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Di- and Trifluorobenzenes in Reactions with Me_2EM (E = P, N; M = $SiMe_3$, $SnMe_3$, Li) Reagents: Evidence for a Concerted Mechanism of Aromatic Nucleophilic Substitution

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In Table 6 of the original article,[1] *the data given for compound* ***12*** *are wrong, the new Table 6 below contains the correct data for* ***12****.*

The Authors

Table 6. Experimental and X-ray crystallographic data for compounds **12**, **18**, **19** and **21**–**23**.

	12	**18**	**19**	**21**	**22**	**23**
Empirical formula	$C_8H_9F_2PS$	$C_{16}H_{20}Cl_2F_2P_2Pd$	$C_{16}H_{18}Cl_2F_4P_2Pd$	$C_{16}H_{18}Cl_2F_4P_2Pd{\cdot}CHCl_3$	$C_{18}H_{12}Cl_2F_{14}P_2Pd$	$C_{16}H_{20}Cl_4F_2P_2Pd_2$
Formula weight	206.18	489.56	525.54	644.91	733.52	666.86
Temperature [K]	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)
Radiation [Å]	Mo-K_α (0.71073)	Mo-K_α (0.71073)	Mo-K_α (0.71073)	Mo-K_α (0.71073)	Mo-K_α (0.71073)	Mo-K_α (0.71073)
Crystal system	monoclinic	monoclinic	triclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1$	$P2_1/c$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$P2_1/n$
Cell dimensions						
a [pm]	768.20(10)	715.60(10)	796.8(2)	956.45(19)	623.6(3)	1364.4(3)
b [pm]	701.10(10)	963.60(10)	901.4(10)	2842.9(6)	748.0(3)	1127.2(2)
c [pm]	863.80(10)	1408.40(10)	1586.3(3)	942.00(19)	2543.6(15)	1571.6(3)
α [°]	90	90	85.47(10)	90	90	90
β [°]	96.470(10)	103.870(10)	80.62(2)	111.74(3)	90.83(3)	114.37(3)
γ [°]	90	90	63.86(10)	90	90	90
Volume [nm^3]	0.46227(10)	0.94285(18)	1.0091(3)	2.3791(8)	1.1862(10)	2.2016(8)
Z	2	2	2	4	2	4
d (calcd.) [Mg/m^3]	1.481	1.724	1.730	1.801	2.054	2.012
μ [mm^{-1}]	0.494	1.450	1.375	1.510	1.260	2.280
Crystal size [mm]	0.60 × 0.50 × 0.20	0.60 × 0.20 × 0.10	0.90 × 0.20 × 0.02	0.40 × 0.20 × 0.20	0.80 × 0.60 × 0.50	0.40 × 0.20 × 0.10
θ range [°]	2.67 to 27.49	2.59 to 27.50	2.52 to 24.99	2.29 to 26.01	2.84 to 27.50	2.44 to 26.05
Range in $h\ k\ l$	$-1 \le h \le 9$	$-9 \le h \le 9$	$-9 \le h \le 1$	$-11 \le h \le 11$	$-1 \le h \le 8$	$-16 \le h \le 16$
	$-8 \le k \le 8$	$-12 \le k \le 12$	$-10 \le k \le 10$	$-34 \le k \le 34$	$-1 \le k \le 9$	$-13 \le k \le 13$
	$-11 \le l \le 11$	$-18 \le l \le 18$	$-18 \le l \le 18$	$-11 \le l \le 11$	$-33 \le l \le 32$	$-19 \le l \le 19$
Refl. collected	2654	8562	4454	25010	3975	14946
Independent refl.	1388, R_{int} = 0.0222	2176, R_{int} = 0.0292	3551, R_{int} = 0.0335	4360, R_{int} = 0.0496	2705, R_{int} = 0.0403	4280, R_{int} = 0.0342
Refl. [$I > 2\sigma(I)$]	1359					
Restr. / parameters	1 / 111					
R_1[a] [$I > 2\sigma(I)$]	0.0237	0.0177	0.0542	0.0274	0.0515	0.0235
wR_2[b] [$I > 2\sigma(I)$]	0.0645	0.0435	0.1274	0.0758	0.1311	0.0499
R_1[a] (all data)	0.0245	0.0198	0.0873	0.0346	0.0585	0.0375
wR_2[b] (all data)	0.0651	0.0444	0.1274	0.0786	0.1396	0.0556
GooF[c] (F_o^2)	1.078	1.076	0.983	1.080	1.156	0.992
Absolute structure parameter	–0.10(9)					
Largest diff. peak [e Å^{-3}]	0.271	0.376	0.812	0.467	1.021	0.450
Largest diff. hole [e Å^{-3}]	–0.219	–0.434	–1.462	–0.484	–1.358	–0.413

[a] $R_1 = \Sigma||F_{obsd.}| - |F_{calcd.}||/\Sigma|F_{obsd.}|$. [b] $wR_2 = \{\Sigma[w(F_{obsd.}^2 - F_{calcd.}^2)^2]/\Sigma[w(F_{obsd.}^2)^2]\}^{1/2}$. [c] $\mathrm{GooF} = \{\Sigma[w(F_{obsd.}^2 - F_{calcd.}^2)/(n-p)\}^{1/2}$.

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