Supporting Information

Highly Efficient Palladium Precatalysts of Homoscorpionate Bispyrazolyl Ligands for the More Challenging Suzuki–Miyaura Cross–Coupling of Aryl Chlorides

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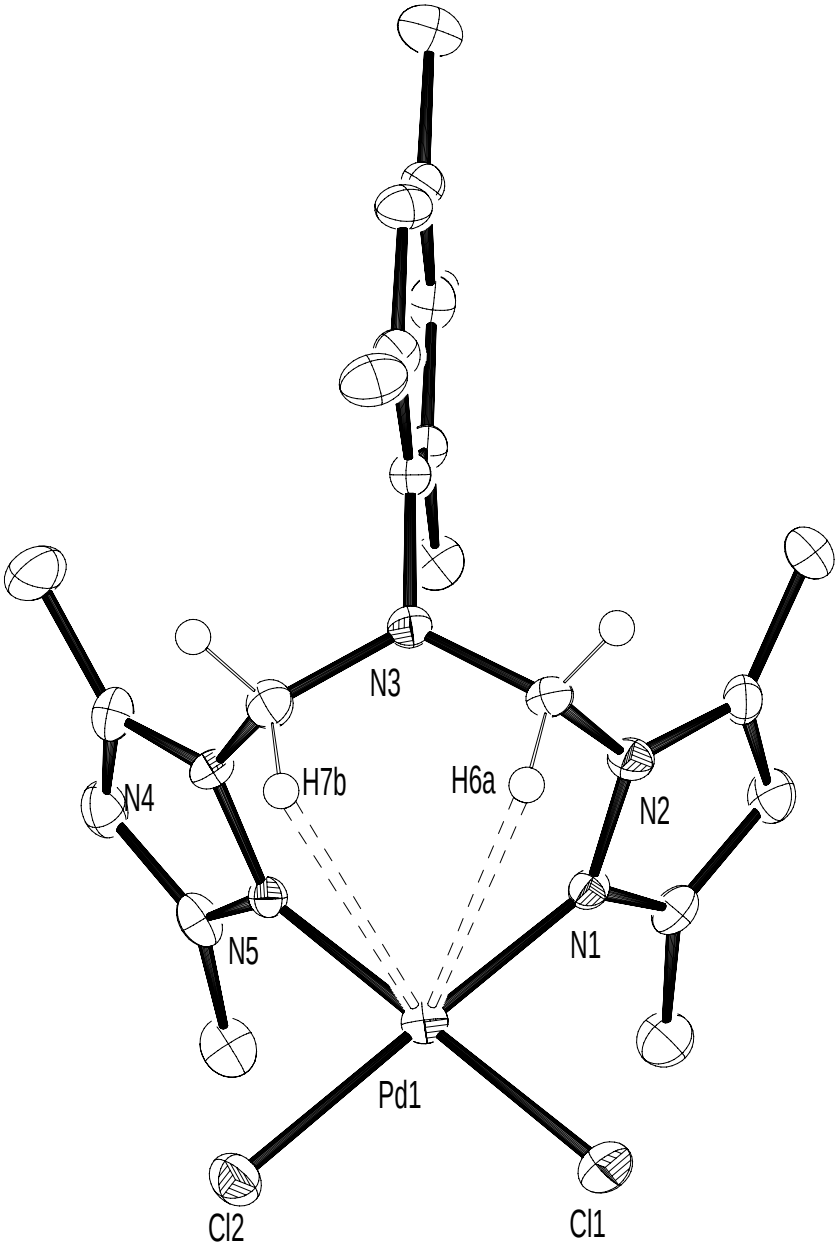


Figure S1. ORTEP of **2** shown with 50 % probability ellipsoids. Selected bond lengths (Å) and angles (^{o}): Pd1-N1 2.0448(18), Pd1-N5 2.0459(18), Pd1-Cl1 2.2810(7), Pd1-Cl2 2.2824(8), Pd1-H6A 2.8436, Pd1-H7B 2.8463, N1-N2 1.366(2), N1-Pd1-N5 92.23(7), N1-Pd1-Cl1 88.42(5), N5-Pd1-Cl1 178.84(6), N1-Pd1-Cl2 178.65(5), N5-Pd1-Cl2 88.01(5).

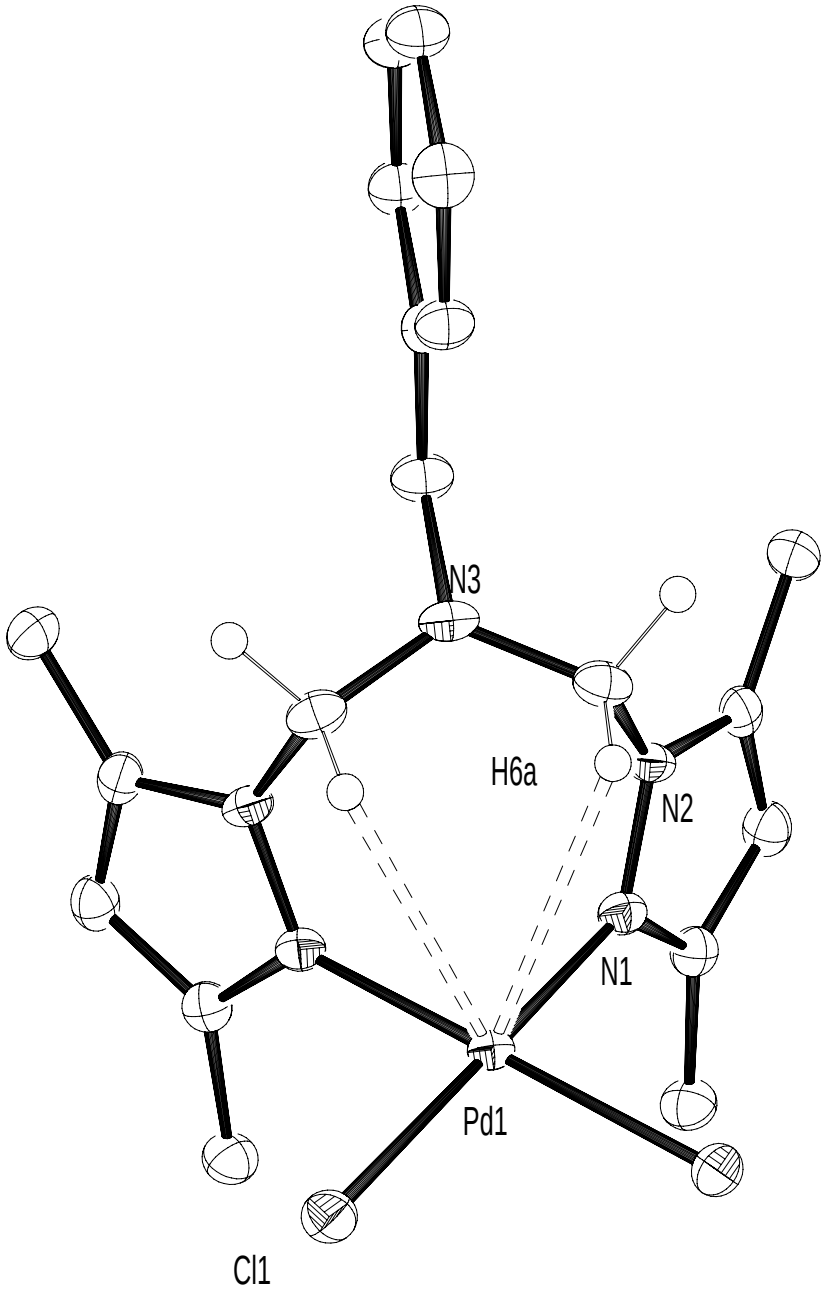


Figure S2. ORTEP of **3** shown with 50 % probability ellipsoids. Selected bond lengths (Å) and angles (°): Pd1-N1 2.0217(15), Pd1-Cl1 2.2866(5), Pd1-H6A 2.8458, N1-N2 1.362(2), N1-Pd1-N1 90.76(9), N1-Pd1-Cl1 177.99(4), Cl1-Pd1-Cl1 92.76(2).

