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Supporting Information for

Synthesis and Molecular Structure of a Palladium Complex Containing a λ^5-Phosphinine–Based SPS Pincer Ligand.

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X-Ray Structural Data for 4:

Theoretical Data:

Geometry optimizations were carried out by means of pure gradient-corrected exchange functional and the Lee-Yang-Parr nonlocal correlation functional BLYP as implemented in the Gaussian 98 program. A 6-31G(d) basis set was used for H, C, P, and S atoms. A relativistic effective core potential (ECP) of Hay and Wadt with a (441/2111/41) split-valence basis set was used for Pd, and Stuttgart pseudopotential with a (31/31/1) basis set was used for Cl. Vibrational frequencies of the stationnary points were calculated at B3LYP with numerical second derivatives of the energy with respect to the coordinates. The structures calculated were located at minima on the potential-energy surface. The bonding situation of the optimized structures were analyzed using the natural bond orbital (NBO) method developed by Weinhold.

Table 6: Distances and angles and NBO charges for the parent phosphinine C_5H_5P **I** (2 pages).

Table 7: Distances and angles and NBO charges for the parent phosphinine 2-diphenylphosphinophosphinine $C_5H_4PH_2$ **II** (2 pages).

Table 8: Distances and angles and NBO charges for the 2,6-bis(diphenylphosphino)phosphinine $C_5H_3P(PH_2)_2$ **III** (2 pages).

Table 9: Distances and angles and NBO charges for the 2,6-bis(diphenylphosphinosulfide)phosphinine $C_5H_3(PH_2S)_2$ **III** (3 pages).

Table 10: Distances and angles and NBO charges for the Pd(2,6-$C_5H_3(PH_2S)_2$)Cl] complex **V** (3 pages).

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Table of crystal data.

Compound **4**
Molecular formula C42H33Cl4P3PdS2
Molecular weight 942.91
Crystal habit orange cube
Crystal dimensions(mm) 0.20x0.20x0.20
Crystal system 'Monoclinic'
Space group 'P21/c
a(Å) 14.316(5)
b(Å) 22.241(5)
c(Å) 14.356(5)
α(°) 90.000(5)
β(°) 117.510(5)
γ(°) 90.000(5)
V(Å3) 4054(2)
Z 4
d(g-cm-3) 1.545
F000 1904
μ(cm-1) 0.974
Absorbtion corrections ? ; 0.8291 min, 0.8291 max
Diffractometer KappaCCD
X-ray source MoKa
λ(Å) 0.71069
Monochromator graphite
T (K) 150.0(10)
Scan mode 'phi
Maximum θ 27.48
HKL ranges -18 18 ; -28 26 ; -18 18
Reflections measured 16947
Independant reflections 9282
Rint 0.0274
Reflections used 7399
Criterion >2sigma(I)
Refinement type Fsqd
Hydrogen atoms mixed
Parameters refined 469
Reflections / parameter 15
wR2 0.1025
R1 0.0369
Flack's parameter not applicable
Weights a, b1 0.0581 ; 0.0000
GoF 1.056
difference peak / hole (e Å-3) 1.290(0.090) / -0.960(0.090)

Note: pseudo orthorhombic C cell; really monoclinic !

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Table 2 : Atomic coordinates (A x 10^4) nd equivalent isotropic displacement parameters (A^2 x 10^3)

atom	x	y	z	U(eq)
Pd(1)	8113(1)	3574(1)	1756(1)	18(1)
Cl(1)	6597(1)	2719(1)	-432(1)	26(1)
Cl(2)	9319(1)	4389(1)	2306(1)	26(1)
S(1)	6663(1)	4203(1)	981(1)	26(1)
S(2)	9463(1)	2883(1)	2618(1)	24(1)
P(1)	6974(1)	2845(1)	1180(1)	17(1)
P(2)	5487(1)	3749(1)	1097(1)	19(1)
P(3)	8788(1)	2053(1)	2261(1)	18(1)
C(1)	5767(2)	2966(1)	1172(2)	19(1)
C(2)	5204(2)	2473(1)	1275(2)	19(1)
C(3)	5640(2)	1895(1)	1541(2)	21(1)
C(4)	6689(2)	1737(1)	1832(2)	18(1)
C(5)	7406(2)	2140(1)	1766(2)	17(1)
C(6)	5370(2)	3993(1)	2236(2)	22(1)
C(7)	5202(2)	4608(1)	2333(2)	31(1)
C(8)	5115(2)	4809(1)	3205(2)	37(1)
C(9)	5182(2)	4405(1)	3961(2)	39(1)
C(10)	5361(2)	3804(1)	3880(2)	35(1)
C(11)	5460(2)	3599(1)	3013(2)	26(1)
C(12)	4304(2)	3969(1)	-58(2)	22(1)
C(13)	4300(2)	3925(1)	-1023(2)	29(1)
C(14)	3402(2)	4090(1)	-1934(2)	34(1)
C(15)	2533(2)	4309(1)	-1869(2)	33(1)
C(16)	2536(2)	4349(1)	-912(2)	31(1)
C(17)	3414(2)	4176(1)	2(2)	24(1)
C(18)	4117(2)	2536(1)	1146(2)	22(1)
C(19)	3289(2)	2747(1)	212(2)	28(1)
C(20)	2286(2)	2793(1)	115(2)	39(1)
C(21)	2082(2)	2617(1)	921(3)	42(1)
C(22)	2883(2)	2394(1)	1840(2)	39(1)
C(23)	3894(2)	2355(1)	1954(2)	28(1)
C(24)	7012(2)	1118(1)	2274(2)	18(1)
C(25)	7072(2)	983(1)	3252(2)	24(1)
C(26)	7362(2)	411(1)	3679(2)	28(1)
C(27)	7581(2)	-32(1)	3138(2)	28(1)
C(28)	7516(2)	98(1)	2163(2)	29(1)
C(29)	7242(2)	668(1)	1744(2)	24(1)
C(30)	9343(2)	1617(1)	3447(2)	19(1)
C(31)	9318(2)	1872(1)	4330(2)	24(1)
C(32)	9704(2)	1547(1)	5251(2)	30(1)
C(33)	10101(2)	977(1)	5308(2)	32(1)
C(34)	10122(2)	724(1)	4442(2)	29(1)
C(35)	9735(2)	1045(1)	3497(2)	22(1)
C(36)	9094(2)	1690(1)	1310(2)	21(1)
C(37)	8303(2)	1481(1)	359(2)	25(1)
C(38)	8568(2)	1201(1)	-358(2)	35(1)
C(39)	9602(2)	1139(1)	-128(2)	37(1)
C(40)	10401(2)	1356(1)	817(2)	35(1)
C(41)	10148(2)	1627(1)	1538(2)	30(1)
C(42)	1847(3)	1286(1)	-907(2)	42(1)
Cl(3)	2388(1)	1536(1)	-1706(1)	64(1)
Cl(4)	2721(1)	835(1)	136(1)	73(1)

U(eq) is defined as 1/3 the trace of the Uij tensor.

