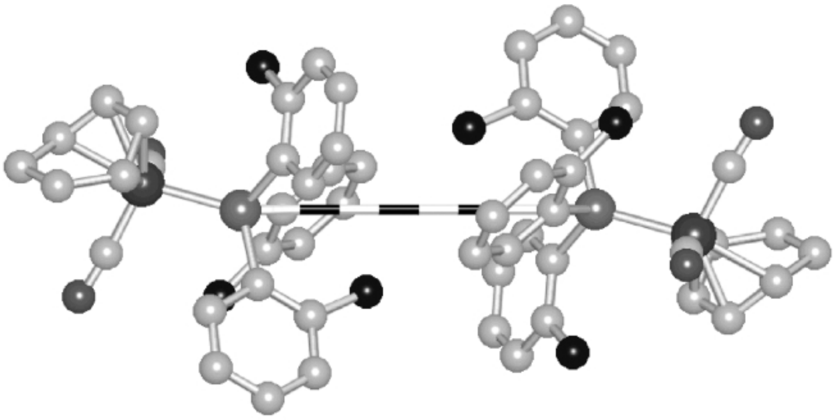

Fig. 3 The interaction zone in $[(o\text{-}CH_3C_6H_4)_3P]Fe(CO)_2L$ ($L = \eta^4$-cyclohexadiene) [JIVDOH]. The methyl carbon atoms are black, clearly illustrating that there are two lying in the interaction zone and four directed away. All hydrogen atoms are omitted.

Structural Data Base (CSD, October, 1999, v5.18)[7,8] to locate examples of substituted PPh_3 groups. We then investigated the possibility of 6PE formation, applying search criteria similar to those previously established for unsubstituted PPh_3 groups, namely $P\cdots P < 8$ Å, and both distal $C\text{–}P\cdots P$ angles about 160–180°. For those examples with no distal atom on P, the six $C\text{–}P\cdots P$ angles are all <70°.

These definitions were used to investigate the possible existence of 6PE for substituted groups. The region between the P atoms for each instance fulfilling the criteria was inspected to determine the nature of the interactions occurring.

o-Substituted PPh_3

A search of the CSD revealed 66 structures with a substituent in one *ortho* position of each ring of PPh_3. Of these, the 6PE criteria were fulfilled in 28 cases. 24 of these examples had CH_3 substituents, while the remaining four had Pr^i, $P(CH_3)_2$, $P(N(CH_3)_2)_2S$ and CHO. Fig. 2 illustrates one such substituted 6PE (in the structure $(o\text{-}CH_3C_6H_4)_3P[(CH_3CN)\text{-}Cu(\mu\text{-}I)_2Cu(NCCH_3)]P(o\text{-}CH_3C_6H_4)_3$ with CSD refcode [LEJYII]) where all substituents are located away from the edge-to-face phenyl interaction zone, so this is named 6-substitution, $(6\text{-})_6$.

Fig. 3 shows the one example, $[(o\text{-}CH_3C_6H_4)_3P]Fe(CO)_2L$ ($L = \eta^4$-cyclohexadiene) [JIVDOH] with *o*-substitution where there are substituents in the interaction zone. Two of the six phenyl rings have 2- as distinct from 6-substitution so this mode of substitution is labelled $(2\text{-})_2(6\text{-})_4$. The $P\cdots P$ distance is longer than most at 7.95 Å, accommodating the additional bulk of the methyl group. This is not a 6PE, because there are no EF motifs. The C atoms of the 2-methyl groups are 4.1–4.5 Å from the C atoms of a phenyl ring on the other molecule, giving rise to a methyl···face (MF) interaction.[9] A sample of 500 structures from the CSD revealed that when a methyl group is located over the centre of a phenyl ring, the mean $C_{methyl}\cdots C_{phenyl}$ distance is about 4 Å. The $C_{methyl}\cdots C_{phenyl}$ distances here indicate that the MF motif is not optimum, but as we shall see from energy calculations, the interaction is still attractive. The 2-substitution has destroyed the $(EF)_6$ of the 6PE, replacing it by $(MF)_2$.

m-Substituted PPh_3

The CSD contains 28 structures with a substituent in one *meta*-position in each ring of PPh_3. Of these, the 6PE motif could be identified in six cases, all with a methyl substituent. Three of these six structures have the substituent pattern $(3\text{-})_2(5\text{-})_4$, while the other three structures are (3-)$_4$(5-)$_2$. An example of the (3-)$_2$(5-)$_4$ configuration, [JAYCER], [(*o*-$CH_3C_6H_4$)$_3$PO][4-$MeC_6H_4SO_2NH_2$] is shown in Fig. 4. Two of the EF aryl interactions are replaced by methyl···face interactions (MF), but a concerted cycle of interactions is retained. The sequence of local interactions around the cycle is EF, EF, MF, EF, EF, MF, so, rather than being termed a 6PE (or (EF)$_6$), this motif could be considered to be (EF)$_4$(MF)$_2$. The shortest $C_{methyl}\cdots C_{phenyl}$ distance is 3.67 Å. The orientation of the C_{phenyl}–C_{methyl} bond to the plane of the phenyl face towards which it is directed indicates that one or two, but not three hydrogen atoms are involved in the interaction.‡[9]