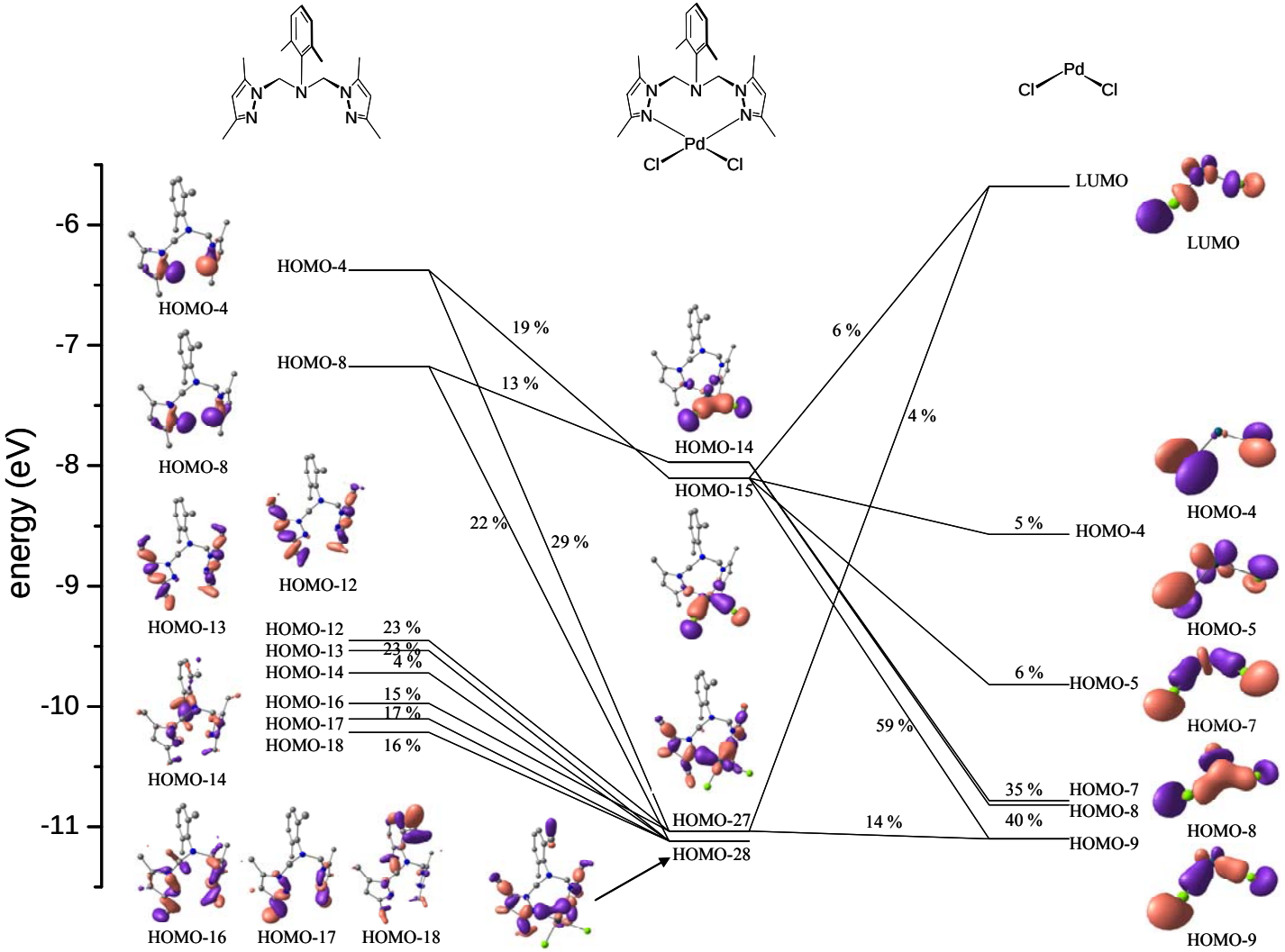


Figure S3. Detailed orbital interaction diagram showing major contributions to the pyrazole─palladium bond in **1**.