Table 3 : Bond lengths (Å) and and bond angles (°)

Pd(1)-P(1)	2.1746(8	Pd(1)-S(1)	2.317(1)
Pd(1)-S(2)	2.3277(8	Pd(1)-Cl(2)	2.3720(8)
Cl(1)-P(1)	2.139(1)	S(1)-P(2)	2.036(1)
S(2)-P(3)	2.036(1)	P(1)-C(1)	1.743(3)
P(1)-C(5)	1.754(2)	P(2)-C(1)	1.779(2)
P(2)-C(6)	1.802(2)	P(2)-C(12)	1.807(2)
P(3)-C(5)	1.777(3)	P(3)-C(30)	1.795(2)
P(3)-C(36)	1.807(2)	C(1)-C(2)	1.409(3)
C(2)-C(3)	1.402(3)	C(2)-C(18)	1.486(3)
C(3)-C(4)	1.405(3)	C(4)-C(5)	1.398(3)
C(4)-C(24)	1.497(3)	C(6)-C(11)	1.377(3)
C(6)-C(7)	1.406(4)	C(7)-C(8)	1.388(4)
C(8)-C(9)	1.377(4)	C(9)-C(10)	1.378(4)
C(10)-C(11)	1.392(4)	C(12)-C(13)	1.386(3)
C(12)-C(17)	1.395(4)	C(13)-C(14)	1.395(4)
C(14)-C(15)	1.378(4)	C(15)-C(16)	1.376(4)
C(16)-C(17)	1.388(3)	C(18)-C(19)	1.398(3)
C(18)-C(23)	1.398(3)	C(19)-C(20)	1.380(4)
C(20)-C(21)	1.375(4)	C(21)-C(22)	1.380(4)
C(22)-C(23)	1.381(4)	C(24)-C(29)	1.385(3)
C(24)-C(25)	1.399(3)	C(25)-C(26)	1.391(3)
C(26)-C(27)	1.378(4)	C(27)-C(28)	1.390(4)
C(28)-C(29)	1.380(4)	C(30)-C(35)	1.378(3)
C(30)-C(31)	1.404(3)	C(31)-C(32)	1.380(3)
C(32)-C(33)	1.375(4)	C(33)-C(34)	1.378(4)
C(34)-C(35)	1.402(3)	C(36)-C(37)	1.391(3)
C(36)-C(41)	1.396(4)	C(37)-C(38)	1.396(4)
C(38)-C(39)	1.366(4)	C(39)-C(40)	1.396(4)
C(40)-C(41)	1.382(4)	C(42)-Cl(3)	1.744(3)
C(42)-Cl(4)	1.756(3)		

P(1)-Pd(1)-S(1)	85.33(3)	P(1)-Pd(1)-S(2)	90.13(3)
S(1)-Pd(1)-S(2)	173.36(2)	P(1)-Pd(1)-Cl(2)	177.34(2)
S(1)-Pd(1)-Cl(2)	92.97(3)	S(2)-Pd(1)-Cl(2)	91.73(3)
P(2)-S(1)-Pd(1)	104.64(4)	P(3)-S(2)-Pd(1)	106.51(4)
C(1)-P(1)-C(5)	105.7(1)	C(1)-P(1)-Cl(1)	105.07(8)
C(5)-P(1)-Cl(1)	104.96(8)	C(1)-P(1)-Pd(1)	117.0(1)
C(5)-P(1)-Pd(1)	116.6(1)	Cl(1)-P(1)-Pd(1)	106.26(3)
C(1)-P(2)-C(6)	110.7(1)	C(1)-P(2)-C(12)	114.2(1)
C(6)-P(2)-C(12)	108.1(1)	C(1)-P(2)-S(1)	108.6(1)
C(6)-P(2)-S(1)	110.6(1)	C(12)-P(2)-S(1)	104.5(1)
C(5)-P(3)-C(30)	111.2(1)	C(5)-P(3)-C(36)	111.1(1)
C(30)-P(3)-C(36)	108.6(1)	C(5)-P(3)-S(2)	108.31(8)
C(30)-P(3)-S(2)	107.49(8)	C(36)-P(3)-S(2)	110.1(1)
C(2)-C(1)-P(1)	119.5(2)	C(2)-C(1)-P(2)	130.1(2)
P(1)-C(1)-P(2)	110.3(1)	C(3)-C(2)-C(1)	122.6(2)
C(3)-C(2)-C(18)	115.4(2)	C(1)-C(2)-C(18)	122.0(2)
C(2)-C(3)-C(4)	126.2(2)	C(5)-C(4)-C(3)	122.4(2)
C(5)-C(4)-C(24)	121.7(2)	C(3)-C(4)-C(24)	115.8(2)
C(4)-C(5)-P(1)	119.9(2)	C(4)-C(5)-P(3)	128.3(2)
P(1)-C(5)-P(3)	111.7(1)	C(11)-C(6)-C(7)	119.7(2)
C(11)-C(6)-P(2)	122.0(2)	C(7)-C(6)-P(2)	118.3(2)
C(8)-C(7)-C(6)	119.5(3)	C(9)-C(8)-C(7)	119.9(3)
C(8)-C(9)-C(10)	120.9(3)	C(9)-C(10)-C(11)	119.5(3)
C(6)-C(11)-C(10)	120.4(2)	C(13)-C(12)-C(17)	120.2(2)
C(13)-C(12)-P(2)	117.9(2)	C(17)-C(12)-P(2)	121.9(2)
C(12)-C(13)-C(14)	119.6(3)	C(15)-C(14)-C(13)	120.0(3)
C(16)-C(15)-C(14)	120.3(3)	C(15)-C(16)-C(17)	120.6(3)
C(16)-C(17)-C(12)	119.2(2)	C(19)-C(18)-C(23)	118.3(2)
C(19)-C(18)-C(2)	121.8(2)	C(23)-C(18)-C(2)	119.8(2)
C(20)-C(19)-C(18)	120.3(3)	C(21)-C(20)-C(19)	120.6(3)
C(20)-C(21)-C(22)	120.1(3)	C(21)-C(22)-C(23)	119.9(3)
C(22)-C(23)-C(18)	120.8(3)	C(29)-C(24)-C(25)	118.5(2)
C(29)-C(24)-C(4)	122.4(2)	C(25)-C(24)-C(4)	119.1(2)
C(26)-C(25)-C(24)	120.4(2)	C(27)-C(26)-C(25)	120.3(2)
C(26)-C(27)-C(28)	119.5(2)	C(29)-C(28)-C(27)	120.2(2)

C(28)-C(29)-C(24)	121.1(2)	C(35)-C(30)-C(31)	120.3(2)
C(35)-C(30)-P(3)	122.7(2)	C(31)-C(30)-P(3)	116.9(2)
C(32)-C(31)-C(30)	119.2(2)	C(33)-C(32)-C(31)	120.8(2)
C(32)-C(33)-C(34)	120.3(2)	C(33)-C(34)-C(35)	120.0(3)
C(30)-C(35)-C(34)	119.4(2)	C(37)-C(36)-C(41)	119.9(2)
C(37)-C(36)-P(3)	121.3(2)	C(41)-C(36)-P(3)	118.8(2)
C(36)-C(37)-C(38)	119.8(3)	C(39)-C(38)-C(37)	120.0(3)
C(38)-C(39)-C(40)	120.7(2)	C(41)-C(40)-C(39)	119.8(3)
C(40)-C(41)-C(36)	119.8(3)	Cl(3)-C(42)-Cl(4)	112.6(2)

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Table 4 : Anisotropic displacement parameters.