An example of (3-)$_4$(5-)$_2$ substitution and embrace formation is shown in Fig. 5 for the structure (*m*-$CH_3C_6H_4$)$_3$P[ClCu(μ-L)$_2$CuCl]P(*m*-$CH_3C_6H_4$)$_3$ (L = 2-benzimidazolethione) [KUTSIB]. As for [JAYCER] above, the local interactions occurring between the six aromatic rings are a combination of EF and MF, as (EF)$_2$(MF)$_4$. The shortest $C_{methyl}\cdots C_{phenyl}$ distances are 3.54 and 3.62 Å for the two independent methyl groups.

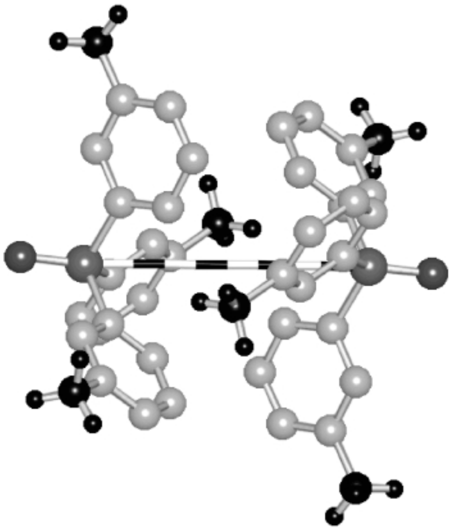

Fig. 4 The structure [(*o*-$CH_3C_6H_4$)$_3$PO][4-$MeC_6H_4SO_2NH_2$] [JAYCER], illustrating (3-)$_2$(5-)$_4$ substitution and the formation of a (EF)$_4$(MF)$_2$: both 3- and 5-CH_3 are coloured black.

4-Substituted PPh_3

A search of the CSD revealed 105 crystal structures with a substituent in the 4-position of each ring of PPh_3. 28 of these structures incorporated the 6PE motif. This frequency of occurrence of the 6PE is similar to the 30% found for unsubstituted PPh_3 groups in $MPPh_3$ compounds.[1,3,10] The substituents in the structures containing 6PE were CH_3 (×17), OCH_3 (×4), F (×3), Cl (×1), SO_3 (×2) and $N(CH_3)_2$ (×1). The 4-position on a phenyl ring is not involved in 6PE formation. This is clear from Fig. 6, where the bulky $N(CH_3)_2$ groups in the 4-positions of the structure [{4-$(CH_3)_2NC_6H_4$}$_3$P]AuCl [YAKMEC] are located around the 6PE, but do not impede its formation.

There are many structures in the CSD which contain two, three or five substituents on each ring of a PPh_3 moiety. Those with two substituents have them in both *o*-positions, or both *m*-positions, while tri-substituted phenyl rings use the *o*- and 4-positions. There are no examples of 6PE (or analogous embrace) formation with these compounds.

Pentasubstituted compounds (8 examples) are all fluorinated. Among these, there is one example of 6PE formation (although it is slightly offset) in [$(C_6F_5)_3P$]$_2Cl_2$Pt [VUBRIT], shown in

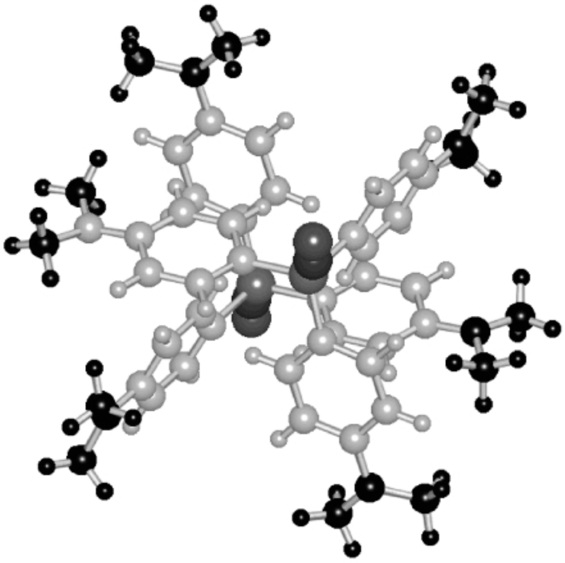

Fig. 6 View almost along the pseudo threefold axis of the 6PE of [{4-$(CH_3)_2NC_6H_4$}$_3$P]AuCl [YAKMEC], where the 4-substituents are large $N(CH_3)_2$ groups (coloured black). The substituents overhang the periphery of the embrace and so do not influence its formation.