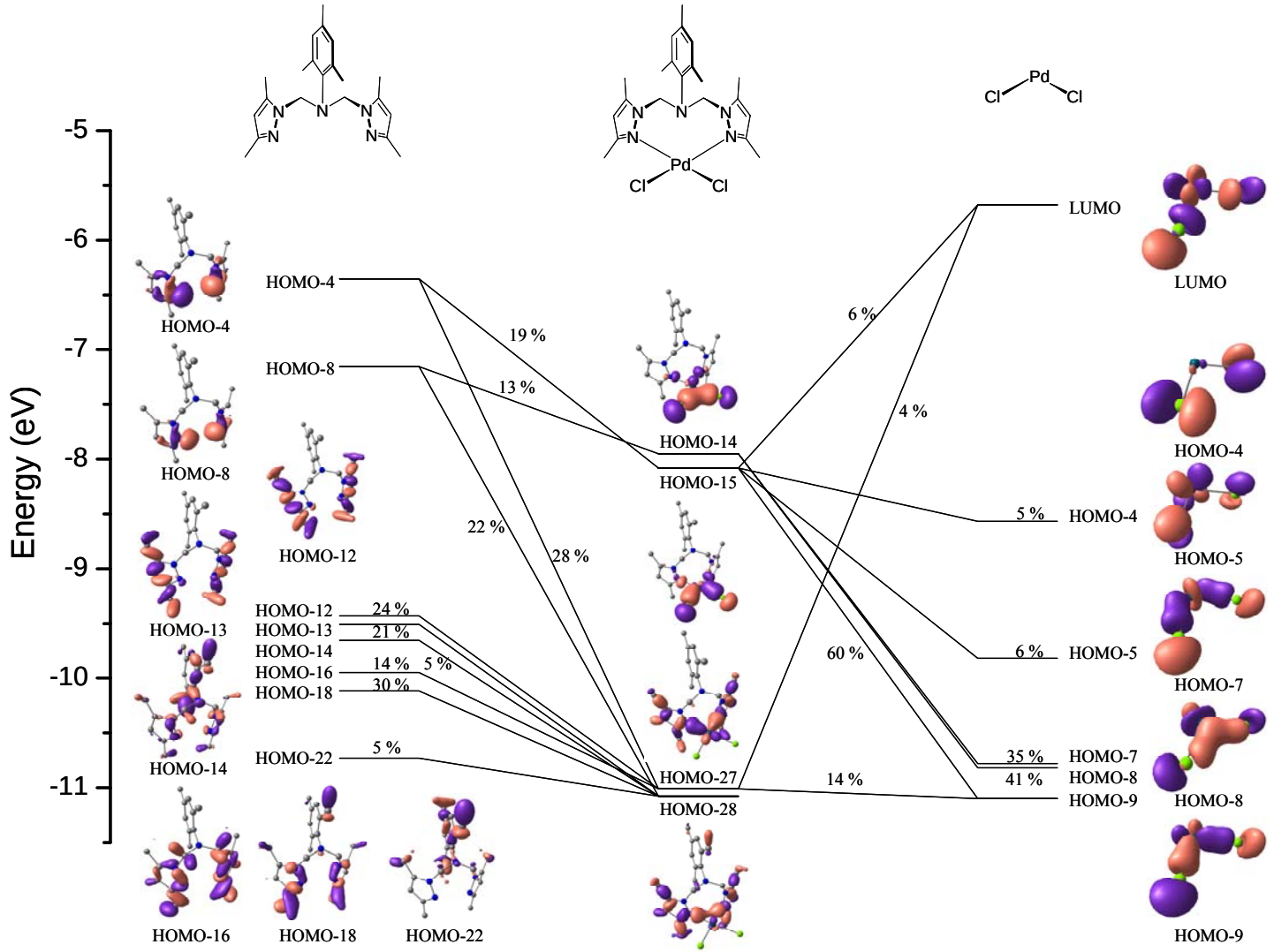


Figure S4. Detailed orbital interaction diagram showing major contributions to the pyrazole─palladium bond in **2**.

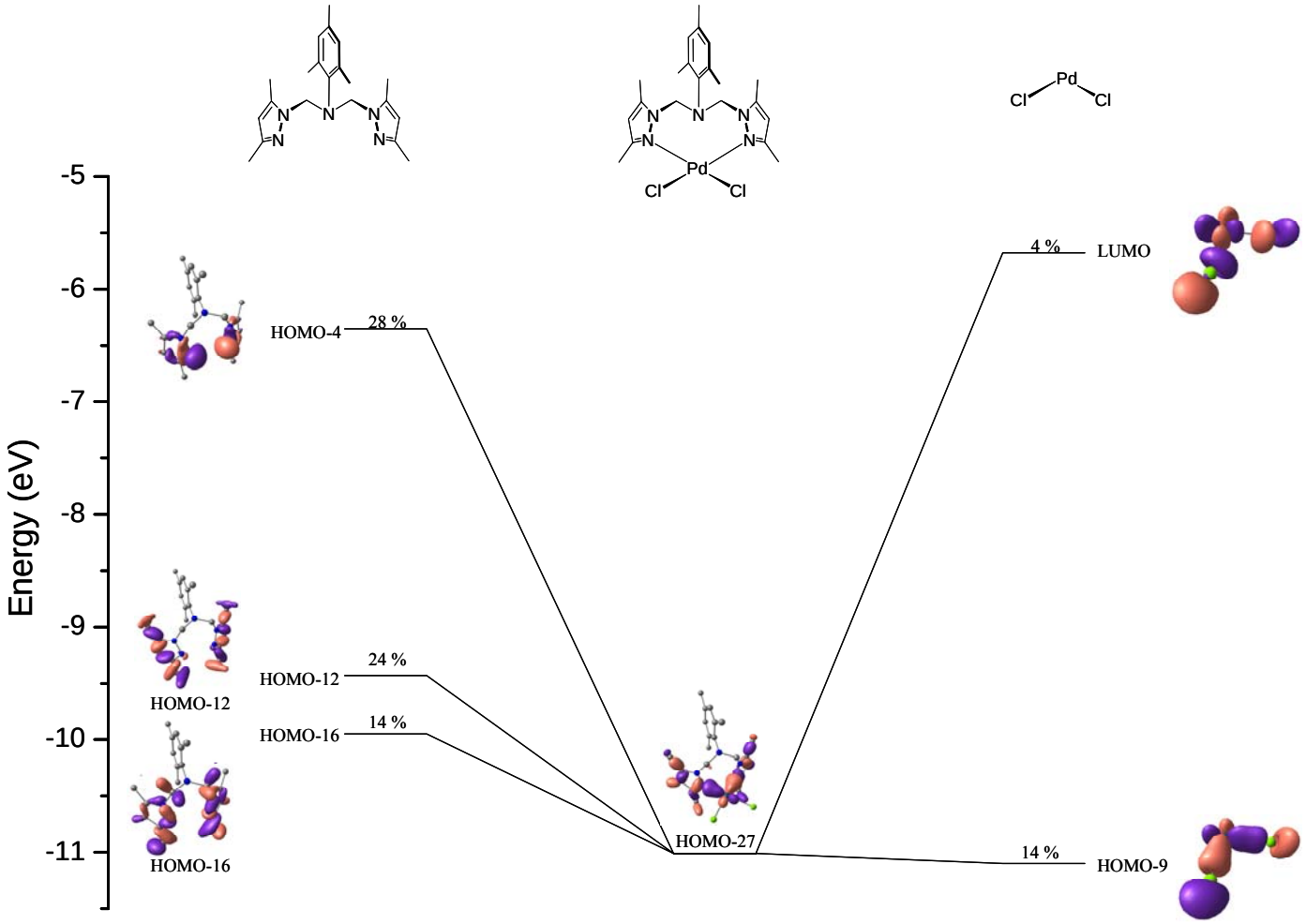


Figure S5. Simplified orbital interaction diagram showing major contributions to the pyrazole─palladium bonding orbital HOMO-27 in **2**.