atom	U11	U22	U33	U23	U13	U12
Pd(1)	18(1)	15(1)	22(1)	1(1)	10(1)	-1(1)
Cl(1)	33(1)	23(1)	21(1)	2(1)	13(1)	1(1)
Cl(2)	24(1)	20(1)	31(1)	0(1)	12(1)	-5(1)
S(1)	23(1)	17(1)	40(1)	8(1)	16(1)	2(1)
S(2)	18(1)	20(1)	30(1)	3(1)	8(1)	-1(1)
P(1)	18(1)	14(1)	20(1)	1(1)	9(1)	0(1)
P(2)	18(1)	16(1)	22(1)	2(1)	9(1)	2(1)
P(3)	17(1)	18(1)	19(1)	2(1)	9(1)	1(1)
C(1)	18(1)	16(1)	20(1)	4(1)	7(1)	3(1)
C(2)	16(1)	19(1)	18(1)	0(1)	6(1)	2(1)
C(3)	20(1)	16(1)	28(1)	-1(1)	11(1)	-1(1)
C(4)	20(1)	16(1)	19(1)	-2(1)	9(1)	0(1)
C(5)	20(1)	16(1)	16(1)	1(1)	8(1)	0(1)
C(6)	17(1)	23(1)	24(1)	-4(1)	7(1)	3(1)
C(7)	33(2)	22(1)	33(1)	-3(1)	10(1)	4(1)
C(8)	34(2)	31(2)	37(2)	-10(1)	8(1)	7(1)
C(9)	37(2)	48(2)	25(1)	-8(1)	9(1)	13(2)
C(10)	39(2)	38(2)	24(1)	2(1)	12(1)	5(1)
C(11)	25(2)	26(1)	24(1)	-2(1)	7(1)	3(1)
C(12)	22(1)	15(1)	26(1)	3(1)	7(1)	2(1)
C(13)	32(2)	25(1)	28(1)	3(1)	13(1)	6(1)
C(14)	40(2)	30(2)	25(1)	3(1)	9(1)	1(1)
C(15)	29(2)	23(1)	28(1)	0(1)	-3(1)	0(1)
C(16)	19(2)	23(1)	42(2)	-3(1)	6(1)	0(1)
C(17)	23(1)	18(1)	28(1)	-1(1)	10(1)	0(1)
C(18)	20(1)	15(1)	31(1)	-3(1)	13(1)	1(1)
C(19)	23(2)	17(1)	34(1)	0(1)	7(1)	-4(1)
C(20)	17(2)	26(2)	55(2)	10(1)	-1(1)	3(1)
C(21)	22(2)	31(2)	76(2)	4(2)	25(2)	2(1)
C(22)	33(2)	36(2)	55(2)	-2(1)	28(2)	-1(1)
C(23)	22(2)	32(2)	32(1)	2(1)	13(1)	1(1)
C(24)	13(1)	14(1)	25(1)	0(1)	7(1)	-1(1)
C(25)	30(2)	20(1)	29(1)	-1(1)	19(1)	0(1)
C(26)	33(2)	25(1)	27(1)	6(1)	15(1)	0(1)
C(27)	25(2)	15(1)	40(1)	8(1)	11(1)	3(1)
C(28)	34(2)	16(1)	39(2)	-4(1)	18(1)	3(1)
C(29)	26(2)	23(1)	23(1)	-2(1)	12(1)	2(1)
C(30)	16(1)	20(1)	19(1)	3(1)	7(1)	0(1)
C(31)	22(1)	25(1)	25(1)	-3(1)	11(1)	-3(1)
C(32)	32(2)	40(2)	21(1)	0(1)	13(1)	-7(1)
C(33)	24(2)	40(2)	28(1)	14(1)	9(1)	2(1)
C(34)	26(2)	25(1)	39(2)	12(1)	17(1)	5(1)
C(35)	16(1)	25(1)	24(1)	4(1)	10(1)	2(1)
C(36)	21(1)	22(1)	23(1)	6(1)	13(1)	7(1)
C(37)	23(2)	32(2)	22(1)	2(1)	12(1)	5(1)
C(38)	37(2)	41(2)	24(1)	-3(1)	13(1)	3(1)
C(39)	45(2)	45(2)	30(1)	3(1)	26(1)	13(2)
C(40)	29(2)	49(2)	37(2)	5(1)	23(1)	11(1)
C(41)	24(2)	43(2)	24(1)	4(1)	12(1)	6(1)
C(42)	46(2)	36(2)	47(2)	-5(1)	25(2)	-1(2)
Cl(3)	95(1)	41(1)	85(1)	-9(1)	67(1)	-11(1)
Cl(4)	83(1)	91(1)	32(1)	2(1)	15(1)	35(1)

The anisotropic displacement factor exponent takes the form
2 pi^2 [h^2a*^2U(11) +...+ 2hka*b*U(12)]

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Table 5 : Hydrogen coordinates and equivalent isotropic parameters

atom	x	y	z	U(eq)
H(3)	5182	1581	1522	25
H(7)	5149	4884	1806	37
H(8)	5008	5224	3279	44
H(9)	5104	4544	4547	47
H(10)	5417	3529	4412	42
H(11)	5589	3185	2957	31
H(13)	4906	3783	-1064	34
H(14)	3388	4051	-2599	41
H(15)	1930	4432	-2488	40
H(16)	1931	4498	-875	37
H(17)	3407	4198	660	29
H(19)	3416	2858	-358	33
H(20)	1732	2947	-515	47
H(21)	1389	2648	845	50
H(22)	2740	2268	2393	46
H(23)	4443	2202	2588	34
H(25)	6914	1285	3626	29
H(26)	7410	325	4348	34
H(27)	7774	-424	3429	34
H(28)	7659	-206	1782	35
H(29)	7210	753	1082	29
H(31)	9040	2264	4293	29
H(32)	9694	1718	5853	36
H(33)	10362	758	5947	38
H(34)	10400	331	4485	35
H(35)	9742	871	2896	26
H(37)	7585	1527	197	30
H(38)	8029	1054	-1005	42
H(39)	9778	946	-616	44
H(40)	11117	1318	964	42
H(41)	10690	1769	2187	36
H(42A)	1200	1053	-1339	50
H(42B)	1645	1638	-619	50

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Table 6: Distances and angles and NBO charges for the parent phosphinine C_5H_5P **I**.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.746765	0.000000			
3	C	1.746799	2.676360	0.000000		
4	C	2.794383	1.392498	2.916352	0.000000	
5	C	2.794446	2.916466	1.392466	2.453494	0.000000
6	C	3.180012	2.454251	2.454165	1.397438	1.397432
7	H	2.438620	1.088743	3.701553	2.131200	4.002021
8	H	2.438589	3.701503	1.088714	4.001881	2.131132
9	H	3.772206	2.140439	4.002515	1.089028	3.416501
10	H	3.772265	4.002641	2.140425	3.416538	1.089036
11	H	4.267067	3.417300	3.417195	2.142356	2.142300

		6	7	8	9	10
6	C	0.000000				
7	H	3.414094	0.000000			
8	H	3.413991	4.676493	0.000000		
9	H	2.138253	2.424484	5.085792	0.000000	
10	H	2.138297	5.085944	2.424430	4.274156	0.000000
11	H	1.087055	4.271568	4.271441	2.430938	2.430923

		11
11	H	0.000000

Interatomic angles (°):