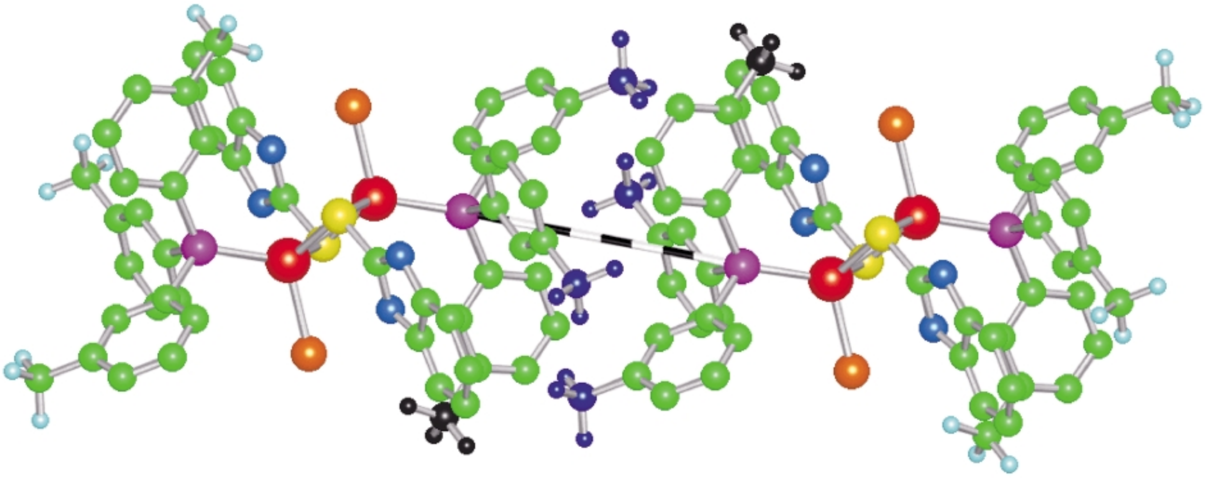

Fig. 5 The (3-)$_4$(5-)$_2$ substitution in (*m*-$CH_3C_6H_4$)$_3$P[ClCu(μ-L)$_2$CuCl]P(*m*-$CH_3C_6H_4$)$_3$ (L = 2-benzimidazolethione) [KUTSIB], and the modified 6PE formed by this molecule. The 3-methyl substituents are blue, while those in the 5-position are black. The central motif is (EF)$_2$(MF)$_4$. The motif is repeated at each end of the molecule leading to a chain structure in the crystal. The overall structure is enhanced by the occurrence of an intramolecular offset face-to-face (OFF) interaction involving the benzimidazole ring.

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‡ We refrain from making definitive comment about H_{methyl} positions, as these are frequently not experimental but included in crystal structures at calculated positions, often with conformational ambiguity for $CH_3C_6H_4$.

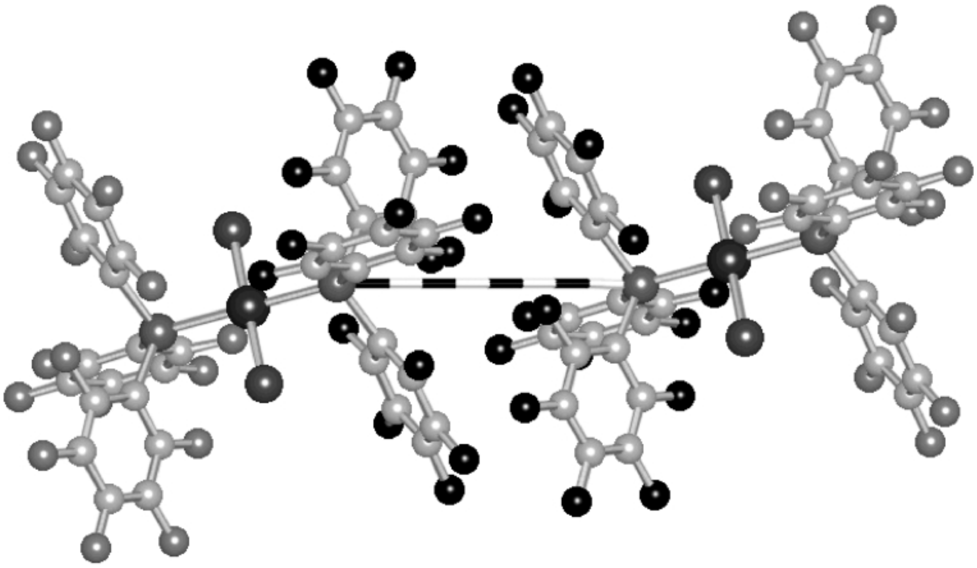

Fig. 7 The 6PE formed by the pentasubstituted compound $[(C_6F_5)_3P]_2Cl_2Pt$ [VUBRIT]. The F atoms of the 6PE have been highlighted black. The symmetrical nature of the molecule leads to formation of chains of embraces.