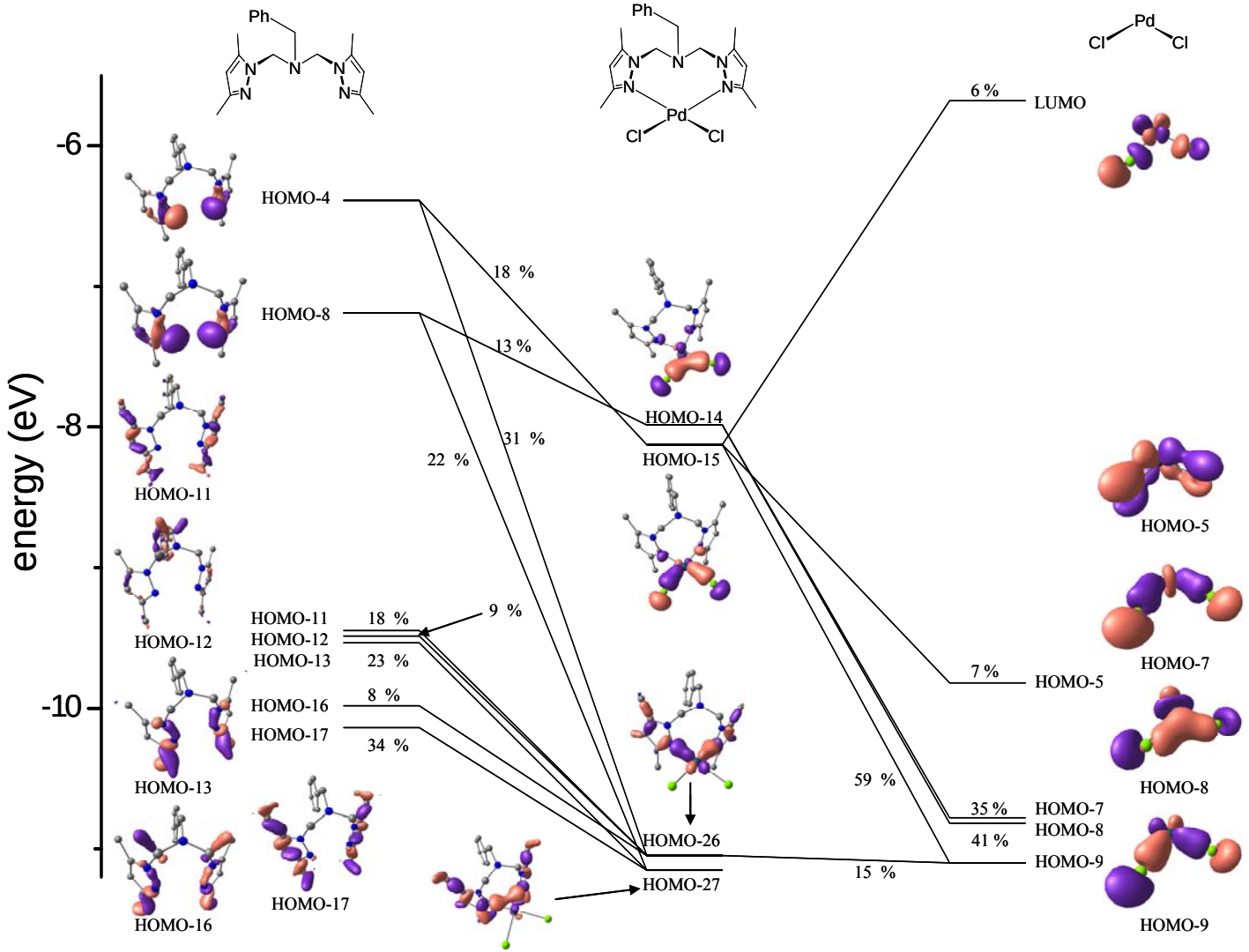


Figure S6. Detailed orbital interaction diagram showing major contributions to the pyrazole─palladium bond in **3**.

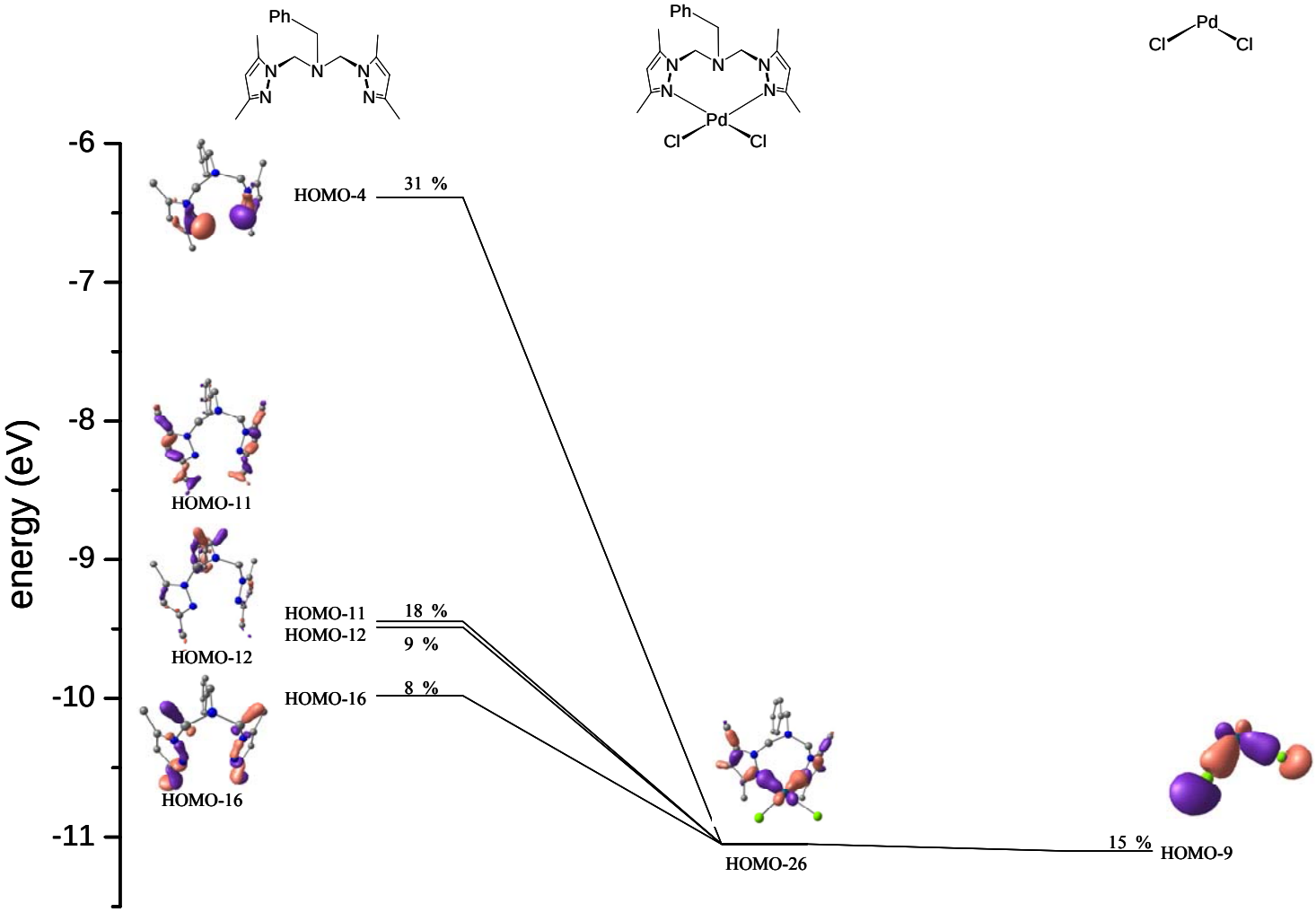


Figure S7. Simplified orbital interaction diagram showing major contributions to the pyrazole─palladium bonding orbital HOMO-26 in **3**.