C2-P1-C3=100.0069	P1-C2-C4=125.4042	C3-P1-C4= 76.0422
C3-C2-C4= 85.4071	C2-P1-C5= 76.0448	P1-C3-C5=125.409
C2-C3-C5= 85.4129	P1-C4-C5= 63.9613	C2-C4-C5= 94.5924
C3-C5-C4= 94.5876	P1-C2-C6= 96.9531	P1-C3-C6= 96.9552
C2-C6-C3= 66.0848	P1-C4-C6= 92.5764	C2-C4-C6=123.2075
C3-C6-C4= 94.4262	P1-C5-C6= 92.5739	C2-C6-C5= 94.4282
C3-C5-C6=123.2029	C4-C6-C5=122.7696	P1-C2-H7=116.7221
C3-P1-H7=123.5086	C3-C2-H7=156.7191	P1-H7-C4= 75.0568
C4-C2-H7=117.8738	C3-C4-H7= 93.0176	C5-P1-H7= 99.5465
C5-C2-H7=174.8616	C5-C4-H7=121.4381	C6-C2-H7=146.3248
C6-C4-H7=150.0532	C2-P1-H8=123.5089	P1-C3-H8=116.7188
C2-C3-H8=156.7149	C4-P1-H8= 99.5442	C4-C3-H8=174.8642
P1-H8-C5= 75.0607	C2-C5-H8= 93.0141	C5-C3-H8=117.8723
C4-C5-H8=121.4339	C6-C3-H8=146.326	C6-C5-H8=150.0491
H7-P1-H8=147.0106	P1-C2-H9=151.9097	C3-C2-H9=111.9127
P1-C4-H9=149.3302	C2-C4-H9=118.6991	C3-C4-H9=175.1291
C5-C2-H9= 83.4934	C5-C4-H9=146.7086	C2-H9-C6= 70.0031
C3-C6-H9=121.1251	C6-C4-H9=118.0934	C5-C6-H9=149.4685
P1-H7-H9=101.7328	H7-C2-H9= 91.3682	H7-C4-H9= 91.8534
C6-H9-H7= 96.6783	P1-C3-H10=151.9147	C2-C3-H10=111.9186
C4-C3-H10= 83.4976	P1-C5-H10=149.3288	C2-C5-H10=175.1324
C3-C5-H10=118.6998	C4-C5-H10=146.7126	C2-C6-H10=121.1257
C3-H10-C6= 69.9997	C4-C6-H10=149.4671	C6-C5-H10=118.0973
P1-H8-H10=101.7375	H8-C3-H10= 91.3665	H8-C5-H10= 91.8536
C6-H10-H8= 96.6748	H9-C6-H10=176.1659	P1-C4-H11=119.0268
C2-C4-H11=149.658	C3-C4-H11= 83.4861	P1-C5-H11=119.0263
C2-C5-H11= 83.4875	C3-C5-H11=149.6553	C4-H11-C5= 69.8667
C2-C6-H11=146.959	C3-C6-H11=146.9562	C4-C6-H11=118.6175
C5-C6-H11=118.6128	H7-C4-H11=176.5036	H8-C5-H11=176.5016
C2-H9-H11= 96.5496	H9-C4-H11= 91.643	C5-H11-H9= 96.4695
H9-C6-H11= 91.9187	H7-H9-H11=123.2249	C3-H10-H11= 96.5464

C4-H11-H10= 96.4699 H10-C5-H11= 91.6449 H10-C6-H11= 91.9154
H8-H10-H11=123.2216 H9-H11-H10=123.0726

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
P 1	0.65826	9.99850	4.29982	0.04342	14.34174
C 2	-0.60301	1.99921	4.58818	0.01562	6.60301
C 3	-0.60302	1.99921	4.58819	0.01562	6.60302
C 4	-0.22908	1.99904	4.21284	0.01720	6.22908
C 5	-0.22902	1.99904	4.21277	0.01720	6.22902
C 6	-0.21655	1.99907	4.20309	0.01439	6.21655
H 7	0.25325	0.00000	0.74586	0.00089	0.74675
H 8	0.25323	0.00000	0.74588	0.00089	0.74677
H 9	0.23877	0.00000	0.75996	0.00128	0.76123
H 10	0.23875	0.00000	0.75998	0.00128	0.76125
H 11	0.23842	0.00000	0.76067	0.00091	0.76158
* Total *	0.00000	19.99407	29.87724	0.12870	50.00000

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Table 7: Distances and angles and NBO charges for the parent phosphinine 2-diphenylphosphinophosphinine $C_5H_4PH_2$ **II**.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.757956	0.000000			
3	C	1.746538	2.705715	0.000000		
4	C	2.786324	1.400960	2.915771	0.000000	
5	C	2.795053	2.951113	1.393614	2.458976	0.000000
6	C	3.172144	2.475497	2.451203	1.398868	1.398596
7	H	2.436234	3.728055	1.089496	4.002615	2.135347
8	H	3.772231	2.146938	4.002138	1.090746	3.415674
9	H	3.774542	4.037066	2.144089	3.422314	1.089052
10	H	4.259504	3.432261	3.416742	2.139971	2.144490
11	P	3.132784	1.858733	4.492482	2.783171	4.799869
12	H	2.931573	2.485357	4.599607	3.769111	5.282769
13	H	3.592686	2.497892	4.912921	3.310626	5.220021

		6	7	8	9	10
6	C	0.000000				
7	H	3.415152	0.000000			
8	H	2.131416	5.086439	0.000000		
9	H	2.141383	2.433900	4.270825	0.000000	
10	H	1.087380	4.277091	2.412858	2.436711	0.000000
11	P	4.130842	5.444604	2.840552	5.880394	4.912599
12	H	4.956383	5.362653	4.098162	6.363938	5.884698
13	H	4.573076	5.825641	3.336475	6.269861	5.314486

		11	12	13
11	P	0.000000		
12	H	1.422171	0.000000	
13	H	1.426859	2.075631	0.000000

Interatomic angles (°):

C2-P1-C3=101.0798	P1-C2-C4=123.3865	C3-P1-C4= 76.2566
C3-C2-C4= 84.0805	C2-P1-C5= 77.1015	P1-C3-C5=125.3975
C2-C3-C5= 85.7873	P1-C4-C5= 64.0426	C2-C4-C5= 95.8297
C3-C5-C4= 94.2926	P1-C2-C6= 95.5648	P1-C3-C6= 96.732
C2-C6-C3= 66.6214	P1-C4-C6= 92.515	C2-C4-C6=124.2967
C3-C6-C4= 94.4869	P1-C5-C6= 92.1558	C2-C6-C5= 95.1778
C3-C5-C6=122.7733	C4-C6-C5=123.0443	C2-P1-H7=124.6719
P1-C3-H7=116.4958	C2-C3-H7=156.1073	C4-P1-H7= 99.8483
C4-C3-H7=175.3144	P1-H7-C5= 75.0584	C2-C5-H7= 92.8635
C5-C3-H7=118.1052	C4-C5-H7=121.038	C6-C3-H7=146.7723
C6-C5-H7=149.5187	P1-C2-H8=149.8913	C3-C2-H8=110.5956
P1-C4-H8=150.2345	C2-C4-H8=118.4711	C3-C4-H8=173.9804
C5-C2-H8= 82.511	C5-C4-H8=145.684	C2-H8-C6= 70.7045
C3-C6-H8=121.5396	C6-C4-H8=117.2314	C5-C6-H8=150.0885
P1-C3-H9=151.7864	C2-C3-H9=112.1784	C4-C3-H9= 83.6329
P1-C5-H9=149.561	C2-C5-H9=174.9416	C3-C5-H9=118.9422
C4-C5-H9=146.7611	C2-C6-H9=121.7842	C3-H9-C6= 69.7767
C4-C6-H9=149.648	C6-C5-H9=118.2831	P1-H7-H9=101.6171
H7-C3-H9= 91.7141	H7-C5-H9= 92.1949	C6-H9-H7= 96.3554
H8-C6-H9=176.5161	P1-C4-H10=119.1033	C2-C4-H10=150.8821
C3-C4-H10= 83.526	P1-C5-H10=118.5657	C2-C5-H10= 83.0686
C3-C5-H10=149.1807	C4-H10-C5= 70.0492	C2-C6-H10=146.128
C3-C6-H10=147.2488	C4-C6-H10=118.2567	C5-C6-H10=118.6939