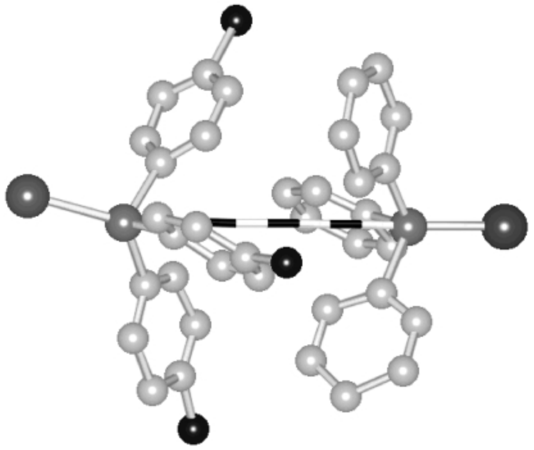

Fig. 8 The unsymmetrical 6PE formed by $[\{(4\text{-}CH_3C_6H_4)_3P\}_2\text{-}Re(AuHPPh_3)_4][BPh_4]$ [GACTAF], highlighted by the black and white rod linking the P atoms. The three 4-methyl groups on the left-hand partner are coloured black. Most of the molecular structure has been omitted for clarity, but the formation of unsymmetrical 6PE at both ends of the molecule generates chains of cations in the crystal structure.

Fig. 7. So far, we have only given examples of 6PE formed by compounds where the three phenyl rings have identical substitution and the two molecules forming the motif are the same substituted PPh_3 group. In $[\{(4\text{-}CH_3C_6H_4)_3P\}_2\text{-}Re(AuHPPh_3)_4][BPh_4]$ [GACTAF], there is 6PE formation which is unsymmetrical in the sense that one partner in the 6PE has three 4-substituted phenyl rings while the other has none (Fig. 8). Both ends of the molecule participate in this type of hetero-molecular embrace, leading to chains of cations in the crystal structure. We note that this molecule with different ligands could have associated with two different symmetrical 6PE, but used one unsymmetrical 6PE. As anticipated for a molecule so intensely covered with aromatic rings, there is much intramolecular aryl···aryl interaction. The $[BPh_4]^-$ counter-ion is disordered (a relatively rare phenomenon), indicating that its orientation is inadequately fixed by phenyl···phenyl forces.

There are many examples in the CSD where substitution occurs on only one ring of PPh_3. Some of these compounds also illustrate examples of 6PE formation. As noted above, if these substituents are in the 4-position, they do not impede 6PE formation. In other instances of unsymmetric substitution, the substituent is generally (but not always) in the 6-position and therefore out of the interaction zone.

Frequently, the 6-position substitution is part of a chelate ring, so that these compounds have a tied-back phenyl ring. Despite this, 6PE formation is still prevalent among these compounds. Most of them have either a five- or six-membered chelate ring. Two examples are shown in Fig. 9.

As is common with "data-mining" of this type, some interesting and beautiful structures come to light. We will conclude with three examples which include substituted PPh_3 groups involved in 6PE formation.

The first shows a combination of multiple phenyl embrace with hydrogen bonding. The compound, $[(m\text{-}COOHC_6H_4)\text{-}(Ph)_2P]_2PtCl_2\cdot 2H_2O$ [ZUFJAL] forms a good 6PE, and in addition, the 5-COOH substituent (away from the interaction zone of the 6PE) forms a hydrogen bonded dimer with another molecule (dashed red lines in Fig. 10). As is common for highly phenylated molecules, there are intramolecular offset face-to-face (OFF) phenyl···phenyl interactions.

Close inspection of the conformation of the PPh_3 group in ZUFJAL shows it to be approximately that of an orthogonal flipper. This conformation, which we have defined previously,[10] does not have all torsion angles for the three phenyl rings approximately equal, as would be expected for a rotor conformation. Instead, the group (ignoring the carboxyl substituent) has approximate mirror symmetry. Despite this, it is still possible for groups with this geometry to associate in pairs in a sixfold phenyl embrace: details are presented in Supplementary Information Fig. S1.