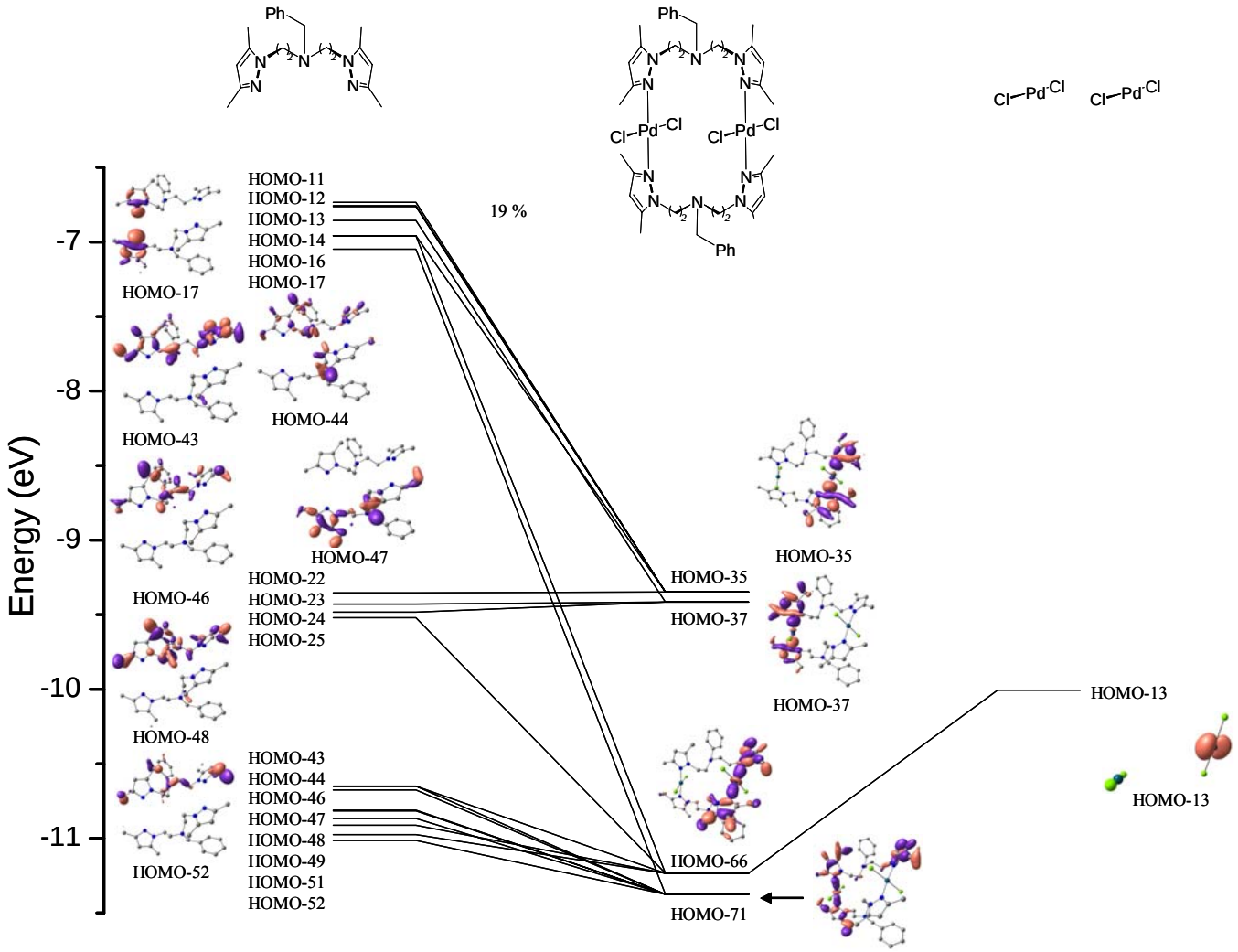


Figure S8. Detailed orbital interaction diagram showing major contributions to the pyrazole─palladium bond in **4**.

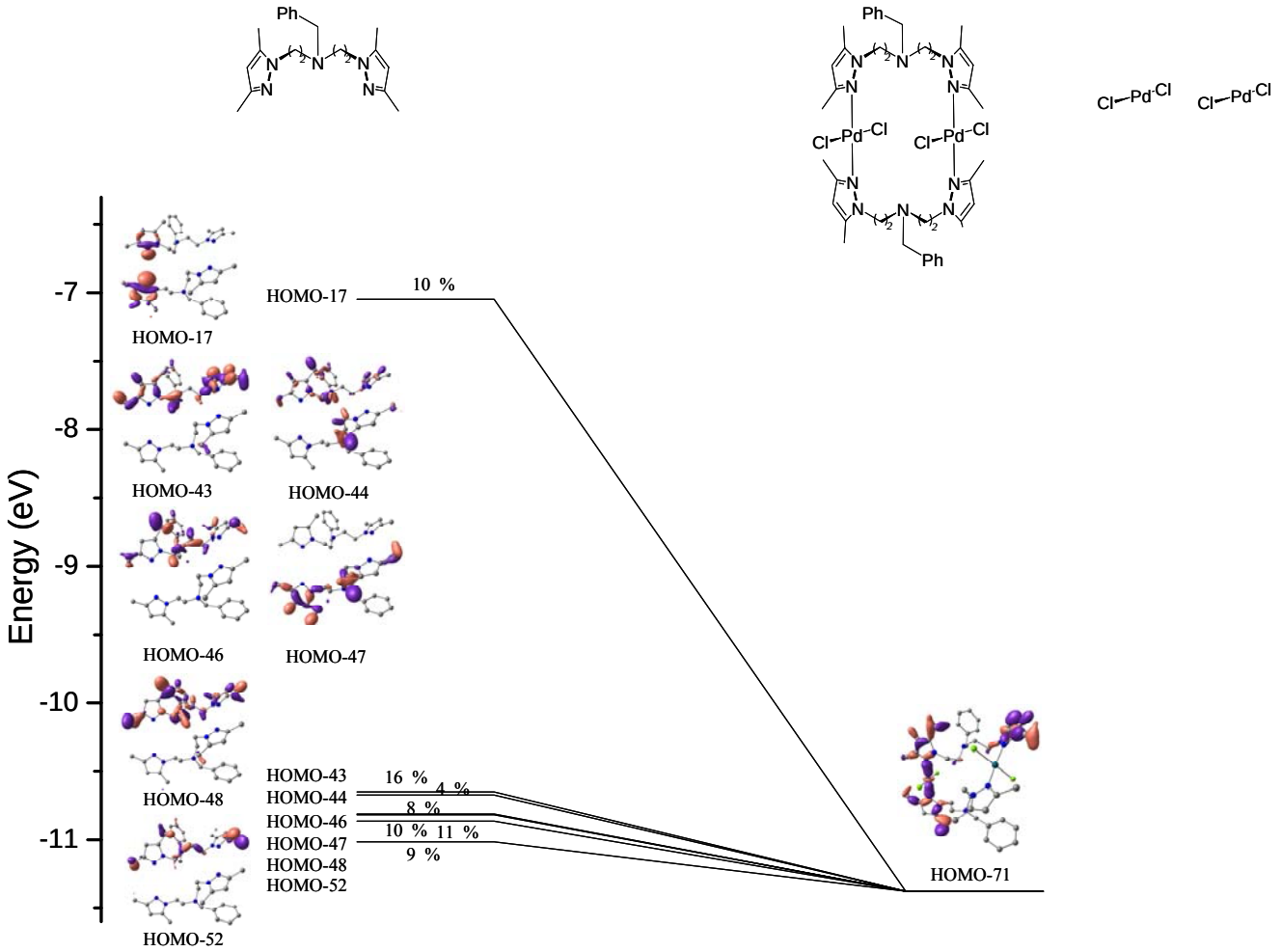


Figure S9. Simplified orbital interaction diagram showing major contributions to the pyrazole─palladium bonding orbital HOMO-71 in **4**.