H7-C5-H10=175.8945	C2-H8-H10= 97.4825	H8-C4-H10= 90.6466
C5-H10-H8= 96.9159	H8-C6-H10= 91.1935	C3-H9-H10= 96.2604
C4-H10-H9= 96.5807	H9-C5-H10= 91.8733	H9-C6-H10= 92.0876
H7-H9-H10=122.8382	H8-H10-H9=123.4436	P1-C2-P11=120.0148
C3-C2-P11=159.2603	P1-C4-P11= 68.4563	C4-C2-P11=116.5572
C3-C4-P11=104.0298	C5-C2-P11=172.4192	C5-C4-P11=132.4943
C6-C2-P11=144.3814	C6-C4-P11=160.9691	H8-C2-P11= 90.0323
H8-C4-P11= 81.7898	C6-H8-P11=111.5727	H10-C4-P11=172.434
H10-H8-P11=138.3523	P1-C2-H12= 85.581	C3-P1-H12=158.26
C3-C2-H12=124.7106	C4-P1-H12= 82.4322	C4-C2-H12=150.5929
C5-P1-H12=134.5728	C5-C2-H12=152.5838	C6-C2-H12=175.1346
H7-P1-H12=174.9562	H8-C2-H12=124.2658	P1-H12-P11= 84.4782
C2-P11-H12= 97.6035	C4-P11-H12=124.0948	H8-P11-H12=146.0687
P1-C2-H13=114.0386	C3-C2-H13=141.4849	C4-C2-H13=113.2083
C5-C2-H13=146.5423	C6-C2-H13=133.7083	H8-C2-H13= 91.5133
C2-P11-H13= 98.1138	C4-P11-H13= 98.5315	H8-P11-H13= 97.2815
P1-H12-H13= 90.0237	C2-H12-H13= 65.6998	H12-P11-H13= 93.5281

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
P 1	0.69597	9.99828	4.26496	0.04079	14.30403
C 2	-0.71427	1.99917	4.69315	0.02195	6.71427
C 3	-0.60829	1.99925	4.59127	0.01777	6.60829
C 4	-0.22963	1.99899	4.20923	0.02140	6.22963
C 5	-0.23227	1.99907	4.21362	0.01959	6.23227
C 6	-0.22158	1.99910	4.20587	0.01661	6.22158
H 7	0.26235	0.00000	0.73699	0.00066	0.73765
H 8	0.24386	0.00000	0.75441	0.00173	0.75614
H 9	0.24526	0.00000	0.75351	0.00123	0.75474
H 10	0.24708	0.00000	0.75210	0.00082	0.75292
P 11	0.32654	9.99881	4.62708	0.04757	14.67346
H 12	-0.00757	0.00000	1.00662	0.00095	1.00757
H 13	-0.00746	0.00000	1.00617	0.00130	1.00746
* Total *	0.00000	29.99268	35.81496	0.19236	66.00000

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Table 8: Distances and angles and NBO charges for the 2,6-bis(diphenylphosphino)phosphinine $C_5H_3P(PH_2)_2$ **III**.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.756828	0.000000			
3	C	1.756773	2.733783	0.000000		
4	C	2.783565	1.399857	2.947572	0.000000	
5	C	3.159587	2.468910	2.468876	1.398069	0.000000
6	C	2.783587	2.947628	1.399891	2.461752	1.398033
7	H	3.771079	2.148378	4.033300	1.090478	2.132554
8	H	4.247006	3.427724	3.427735	2.139812	1.087419
9	H	3.771068	4.033359	2.148390	3.418436	2.132568
10	P	3.129731	1.859218	4.517017	2.785709	4.129736
11	H	2.926672	2.485285	4.613601	3.769181	4.949917
12	H	3.587800	2.496233	4.930154	3.314574	4.569541
13	P	3.129663	4.517032	1.859240	4.798159	4.129721
14	H	2.926542	4.613613	2.485320	5.275313	4.949987
15	H	3.588499	4.930516	2.496278	5.208909	4.569018

		6	7	8	9	10
6	C	0.000000				
7	H	3.418399	0.000000			
8	H	2.139821	2.415923	0.000000		
9	H	1.090475	4.263994	2.416021	0.000000	
10	P	4.798189	2.849229	4.916420	5.878090	0.000000
11	H	5.275310	4.104213	5.882552	6.360041	1.422221
12	H	5.209044	3.349932	5.315530	6.251150	1.426635
13	P	2.785744	5.878055	4.916474	2.849229	6.199766
14	H	3.769312	6.360052	5.882693	4.104342	6.026724
15	H	3.313992	6.250950	5.314824	3.348856	6.539732

		11	12	13	14	15
11	H	0.000000				
12	H	2.076096	0.000000			
13	P	6.026755	6.539159	0.000000		
14	H	5.541575	6.304479	1.422221	0.000000	
15	H	6.305050	7.148899	1.426637	2.076123	0.000000

Interatomic angles (°):

C2-P1-C3=102.1661	P1-C2-C4=123.3245	C3-P1-C4= 77.323
C3-C2-C4= 84.4142	P1-C2-C5= 95.2981	P1-C3-C5= 95.3008
C2-C5-C3= 67.235	P1-C4-C5= 92.0628	C2-C4-C5=123.8682
C3-C5-C4= 95.3048	C2-P1-C6= 77.3236	P1-C3-C6=123.3278
C2-C3-C6= 84.4161	P1-C4-C6= 63.7566	C2-C4-C6= 95.5676
C3-C6-C4= 95.564	P1-C6-C5= 92.0627	C2-C5-C6= 95.307
C3-C6-C5=123.8654	C4-C5-C6=123.3868	P1-C2-H7=149.7238
C3-C2-H7=110.8375	P1-C4-H7=150.4976	C2-C4-H7=118.7139
C3-C4-H7=173.7396	C2-H7-C5= 70.4396	C3-C5-H7=122.2848
C5-C4-H7=117.4178	C6-C2-H7= 82.6576	C6-C4-H7=145.7149
C6-C5-H7=150.3723	P1-C4-H8=118.6414	C2-C4-H8=150.4362
C3-C4-H8= 83.0902	C2-C5-H8=146.3795	C3-C5-H8=146.3855
C4-C5-H8=118.3047	P1-C6-H8=118.6402	C2-C6-H8= 83.0883
C3-C6-H8=150.4322	C4-H8-C6= 70.2308	C6-C5-H8=118.3085
C2-H7-H8= 97.178	H7-C4-H8= 90.844	H7-C5-H8= 91.3147
C6-H8-H7= 97.0552	P1-C3-H9=149.7272	C2-C3-H9=110.8396
C4-C3-H9= 82.66	C2-C5-H9=122.2856	C3-H9-C5= 70.438