We have previously shown that the 6PE can be employed in the HA6PE array (the hexagonal array of 6PE) in a wide variety of compounds with threefold symmetry.[11,12] The array has been successfully used to trap anions which do not exist in solution.[6] There are three instances of HA6PE crystal lattice formation with molecules containing substituted PPh_3 groups. They are: [KEPMIZ] $[(6\text{-}CH_3C_6H_4)_3P]AuCl$, [KIFSUN] $[(6\text{-}CH_3C_6H_4)_3P]AlCl_3$ (both of which have the substituent outside the 6PE interaction zone and therefore labelled 6- rather than 2-) and [CANTEQ] $(4\text{-}CH_3C_6H_4)_3P$. In all three, the six-membered ring of lateral P···P interactions is nearly planar.

Finally, there is in the CSD a rare example of a substituted Ph_4P^+ cation. One ring in the cation of structure $[(o\text{-}NH_2C_6H_4)(Ph)_3P]_2[NiCl_4]$ [YABYUV] has an amino substitu-

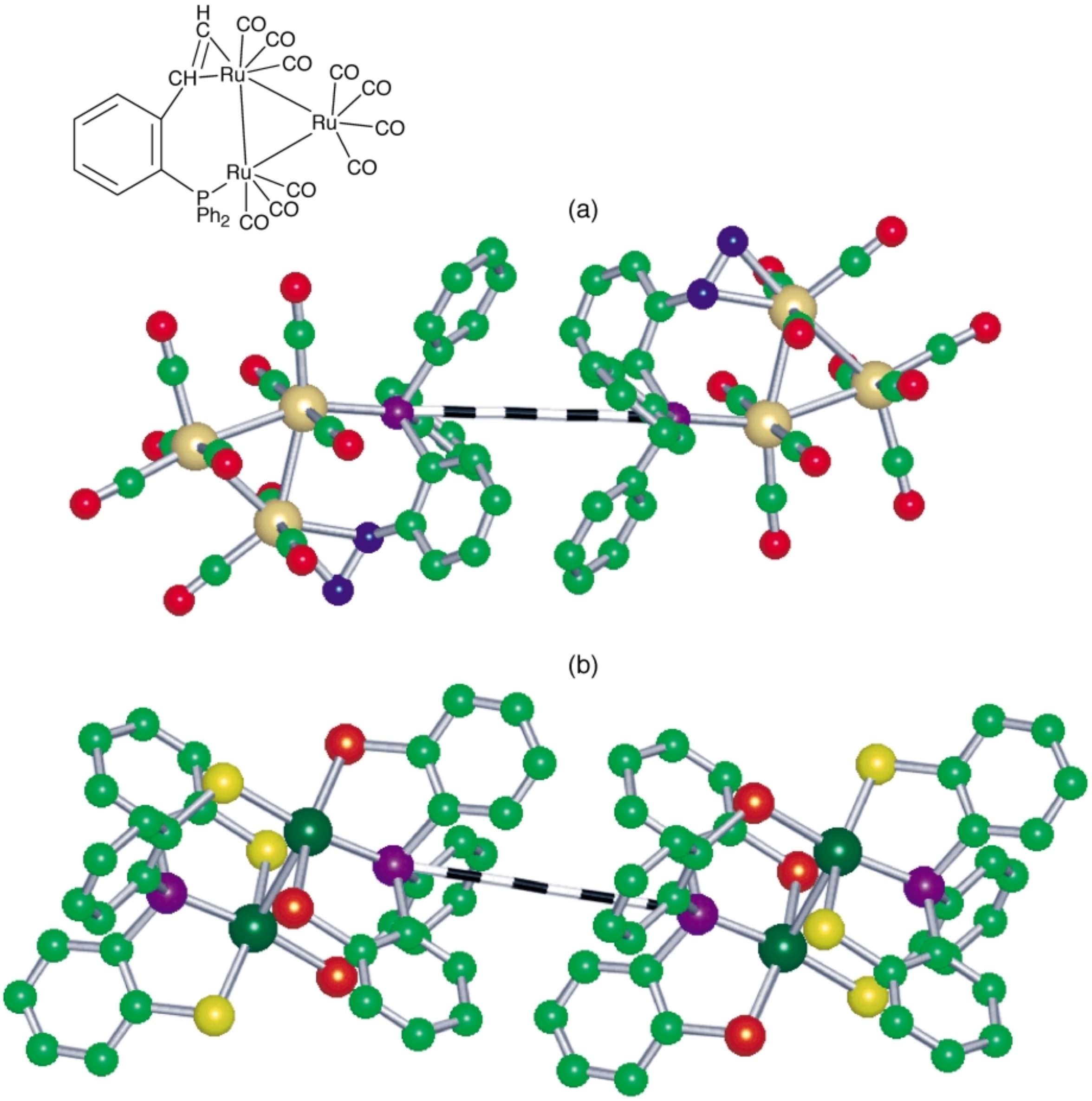

Fig. 9 Tied-back substitution in 6PEs. The bridging 6-substituents are coloured blue. (a) 6PE formed by [BUBZIH] (the formula for [BUBZIH] is shown in the top left corner). The η^2-styryl group chelates to the Ru atom. (b) 6PE formed by $[NBu^n_4]_2[(\mu\text{-}o\text{-}SC_6H_5)_3PNi]_2(CH_3OH)_2$ [KUKYOE]. Ni dark green, S yellow and orange. Each S substituent in the 6-position of each ring coordinates to a Ni atom, two to one Ni and one to the other. Both ends of the molecule form 6PEs, resulting in an infinite chain structure. The S atoms of the ligands involved in the central 6PE are coloured orange.