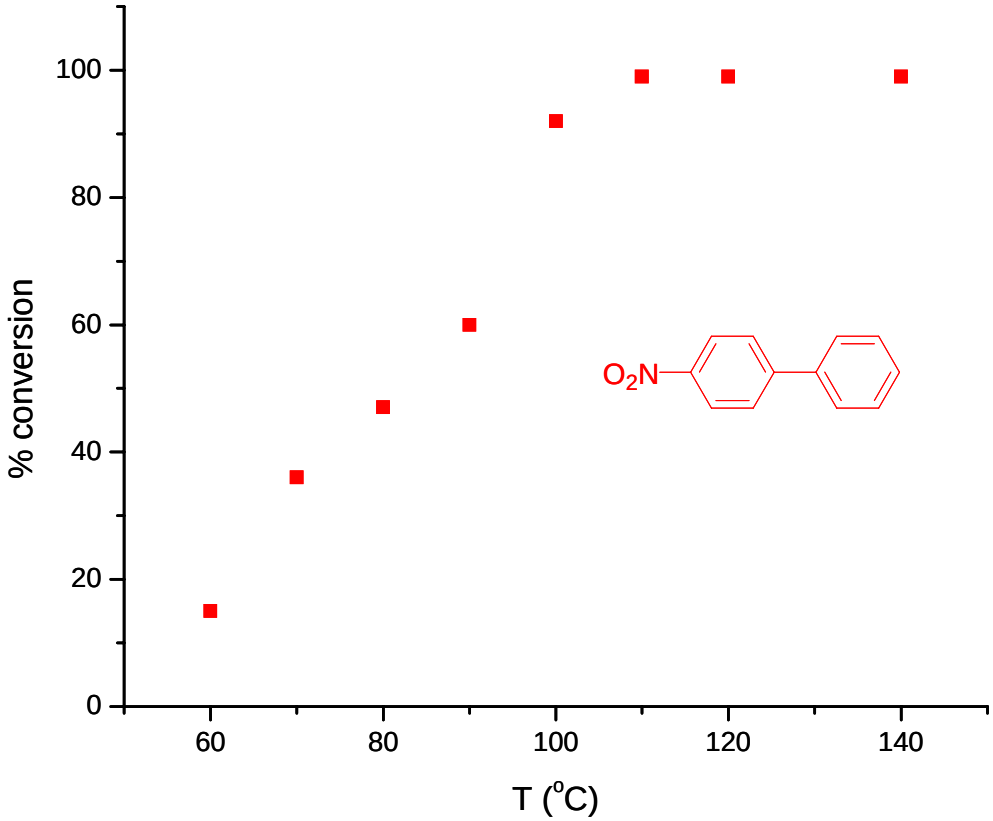


Figure S10. Temperature dependence of the coupling of *p*-$NO_2C_6H_4Cl$ with $PhB(OH)_2$ at 0.5 mol % loading of **3**.

Table S1. X-ray crystallographic data for palladium **1**–**4** complexes.

compound	**1**	**2**	**3**	**4**
lattice	Orthorhombic	Triclinic	Orthorhombic	Triclinic
formula	$C_{22}H_{30}Cl_2N_6Pd$	$C_{25}H_{35}Cl_2N_7Pd$	$C_{19}H_{24}Cl_2N_5Pd$	$C_{44}H_{61}Cl_4N_{11}Pd_2$
formula weight	555.82	610.90	499.73	1098.64
Space group	P 21 21 21	P-1	Pcmn[a]	P-1
a/Å	11.6343(2)	10.688(4)	8.1966(2)	12.8252(1)
b/Å	12.5462(3)	12.313(2)	13.6939(3)	12.8252(1)
c/Å	16.8066(4)	12.6717(12)	18.0046(4)	17.6659(2)
α/°	90	110.583(14)	90	98.513(9)
β/°	90	105.572(19)	90	111.107(8)
γ/°	90	101.64(2)	90	107.462(8)
V/Å^3	2453.20(9)	1420.4(6)	2020.90(8)	2476.5(3)
Z	4	2	4	2
temperature (K)	123(2)	123(2)	123(2)	123(2)
radiation (λ,Å)	0.71073	0.71073	0.71073	0.71073
ρ (calcd.), g cm^{-3}	1.505	1.428	1.642	1.473
μ(Mo Kα), mm^{-1}	0.995	0.868	1.197	0.985
θ max, deg.	32.0906	32.4264	32.4887	32.2149
No. of data	8066	9378	3588	13369
No. of parameters	259	325	138	559
Flack Parameter	-0.02(3)			
R_1	0.0426	0.0350	0.0275	0.0549
wR_2	0.0871	0.0562	0.0652	0.1277
GOF	1.077	0.823	1.032	0.956

[a] The reported space group Pcmn is a non-standard setting of Pmna.

The density functional theory calculations were performed for the palladium **1–4** complexes by using the GAUSSIAN 03[1] suite of quantum chemical programs.

Table S2. B3LYP/SDD, 6-31G(d) optimized coordinates of **1**.

Energy = -2100.5472514 hartree/particle.

N	-0.97522	-1.50413	0.487914
N	0.225668	-1.92987	0.006342
N	1.499391	0.000214	-0.86528
N	0.217392	1.930913	-0.00508
N	-0.9811	1.501609	0.478973
C	-2.60241	-2.17716	2.230229
H	-2.66508	-1.21702	2.754865
H	-2.70832	-2.97702	2.968535
H	-3.4398	-2.22794	1.526607
C	-1.30576	-2.31691	1.497234
C	-0.28685	-3.2739	1.672803
H	-0.26468	-4.07066	2.40251
C	0.671941	-3.00953	0.709007
C	1.959187	-3.7153	0.413553
H	2.108452	-4.51366	1.144916
H	2.821657	-3.04162	0.466995
H	1.953342	-4.17662	-0.5818
C	0.848054	-1.25182	-1.14255
H	1.570438	-1.96659	-1.54377
H	0.051429	-1.10248	-1.87633
C	2.869049	0.002955	-0.42403
C	3.195502	0.01871	0.948358
C	2.15395	0.040772	2.045313
H	2.220117	0.969347	2.625635
H	2.314155	-0.78607	2.747304
H	1.138629	-0.037	1.657325
C	4.552914	0.018355	1.310701
H	4.814285	0.028853	2.366455
C	5.557025	0.004323	0.349602
H	6.600872	0.004076	0.651888
C	5.222013	-0.00999	-1.00503
H	6.006053	-0.02056	-1.75787
C	3.88522	-0.01107	-1.41081
C	3.545178	-0.0269	-2.88455
H	4.456863	-0.01504	-3.48909
H	2.941055	0.838956	-3.17984

H	2.973477	-0.91855	-3.16848
C	0.844069	1.24861	-1.14903
H	0.049166	1.092618	-1.88335
H	1.564821	1.963533	-1.55307
C	1.937579	3.732521	0.386549
H	2.804904	3.065841	0.449309
H	2.079425	4.540203	1.109107
H	1.93078	4.182487	-0.61396
C	0.654743	3.02081	0.687097
C	-0.30707	3.287717	1.647349
H	-0.29158	4.091696	2.369267
C	-1.31898	2.321834	1.479581
C	-2.61853	2.183422	2.207463
H	-3.45409	2.289293	1.507456
H	-2.70322	2.950403	2.982503
H	-2.7083	1.201035	2.683965
Pd	-2.09719	-0.00616	-0.43854
Cl	-3.30146	-1.68749	-1.48678
Cl	-3.30666	1.665138	-1.49717

Table S3. B3LYP/SDD, 6-31G(d) optimized coordinates of **2**.