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C4-C5-H9=150.371	P1-C6-H9=150.4934	C2-C6-H9=173.7437
C3-C6-H9=118.7125	C4-C6-H9=145.7201	C5-C6-H9=117.4221
H7-C5-H9=177.3654	C3-H9-H8= 97.1751	C4-H8-H9= 97.0539
H8-C5-H9= 91.3199	H8-C6-H9= 90.8495	H7-H8-H9=123.881
P1-C2-P10=119.8558	C3-C2-P10=158.7336	P1-C4-P10= 68.3834
C4-C2-P10=116.7623	C3-C4-P10=103.936	C5-C2-P10=144.8078
C5-C4-P10=160.445	C6-C2-P10=172.938	C6-C4-P10=132.1395
H7-C2-P10= 90.3291	H7-C4-P10= 82.1365	C5-H7-P10=111.171
H8-C4-P10=172.9721	H8-H7-P10=137.9099	P1-C2-H11= 85.4175
C3-P1-H11=159.5295	C3-C2-H11=124.186	C4-P1-H11= 82.5701
C4-C2-H11=150.743	C5-C2-H11=175.2375	C6-P1-H11=134.9703
C6-C2-H11=152.2286	H7-C2-H11=124.5256	P1-H11-P10= 84.5345
C2-P10-H11= 97.576	C4-P10-H11=123.9382	H7-P10-H11=145.8088
P1-C2-H12=113.9087	C3-C2-H12=140.9662	C4-C2-H12=113.5793
C5-C2-H12=133.9462	C6-C2-H12=146.1003	H7-C2-H12= 92.0054
C2-P10-H12= 98.0099	C4-P10-H12= 98.6173	H7-P10-H12= 97.5535
P1-H11-H12= 89.9845	C2-H11-H12= 65.6448	H11-P10-H12= 93.5628
P1-C3-P13=119.8533	C2-C3-P13=158.7327	C4-C3-P13=172.9395
C5-C3-P13=144.8077	P1-C6-P13= 68.381	C2-C6-P13=103.9342
C6-C3-P13=116.7614	C4-C6-P13=132.1361	C5-C6-P13=160.4423
H8-C6-P13=172.9758	H9-C3-P13= 90.3281	C5-H9-P13=111.17
H9-C6-P13= 82.1348	H8-H9-P13=137.9076	C2-P1-H14=159.5424
P1-C3-H14= 85.4125	C2-C3-H14=124.1851	C4-P1-H14=134.9779
C4-C3-H14=152.2307	C5-C3-H14=175.2762	C6-P1-H14= 82.5756
C6-C3-H14=150.7512	H9-C3-H14=124.5303	H11-P1-H14=142.4385
P1-H14-P13= 84.5366	C3-P13-H14= 97.5769	C6-P13-H14=123.9447
H9-P13-H14=145.8221	P1-C3-H15=113.9447	C2-C3-H15=140.9873
C4-C3-H15=146.0914	C5-C3-H15=133.9149	C6-C3-H15=113.5409
H9-C3-H15= 91.9654	C3-P13-H15= 98.0113	C6-P13-H15= 98.5876
H9-P13-H15= 97.5022	P1-H14-H15= 90.0113	C3-H14-H15= 65.6451
H14-P13-H15= 93.5643		

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
P 1	0.72449	9.99815	4.23855	0.03881	14.27551
C 2	-0.71206	1.99917	4.69171	0.02119	6.71206
C 3	-0.71208	1.99917	4.69172	0.02119	6.71208
C 4	-0.22723	1.99899	4.20682	0.02143	6.22723
C 5	-0.21652	1.99911	4.20065	0.01677	6.21652
C 6	-0.22723	1.99899	4.20682	0.02143	6.22723
H 7	0.24542	0.00000	0.75294	0.00164	0.75458
H 8	0.24898	0.00000	0.75016	0.00086	0.75102
H 9	0.24541	0.00000	0.75295	0.00164	0.75459
P 10	0.32872	9.99880	4.62519	0.04729	14.67128
H 11	-0.00708	0.00000	1.00618	0.00090	1.00708
H 12	-0.00623	0.00000	1.00497	0.00126	1.00623
P 13	0.32873	9.99880	4.62518	0.04729	14.67127
H 14	-0.00707	0.00000	1.00617	0.00090	1.00707
H 15	-0.00623	0.00000	1.00497	0.00126	1.00623
* Total *	0.00000	39.99117	41.76496	0.24387	82.00000

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Table 9: Distances and angles and NBO charges for the 2,6-bis(diphenylphosphinosulfide)phosphinine $C_5H_3(PH_2S)_2$ **III**.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.751152	0.000000			
3	C	1.751153	2.698157	0.000000		
4	C	2.792195	1.395845	2.929282	0.000000	
5	C	3.172802	2.459366	2.459366	1.397729	0.000000
6	C	2.792195	2.929282	1.395845	2.458091	1.397729
7	H	3.768414	2.136029	4.016474	1.089710	2.145227
8	H	4.259427	3.420255	3.420255	2.140334	1.086626
9	H	3.768413	4.016474	2.136029	3.424552	2.145227
10	P	3.075402	1.847842	4.457939	2.789179	4.125752
11	H	3.249809	2.556644	4.772595	3.643500	4.853129
12	H	3.196879	2.553224	4.750127	3.677172	4.883900
13	P	3.075402	4.457939	1.847842	4.772184	4.125752
14	H	3.249794	4.772589	2.556644	5.297427	4.853138
15	H	3.196895	4.750135	2.553225	5.305330	4.883892
16	S	4.849369	5.934753	3.256432	5.855322	4.811797
17	S	4.849368	3.256432	5.934753	3.443491	4.811798

		6	7	8	9	10
6	C	0.000000				
7	H	3.424553	0.000000			
8	H	2.140334	2.437815	0.000000		
9	H	1.089710	4.287920	2.437815	0.000000	
10	P	4.772184	2.852418	4.923481	5.855954	0.000000
11	H	5.297424	3.837591	5.712324	6.364846	1.415497
12	H	5.305331	3.891374	5.757581	6.376913	1.415239
13	P	2.789179	5.855955	4.923481	2.852417	6.100005
14	H	3.643510	6.364848	5.712337	3.837607	6.225928
15	H	3.677163	6.376912	5.757569	3.891359	6.183857
16	S	3.443490	6.862315	5.259038	2.822864	7.713855
17	S	5.855323	2.822865	5.259039	6.862315	1.962702

		11	12	13	14	15
11	H	0.000000				
12	H	2.170129	0.000000			
13	P	6.225939	6.183846	0.000000		
14	H	6.433889	5.984725	1.415497	0.000000	
15	H	5.984748	6.294232	1.415239	2.170129	0.000000
16	S	7.930550	7.928085	1.962702	2.879609	2.883148
17	S	2.879608	2.883149	7.713855	7.930537	7.928097

		16	17
16	S	0.000000	
17	S	9.124680	0.000000

Interatomic angles (°):

C2-P1-C3=100.7787	P1-C2-C4=124.6774	C3-P1-C4= 76.5042
C3-C2-C4= 85.0668	P1-C2-C5= 96.3432	P1-C3-C5= 96.3432
C2-C5-C3= 66.5348	P1-C4-C5= 92.3251	C2-C4-C5=123.373
C3-C5-C4= 94.8274	C2-P1-C6= 76.5042	P1-C3-C6=124.6774
C2-C3-C6= 85.0668	P1-C6-C4= 63.8852	C2-C4-C6= 94.9331
C3-C6-C4= 94.9331	P1-C6-C5= 92.3251	C2-C5-C6= 94.8274
C3-C6-C5=123.373	C4-C5-C6=123.12	P1-C2-H7=151.4572