ent. Just as we have found previously, the cations still associate, with two different types of chain formed. One is analogous to the zig-zag infinite chain, the ZZI6PE, which we have described.[13] Each cation participates in two 6PE [Fig. 11(a)]. In both embraces, the substituent is located outside the interaction zone. For the 6PE with a P···P distance of 6.34 Å, the amino substituent is located on the distal ring. For the other 6PE (P···P = 6.08 Å), the substituent is (necessarily) located on one of the three rings, but is located away from the interaction zone, which, as noted above, is common for *o*-substitution.

The second distinct chain in [YABYUV] has cations taking part in two different alternating motifs [Fig. 11(b)]. The first is a 6PE and the second is an OFF interaction between the distal rings of the 6PE. We have previously observed this chain,[14] although its occurrence is rare. The 6PE (P···P = 6.28 Å) is similar to that with P···P = 6.08 Å in the ZZI6PE chain in that the substituted ring participates in the embrace, but the amine group is disposed away from the interaction zone. The OFF interaction involves only the two substituted rings.

Calculated energies

We have estimated the intermolecular energies (using the summed atom–atom energy approximation) for the $\{PPh_3\}_2$ pair in some of the embraces pictured above. Our intermolecular potential for atoms with charges q_i, q_j separated by d_{ij} is shown in eqn. (1), with a distance-dependent permittivity,

$$E_{ij} = e^{a}{}_{ij}\,[(d_{ij}/d^{a}{}_{ij})^{-12} - 2(d_{ij}/d^{a}{}_{ij})^{-6}] + q_i{\cdot}q_j/\varepsilon{\cdot}d_{ij} \qquad (1)$$

$\varepsilon = 1d$. Atom charges used are P −0.13, C_{ipso} −0.02, C −0.08, C_{Me} −0.20, H 0.10. The atom parameters e^a and d^a are obtained by analyses described and justified in detail in a separate paper.[15] The van der Waals parameters (e^a/kcal mol^{-1}, r^a/Å) used for the calculations reported in this paper are: C 0.08, 1.95; H 0.02, 1.62; P 0.20, 2.10.

We have previously reported that a good 6PE between PPh_3 has attractive energy of around 11 kcal mol^{-1}.[10] Table 1 contains the calculated energies for some of the embraces pictured above where methyl substitution occurs, and confirms that there