Energy = -2139.8649961 hartree/particle.

N	-1.1728	1.500606	0.485306
N	0.006876	1.932972	-0.04049
N	1.257412	0.001974	-0.94241
N	0.009754	-1.93179	-0.04266
N	-1.17311	-1.50654	0.482047
C	-2.74687	2.175065	2.274622
H	-3.60688	2.306057	1.609224
H	-2.79367	2.924805	3.06953
H	-2.8304	1.182631	2.730769
C	-1.47407	2.316265	1.50141
C	-0.45663	3.281154	1.637097
H	-0.41463	4.081314	2.362183
C	0.469757	3.018713	0.641415
C	1.741706	3.731073	0.298709
H	2.608439	3.061023	0.31776
H	1.914997	4.528608	1.025686
H	1.69572	4.194333	-0.69469
C	0.596457	1.251541	-1.20462
H	-0.22033	1.098841	-1.91509
H	1.305511	1.966508	-1.62877
C	0.596835	-1.24752	-1.20631

H	1.305762	-1.96107	-1.63309
H	-0.22116	-1.0939	-1.91519
C	1.752394	-3.72295	0.294372
H	1.707016	-4.18739	-0.69852
H	1.930272	-4.51899	1.021881
H	2.616099	-3.049	0.311529
C	0.477728	-3.01602	0.638253
C	-0.44798	-3.28435	1.632803
H	-0.40271	-4.0855	2.356607
C	-1.47024	-2.32446	1.497743
C	-2.73825	-2.18486	2.279506
H	-2.75785	-1.24812	2.84849
H	-2.83996	-3.01355	2.985977
H	-3.59969	-2.18495	1.603904
C	2.633978	0.001814	-0.5237
C	3.638114	0.001645	-1.52391
C	3.276872	0.001915	-2.99268
H	4.179303	0.001982	-3.61108
H	2.684188	0.880827	-3.27286
H	2.684143	-0.87685	-3.27323
C	4.978242	0.001098	-1.13922
H	5.746964	0.000785	-1.90954
C	5.35972	0.000951	0.210227
C	6.82054	0.001044	0.596685
H	6.947294	-0.00598	1.683598
H	7.336532	0.88632	0.20474
H	7.339919	-0.87676	0.192726
C	4.354047	0.00122	1.174526
H	4.629172	0.001027	2.227699
C	2.989509	0.001527	0.83893
C	1.973979	0.000624	1.960263
H	0.947768	0.007448	1.593877
H	2.107808	0.877694	2.60485
H	2.098929	-0.88461	2.595499
Pd	-2.32588	-0.00144	-0.39485
Cl	-3.57375	1.677318	-1.39603
Cl	-3.57686	-1.67501	-1.4005

Table S4. B3LYP/SDD, 6-31G(d) optimized coordinates of **3**.

Energy = -2061.2262513 hartree/particle.

N	-0.73694	-1.49678	0.356871
N	0.249352	-1.90526	-0.49061
N	1.136738	-1.3E-05	-1.80625

N	0.249432	1.905201	-0.49053
N	-0.73661	1.496478	0.357133
C	-1.69004	-2.18164	2.539121
H	-1.55301	-1.24641	3.094163
H	-1.57294	-3.0127	3.240444
H	-2.71088	-2.19013	2.143785
C	-0.70436	-2.30686	1.420387
C	0.33248	-3.24583	1.254435
H	0.608301	-4.03502	1.939116
C	0.918926	-2.97329	0.03033
C	2.061967	-3.65261	-0.65655
H	2.389738	-4.50254	-0.05274
H	2.920124	-2.98194	-0.78138
H	1.781674	-4.0383	-1.64423
C	0.422993	-1.24547	-1.79661
H	0.946438	-1.97142	-2.42517
H	-0.58507	-1.09986	-2.19363
C	2.584765	-1.6E-05	-1.93756
C	0.423007	1.245455	-1.79655
H	-0.58506	1.099864	-2.19355
H	0.946439	1.971426	-2.4251
C	2.061789	3.652808	-0.65664
H	2.920082	2.982293	-0.78141
H	2.389389	4.502882	-0.05294
H	1.781401	4.038318	-1.64437
C	0.918912	2.973316	0.030343
C	0.332641	3.245698	1.254572
H	0.608452	4.034908	1.939238
C	-0.70398	2.306526	1.420675
C	-1.68944	2.181084	2.539579
H	-2.71037	2.189953	2.144474
H	-1.57201	3.011851	3.241201
H	-1.5525	1.245611	3.094216
C	3.431077	-3.1E-05	-0.66325
C	4.828623	-4.5E-05	-0.79635
C	2.878039	-3.3E-05	0.620957
C	5.653887	-6.2E-05	0.326838
C	3.705405	-5.2E-05	1.748794
C	5.092289	-6.7E-05	1.607206
H	5.273774	-4.2E-05	-1.79019
H	1.800256	-1.4E-05	0.742871
H	6.733731	-7.6E-05	0.204045
H	3.258288	-5.5E-05	2.7393
H	5.733064	-8.3E-05	2.484674
H	2.866567	-0.87394	-2.54275
H	2.866581	0.873902	-2.54275

Pd	-2.10586	0.000035	-0.13297
Cl	-3.60023	-1.67545	-0.71327
Cl	-3.59982	1.67599	-0.71295

Table S5. B3LYP/SDD, 6-31G(d) optimized coordinates of **4**.

Energy = -4279.7339465 hartree/particle.

N	-3.53407	1.399762	1.410156
N	-2.29914	1.898826	1.69477
N	-0.44771	2.980823	-0.55666
N	3.3453	2.875467	-0.90876
N	3.999458	2.103403	0.002489
N	3.219354	-1.70766	1.340263
N	2.030958	-2.35485	1.505082
N	-0.03864	-3.47182	-0.76455
N	-3.75984	-2.86546	-1.3639
N	-4.49599	-2.10624	-0.50626
C	-5.9054	1.95913	1.889528
H	-6.22043	1.879565	0.843926
H	-6.45713	2.776804	2.362246
H	-6.17512	1.025521	2.396557
C	-4.43383	2.213286	1.980627
C	-3.75659	3.253549	2.63813
H	-4.20105	4.061721	3.200803
C	-2.40114	3.029387	2.440012
C	-1.21542	3.805627	2.919646
H	-0.5246	3.180838	3.497771
H	-1.55314	4.620346	3.565523
H	-0.65549	4.237493	2.083811
C	-1.1043	1.268018	1.15
H	-1.23709	0.191801	1.277151
H	-0.25544	1.565772	1.76927
C	-0.87269	1.600456	-0.33309
H	-0.14768	0.866636	-0.72523
H	-1.80882	1.430938	-0.87257
C	-0.9642	3.573386	-1.79851
H	-2.01768	3.27915	-1.87206
H	-0.47208	3.174541	-2.70488
C	-0.8702	5.088248	-1.81273
C	-1.44092	5.843302	-0.77745
H	-1.93388	5.326469	0.041303
C	-1.38282	7.23608	-0.79815
H	-1.83289	7.807468	0.00964
C	-0.75462	7.899272	-1.85696