C3-C2-H7=111.8468	P1-C4-H7=149.0172	C2-C4-H7=117.9696
C3-C4-H7=175.4371	C2-H7-C5= 70.1218	C3-C5-H7=121.2982
C5-C4-H7=118.6573	C6-C2-H7= 83.5041	C6-C4-H7=147.0972
C6-C5-H7=149.5909	P1-C4-H8=118.8394	C2-C4-H8=149.8872
C3-C4-H8= 83.2972	C2-C5-H8=146.7326	C3-C5-H8=146.7326
C4-C5-H8=118.44	P1-C6-H8=118.8394	C2-C6-H8= 83.2972
C3-C6-H8=149.8872	C4-H8-C6= 70.0916	C6-C5-H8=118.44
C2-H7-H8= 96.5755	H7-C4-H8= 92.1432	H7-C5-H8= 91.969
C6-H8-H7= 96.623	P1-C3-H9=151.4572	C2-C3-H9=111.8468
C4-C3-H9= 83.504	C2-C5-H9=121.2982	C3-H9-C5= 70.1218
C4-C5-H9=149.5909	P1-C6-H9=149.0172	C2-C6-H9=175.4371
C3-C6-H9=117.9696	C4-C6-H9=147.0972	C5-C6-H9=118.6573
H7-C5-H9=176.0619	C3-H9-H8= 96.5755	C4-H8-H9= 96.623
H8-C5-H9= 91.969	H8-C6-H9= 92.1432	H7-H8-H9=123.1545
P1-C2-P10=117.3876	C3-C2-P10=156.9971	P1-C4-P10= 66.8728
C4-C2-P10=117.9346	C3-C4-P10=102.4148	C5-C2-P10=146.2678
C5-C4-P10=159.1959	C6-C2-P10=174.6492	C6-C4-P10=130.7571
H7-C2-P10= 91.1552	H7-C4-P10= 82.1457	C5-H7-P10=110.4882
H8-C4-P10=174.2813	H8-H7-P10=136.9412	P1-C2-H11= 96.1437
C3-C2-H11=130.506	C4-C2-H11=132.1563	C5-C2-H11=150.712
C6-C2-H11=149.8019	H7-C2-H11=109.4008	C2-P10-H11=102.3433
C4-P10-H11=116.2465	H7-P10-H11=124.6151	P1-C2-H12= 94.0692
C3-C2-H12=129.5044	C4-C2-H12=135.1609	C5-C2-H12=153.9732
C6-C2-H12=150.7179	H7-C2-H12=111.8595	C2-P10-H12=102.1579
C4-P10-H12=118.2702	H7-P10-H12=128.2972	C2-H12-H11= 64.9505
H11-P10-H12=100.1045	P1-C3-P13=117.3877	C2-C3-P13=156.9971
C4-C3-P13=174.6492	C5-C3-P13=146.2677	P1-C6-P13= 66.8729
C2-C6-P13=102.4148	C6-C3-P13=117.9346	C4-C6-P13=130.7571
C5-C6-P13=159.1959	H8-C6-P13=174.2813	H9-C3-P13= 91.1552
C5-H9-P13=110.4883	H9-C6-P13= 82.1456	H8-H9-P13=136.9412
P1-C3-H14= 96.1431	C2-C3-H14=130.5057	C4-C3-H14=149.8021
C5-C3-H14=150.7128	C6-C3-H14=132.1572	H9-C3-H14=109.4015
C3-P13-H14=102.3433	C6-P13-H14=116.2471	H9-P13-H14=124.6161
P1-C3-H15= 94.0698	C2-C3-H15=129.5047	C4-C3-H15=150.7177
C5-C3-H15=153.9723	C6-C3-H15=135.1601	H9-C3-H15=111.8588
C3-P13-H15=102.158	C6-P13-H15=118.2697	H9-P13-H15=128.2962
C3-H15-H14= 64.9505	H14-P13-H15=100.1046	C3-H9-S16= 80.806
C5-H9-S16=150.9026	C6-H9-S16=116.0482	H8-H9-S16=177.1305
C3-P13-S16=117.3961	C6-P13-S16= 91.1823	H9-S16-P13= 70.579
C3-H14-S16= 73.3282	H9-S16-H14= 84.5876	H14-P13-S16=116.0063
C3-H15-S16= 73.3145	H9-S16-H15= 85.9895	H15-P13-S16=116.2541
H15-H14-S16= 67.9647	C2-H7-S17= 80.8059	C4-H7-S17=116.0481
C5-H7-S17=150.9025	H8-H7-S17=177.1302	C2-P10-S17=117.3961
C4-P10-S17= 91.1823	H7-S17-P10= 70.5789	C2-H11-S17= 73.3282
H7-S17-H11= 84.5871	H11-P10-S17=116.0063	C2-H12-S17= 73.3144
H7-S17-H12= 85.9899	H12-P10-S17=116.2542	H12-H11-S17= 67.9647

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
P 1	0.74734	9.99815	4.21841	0.03611	14.25266
C 2	-0.76489	1.99911	4.74357	0.02221	6.76489
C 3	-0.76489	1.99911	4.74357	0.02221	6.76489

C 4	-0.19357	1.99900	4.17125	0.02332	6.19357
C 5	-0.21058	1.99911	4.19489	0.01658	6.21058
C 6	-0.19357	1.99900	4.17125	0.02332	6.19357
H 7	0.27284	0.00000	0.72526	0.00190	0.72716
H 8	0.25915	0.00000	0.74003	0.00082	0.74085
H 9	0.27284	0.00000	0.72526	0.00190	0.72716
P 10	0.82842	9.99848	4.08110	0.09200	14.17158
H 11	0.00277	0.00000	0.99437	0.00286	0.99723
H 12	0.00270	0.00000	0.99448	0.00283	0.99730
P 13	0.82842	9.99848	4.08110	0.09200	14.17158
H 14	0.00277	0.00000	0.99437	0.00286	0.99723
H 15	0.00270	0.00000	0.99448	0.00283	0.99730
S 16	-0.54622	9.99942	6.52377	0.02302	16.54622
S 17	-0.54622	9.99942	6.52377	0.02302	16.54622
* Total *	0.00000	59.98929	53.62092	0.38979	114.00000

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Table 10: Distances and angles and NBO charges for the Pd(2,6-$C_5H_3(PH_2S)_2$)Cl] complex **V**.

Distance matrix (angstroms):

		1	2	3	4	5
1	P	0.000000				
2	C	1.716972	0.000000			
3	C	1.716975	2.776011	0.000000		
4	C	2.709436	1.400944	2.982332	0.000000	
5	C	2.709439	2.982335	1.400944	2.496989	0.000000
6	C	3.049247	2.466249	2.466247	1.405080	1.405081
7	H	3.710824	4.063694	2.157611	3.442465	1.088189
8	H	4.134524	3.418343	3.418341	2.133360	2.133360
9	H	3.710820	2.157610	4.063690	1.088189	3.442466
10	P	2.887883	1.826522	4.400999	2.936680	4.800547
11	H	3.844792	2.607770	5.209914	3.342085	5.428407
12	H	3.844628	2.607747	5.209782	3.342169	5.428354
13	S	3.191151	3.232670	4.905777	4.606486	5.785119
14	P	2.887894	4.401003	1.826518	4.800541	2.936667
15	H	3.844845	5.209957	2.607780	5.428425	3.342065
16	H	3.844598	5.209747	2.607740	5.428326	3.342168
17	S	3.191184	4.905807	3.232687	5.785142	4.606499
18	Pd	2.171568	3.471788	3.471744	4.743479	4.743451
19	Cl	4.485956	5.669197	5.669124	7.002819	7.002766

		6	7	8	9	10
6	C	0.000000				
7	H	2.135906	0.000000			
8	H	1.085277	2.402474	0.000000		
9	H	2.135905	4.271710	2.402474	0.000000	
10	P	4.222882	5.885537	5.069369	3.157314	0.000000
11	H	4.668144	6.475073	5.364076	3.259333	1.408921
12	H	4.668182	6.475025	5.364167	3.259536	1.408923
13	S	5.650901	6.842613	6.645352	5.086094	2.056315
14	P	4.222872	3.157297	5.069356	5.885531	5.775423
15	H	4.668139	3.259283	5.364057	6.475091	6.656453
16	H	4.668169	3.259556	5.364160	6.474996	6.656154
17	S	5.650920	5.086102	6.645368	6.842637	5.705923
18	Pd	5.220815	5.627169	6.306092	5.627209	3.594033
19	Cl	7.535202	7.817853	8.620479	7.817934	5.308272

		11	12	13	14	15
11	H	0.000000				
12	H	2.206182	0.000000			
13	S	2.919840	2.919868	0.000000		
14	P	6.656404	6.656201	5.705903	0.000000	
15	H	7.328119	7.652769	6.668654	1.408921	0.000000
16	H	7.652695	7.327538	6.668377	1.408924	2.206182
17	S	6.668595	6.668477	4.905091	2.056333	2.919841
18	Pd	4.596527	4.596370	2.456019	3.593962	4.596512
19	Cl	6.186540	6.186448	3.462657	5.308128	6.186441