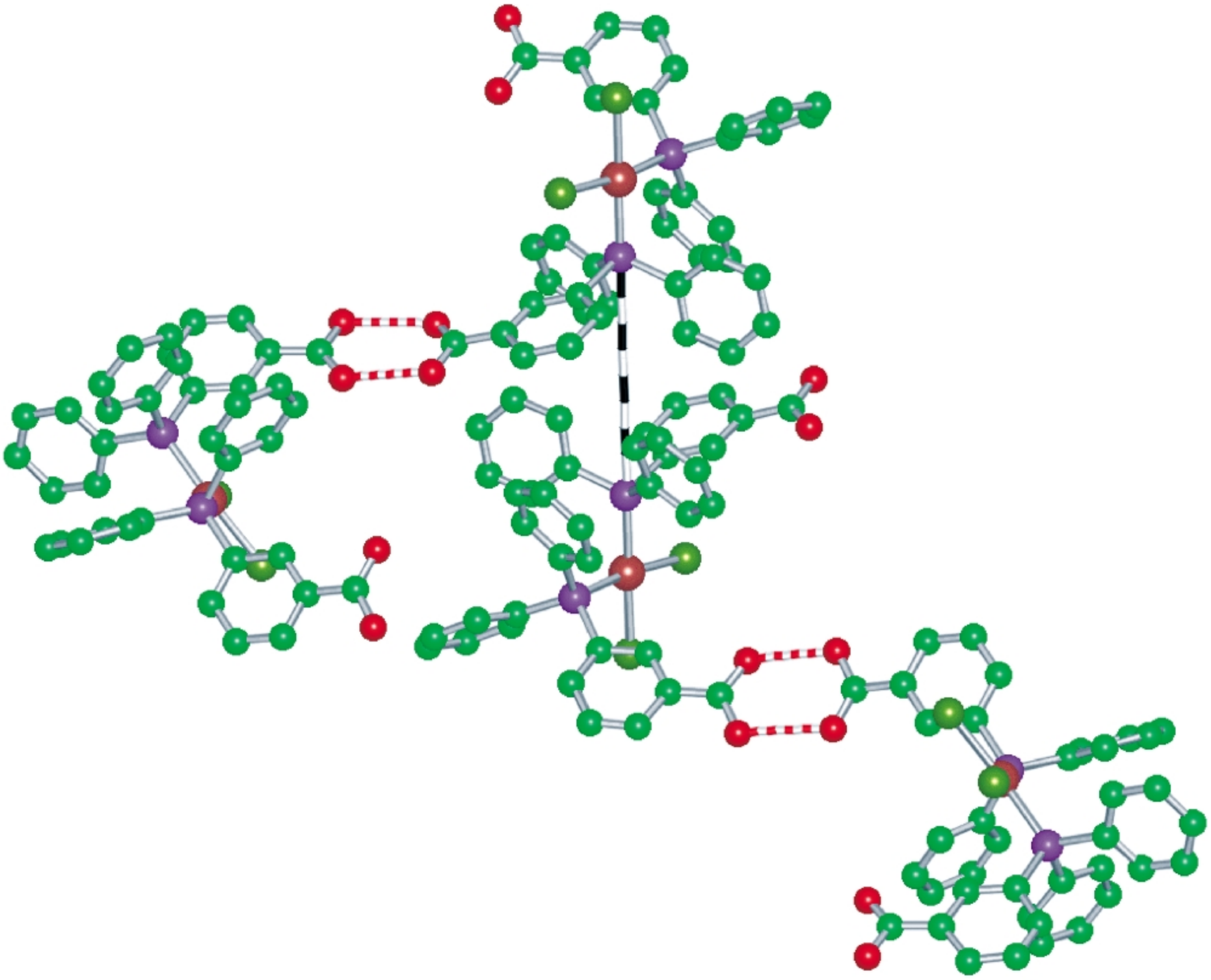

Fig. 10 The 6PE and hydrogen bonding in [(m-COOHC$_6$H$_4$)(Ph)$_2$P]$_2$PtCl$_2$·2H$_2$O [ZUFJAL]. The 6PE is identified by the black and white rod, and the carboxylic acid hydrogen bonded dimer is marked by dashed red lines.

Table 1 Energy for CH$_3$ substituted embraces

REFCODE	Position of CH$_3$ [a]	Energy/kcal mol^{-1} per {PPh$_3$}$_2$		
		Total	van der Waals	Coulombic
[LEJYII]	(6-)$_6$	−13.4	−13.0	−0.5
[JIVDOH]	(2-)$_2$(6-)$_4$	−8.2	−8.7	0.5
[JAYCER]	(3-)$_2$(5-)$_4$	−13.3	−12.6	−0.7
[KUTSIB]	(3-)$_4$(5-)$_2$	−5.3	−4.0	−1.3
[TEZWOK] [b]	(4-)$_6$	−11.9	−11.3	−0.6

[a] Lower numbers represent a substituent in the interaction zone: see Fig. 1. [b] [TEZWOK] = [(4-CH$_3$C$_6$H$_4$)$_3$P]$_2$Pt[Sn(CH$_3$)$_3$]$_2$.

is no impediment unless the methyl substitution dominates the 2- and 3-positions.

In ZUFJAL the calculated energy for the sixfold embrace between two orthogonal flippers (Fig. S1) is −14.3 (−13.0, −1.4) kcal mol^{-1} which is comparable with the energy of the cyclic hydrogen bonded dimer motif which also occurs in these crystals (Fig. 10).

Conclusions

Crystal structures are known for molecules with substitution at the *o*-, *m*- or 4-positions of the phenyl rings in the PPh$_3$ moiety. Substituents in the 4-position are located around the periphery of the group and do not interfere with the embrace, or diminish the frequency of occurrence of the 6PE. The resulting substituted 6PE is of similar energy to a good unsubstituted 6PE.

Substitution of the *o*- or *m*-positions of the phenyl rings in PPh$_3$ does disrupt the (EF)$_6$ composition of the 6PE when these substituents are in the 2- or 3-positions relative to the supramolecular motif. In these cases the search criteria for the 6PE, based on P···P distance and C–P···P angles, can still be fulfilled, but the embraces are (MF)$_2$ or (EF)$_2$(MF)$_4$ or (EF)$_4$-(MF)$_2$ instead of (EF)$_6$. Modified 6PE can retain supramolecular energies comparable with the 11 kcal mol^{-1} of a regular 6PE, but, if four substituents are in the interaction domain the attractive energy reduces to about 5 kcal mol^{-1}. We can find no instances of 6PE with di- or tri-substituted phenyl rings in PPh$_3$. There is one instance of 6PE formed by coordinated P(C$_6$F$_5$)$_3$.

Tertiary motifs based on the 6PE, namely the ZZI6PE and the HA6PE, can be maintained with substituted PPh$_3$, provided that the substituents are outside the interaction zone of the 6PE. There is one instance of a substituted Ph$_4$P$^+$ cation, forming the ZZI6PE motif.

Since substitution need not interfere with the 6PE, heteromolecular 6PE involving two different PAr$_3$ groups are possible, and occur. This destroys the centre of inversion which is normally associated with homo-molecular 6PE. The heteromolecular 6PE could be deployed in the construction of acentric crystals.

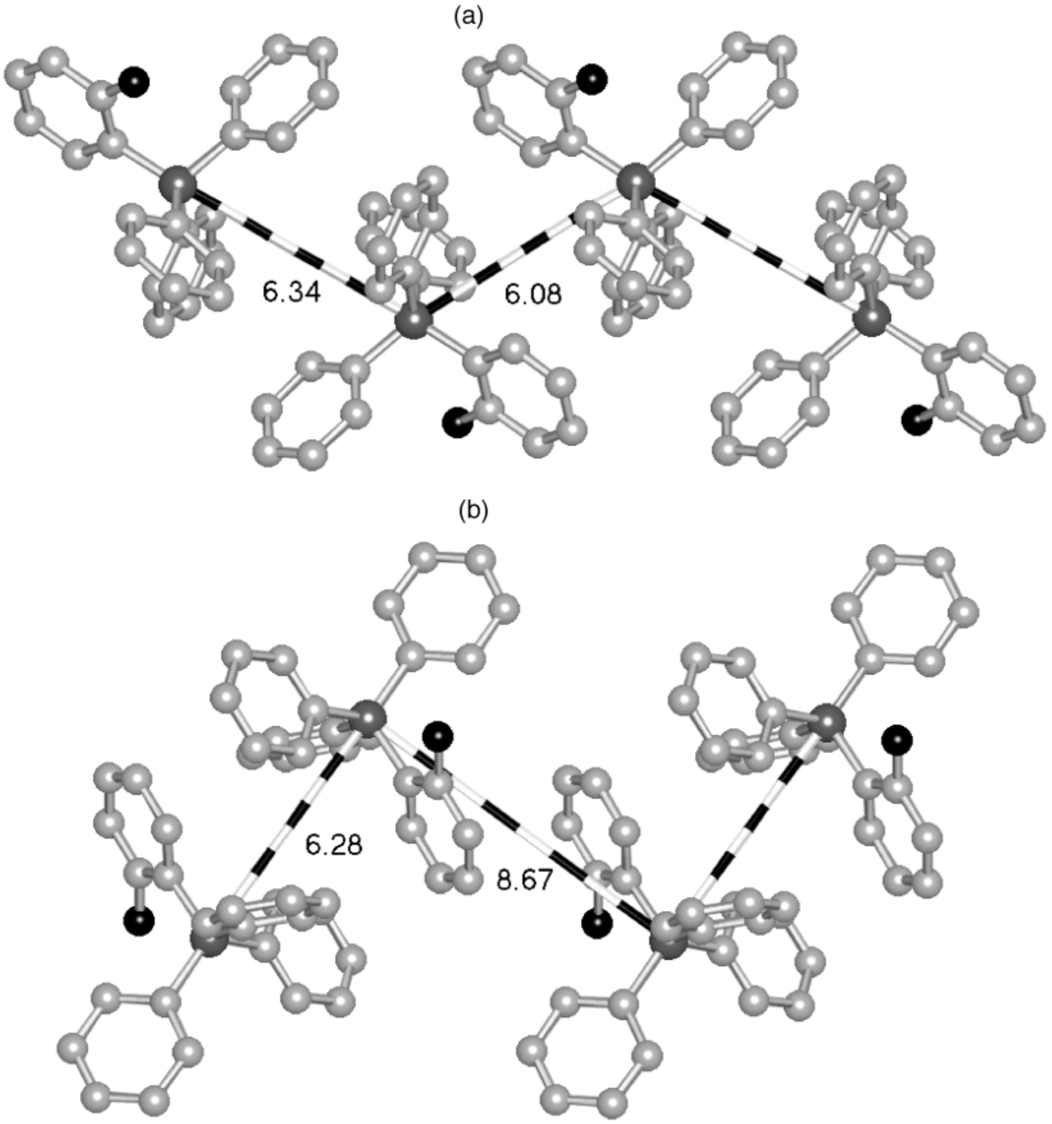

Fig. 11 The two different cation chains in $[(o\text{-}NH_2C_6H_4)(Ph)_3P]_2[NiCl_4]$ [YABYUV]: N is black. (a) The ZZI6PE chain and (b) the chain of alternating 6PE and OFF interactions.

Acknowledgements

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