		16	17	18	19
16	H	0.000000			
17	S	2.919886	0.000000		
18	Pd	4.596243	2.455943	0.000000	
19	Cl	6.186232	3.462465	2.314387	0.000000

Interatomic angles (°):

C2-P1-C3=107.8802	P1-C2-C4=120.3447	C3-P1-C4= 81.3785
C3-C2-C4= 84.2847	C2-P1-C5= 81.3786	P1-C3-C5=120.3448
C2-C3-C5= 84.2849	P1-C4-C5= 62.5617	C2-C4-C5= 95.7153

C3-C5-C4= 95.7151	P1-C2-C6= 91.8102	P1-C3-C6= 91.8102
C2-C6-C3= 68.4994	P1-C4-C6= 89.8692	C2-C4-C6=123.0228
C3-C6-C4= 96.9421	P1-C5-C6= 89.869	C2-C6-C5= 96.9422
C3-C5-C6=123.0226	C4-C6-C5=125.385	P1-C3-H7=146.34
C2-C3-H7=110.2802	C4-C3-H7= 82.4137	P1-C5-H7=152.8069
C2-C5-H7=172.498	C3-C5-H7=119.6533	C4-C5-H7=144.6316
C2-C6-H7=123.8547	C3-H7-C6= 70.1148	C4-C6-H7=152.2975
C6-C5-H7=117.3241	P1-C4-H8=116.7428	C2-C4-H8=149.8964
C3-C4-H8= 82.0476	P1-C5-H8=116.7427	C2-C5-H8= 82.0476
C3-C5-H8=149.8962	C4-H8-C5= 71.6377	C2-C6-H8=145.7503
C3-C6-H8=145.7503	C4-C6-H8=117.3075	C5-C6-H8=117.3075
C3-H7-H8= 96.9691	C4-H8-H7= 98.5696	H7-C5-H8= 90.4504
H7-C6-H8= 90.395	P1-C2-H9=146.34	C3-C2-H9=110.2801
P1-C4-H9=152.8067	C2-C4-H9=119.6531	C3-C4-H9=172.4981
C5-C2-H9= 82.4136	C5-C4-H9=144.6316	C2-H9-C6= 70.1149
C3-C6-H9=123.8546	C6-C4-H9=117.3241	C5-C6-H9=152.2975
H7-C6-H9=179.21	C2-H9-H8= 96.9692	H8-C4-H9= 90.4505
C5-H8-H9= 98.5696	H8-C6-H9= 90.395	H7-H8-H9=125.5015
P1-C2-P10=109.1321	C3-P1-P10=144.5744	C3-C2-P10=145.192
C4-P1-P10= 63.1959	C4-C2-P10=130.5232	C3-C4-P10= 96.064
C5-P1-P10=118.0727	C5-C2-P10=173.0585	C5-C4-P10=123.9305
C6-C2-P10=159.0577	C6-C4-P10=151.238	H8-C4-P10=178.1116
H9-C2-P10=104.5279	H9-C4-P10= 91.4379	P1-C2-H11=124.2042
C3-C2-H11=150.7837	C4-C2-H11=109.229	C5-C2-H11=152.3076
C6-C2-H11=133.8358	H9-C2-H11= 85.7574	P1-P10-H11=123.2139
C2-P10-H11=106.7026	C4-P10-H11= 93.883	P1-C2-H12=124.1957
C3-C2-H12=150.7745	C4-C2-H12=109.2349	C5-C2-H12=152.305
C6-C2-H12=133.8392	H9-C2-H12= 85.7648	P1-P10-H12=123.2032
C2-P10-H12=106.7011	C4-P10-H12= 93.8869	C2-H12-H11= 64.9762
H11-P10-H12=103.0597	P1-P10-S13= 78.4163	C2-P10-S13=112.59
C4-P10-S13=133.8516	C2-H11-S13= 71.3266	H11-P10-S13=113.5159
C2-H12-S13= 71.3264	H12-P10-S13=113.5176	H12-H11-S13= 67.8038
C2-P1-P14=144.5739	P1-C3-P14=109.1328	C2-C3-P14=145.1927
C4-P1-P14=118.0722	C4-C3-P14=173.0592	C5-P1-P14= 63.1954
C2-C5-P14= 96.0643	C5-C3-P14=130.5224	C4-C5-P14=123.9307
C6-C3-P14=159.057	C6-C5-P14=151.2382	H7-C3-P14=104.5272
H7-C5-P14= 91.4377	H8-C5-P14=178.1119	P10-P1-P14=178.7319
P1-C3-H15=124.2067	C2-C3-H15=150.7865	C4-C3-H15=152.3087
C5-C3-H15=109.2275	C6-C3-H15=133.8351	H7-C3-H15= 85.7555
P1-P14-H15=123.2166	C3-P14-H15=106.7034	C5-P14-H15= 93.8826
P1-C3-H16=124.1942	C2-C3-H16=150.7721	C4-C3-H16=152.3035
C5-C3-H16=109.2352	C6-C3-H16=133.839	H7-C3-H16= 85.7656
P1-P14-H16=123.2005	C3-P14-H16=106.7008	C5-P14-H16= 93.8873
C3-H16-H15= 64.9766	H15-P14-H16=103.0598	P1-P14-S17= 78.4168
C3-P14-S17=112.5903	C5-P14-S17=133.8522	C3-H15-S17= 71.3269
H15-P14-S17=113.515	C3-H16-S17= 71.3267	H16-P14-S17=113.5177
H16-H15-S17= 67.8043	C2-P1-Pd18=126.0614	C3-P1-Pd18=126.0584
C4-P1-Pd18=152.5632	C5-P1-Pd18=152.56	P10-P1-Pd18= 89.3673
P1-Pd18-S13= 86.9675	P10-S13-Pd18=105.2489	H11-S13-Pd18=117.2661
H12-S13-Pd18=117.2586	P14-P1-Pd18= 89.3647	P1-Pd18-S17= 86.9706
S13-Pd18-S17=173.9381	P14-S17-Pd18=105.248	H15-S17-Pd18=117.268
H16-S17-Pd18=117.2552	P1-Pd18-Cl19=179.9971	S13-Pd18-Cl19= 93.0333
S17-Pd18-Cl19= 93.0286		

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population			
			Core	Valence	Rydberg	Total
P	1	0.94505	9.99739	3.97649	0.08107	14.05495
C	2	-0.80307	1.99897	4.78566	0.01844	6.80307
C	3	-0.80307	1.99897	4.78566	0.01844	6.80307
C	4	-0.14492	1.99899	4.12613	0.01980	6.14492
C	5	-0.14492	1.99899	4.12613	0.01980	6.14492
C	6	-0.21370	1.99910	4.19969	0.01491	6.21370
H	7	0.27805	0.00000	0.72096	0.00099	0.72195
H	8	0.28182	0.00000	0.71751	0.00067	0.71818
H	9	0.27805	0.00000	0.72096	0.00099	0.72195
P	10	0.88283	9.99820	4.04642	0.07255	14.11717
H	11	0.05409	0.00000	0.94317	0.00274	0.94591
H	12	0.05408	0.00000	0.94318	0.00275	0.94592
S	13	-0.31443	9.99947	6.28708	0.02789	16.31443
P	14	0.88282	9.99820	4.04642	0.07255	14.11718
H	15	0.05409	0.00000	0.94316	0.00274	0.94591
H	16	0.05408	0.00000	0.94318	0.00275	0.94592
S	17	-0.31440	9.99947	6.28704	0.02789	16.31440
Pd	18	0.41353	35.99186	9.55823	0.03638	45.58647
Cl	19	-0.43996	10.00000	7.43175	0.00820	17.43996
* Total *		1.00000	105.97962	69.58883	0.43155	176.00000