H	-0.71147	8.985027	-1.87295
C	-0.18863	7.159035	-2.8948
H	0.296685	7.66496	-3.72548
C	-0.24637	5.761988	-2.86889
H	0.188842	5.189063	-3.68548
C	0.967993	3.222894	-0.29264
H	1.216687	2.845053	0.704378
H	1.134949	4.305499	-0.27377
C	1.969462	2.588414	-1.29565
H	1.873455	1.501991	-1.34477
H	1.828091	2.980797	-2.30569
C	3.625982	5.02239	-2.18401
H	3.54253	4.608921	-3.19708
H	4.359321	5.83221	-2.2157
H	2.654897	5.457676	-1.9228
C	4.076444	3.984465	-1.20482
C	5.244902	3.902048	-0.46387
H	6.061614	4.609359	-0.46598
C	5.161793	2.711189	0.277188
C	6.157668	2.122981	1.226308
H	5.68448	1.883285	2.184193
H	6.971305	2.832232	1.403972
H	6.587974	1.199906	0.821633
C	5.607965	-2.06949	1.9132
H	5.950058	-1.79913	0.909003
H	6.224917	-2.89269	2.285193
H	5.761382	-1.20411	2.568445
C	4.168748	-2.47822	1.889454
C	3.573547	-3.63936	2.409393
H	4.072914	-4.45256	2.915769
C	2.215244	-3.53607	2.149434
C	1.091373	-4.46761	2.473496
H	0.37175	-4.00816	3.162571
H	1.4891	-5.36597	2.952461
H	0.55284	-4.76036	1.566988
C	0.810376	-1.80731	0.928466
H	0.891078	-0.72518	1.037984
H	-0.03024	-2.1347	1.544879
C	0.61267	-2.17546	-0.55367
H	0.05299	-1.3551	-1.03576
H	1.59717	-2.19183	-1.02886
C	0.381374	-4.1345	-2.0126
H	0.364083	-3.44576	-2.87577
H	-0.35762	-4.91784	-2.22163
C	1.75451	-4.77095	-1.90687
C	2.864825	-4.21774	-2.55226

H	2.752011	-3.30867	-3.13754
C	4.125509	-4.81131	-2.43892
H	4.978429	-4.35895	-2.9367
C	4.285169	-5.97293	-1.68455
H	5.263633	-6.43812	-1.59834
C	3.180351	-6.53815	-1.0393
H	3.296955	-7.44701	-0.45433
C	1.927268	-5.93908	-1.14959
H	1.069555	-6.37961	-0.64587
C	-1.4837	-3.46782	-0.5454
H	-1.70388	-3.09313	0.459337
H	-1.83145	-4.5078	-0.57163
C	-2.33107	-2.64572	-1.55678
H	-2.15993	-1.57181	-1.45798
H	-2.09583	-2.9259	-2.58758
C	-3.99339	-4.87952	-2.85021
H	-3.66977	-4.40259	-3.78367
H	-4.78398	-5.59224	-3.09769
H	-3.14328	-5.44789	-2.45501
C	-4.51652	-3.87957	-1.86764
C	-5.77986	-3.74972	-1.31402
H	-6.6364	-4.37994	-1.50478
C	-5.72904	-2.62787	-0.46935
C	-6.81906	-2.02149	0.356764
H	-6.51782	-1.94731	1.407116
H	-7.72257	-2.63501	0.295793
H	-7.05967	-1.01327	0.001893
Pd	-3.91618	-0.36417	0.422129
Pd	3.486213	0.206444	0.621441
Cl	-3.18813	-1.59671	2.29814
Cl	-4.54475	0.838868	-1.50261
Cl	2.584018	1.095949	2.615575
Cl	4.253979	-0.6393	-1.43335

Table S6. Natural charge analyses of the palladium **1** and **2** complexes.

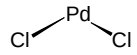
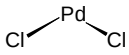
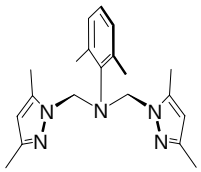
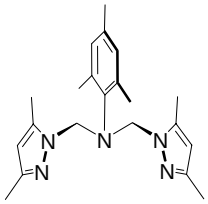
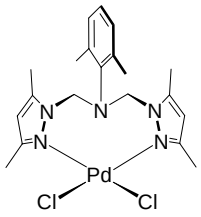
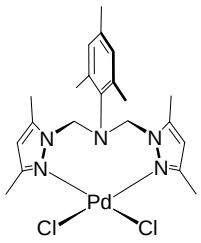
compound/specie	$N_{pyrazole}$	Pd	compound/specie	$N_{pyrazole}$	Pd
		0.654			0.654
	-0.296 -0.296			-0.296 -0.296	
 **1**	-0.319 -0.319	0.621	 **2**	-0.319 -0.319	0.622

Table S7. Natural charge analyses of the palladium **3** and **4** complexes.

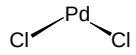
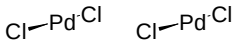
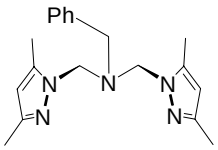
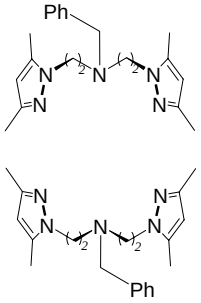
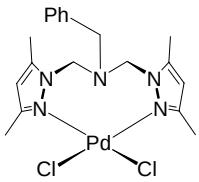
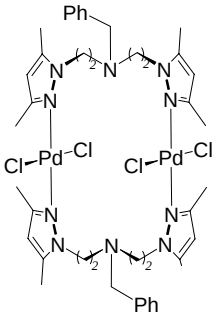
compound/specie	$N_{pyrazole}$	Pd	compound/specie	$N_{pyrazole}$	Pd
		0.654			0.975 0.975
	-0.297 -0.297			-0.319 -0.313 -0.320 -0.309	
	-0.319 -0.319	0.621		-0.305 -0.300 -0.306 -0.296	0.651 0.651
3			**4**		

Table S8. Mulliken charge analyses of the palladium **1** and **2** complexes.

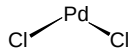
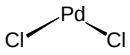
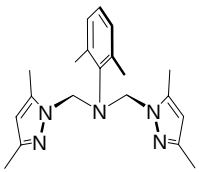
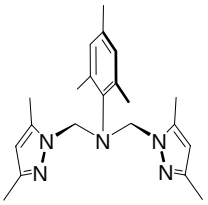
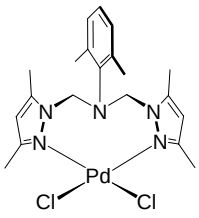
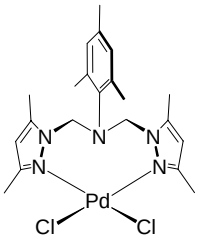
compound/specie	$N_{pyrazole}$	Pd	compound/specie	$N_{pyrazole}$	Pd
		0.269			0.269
	-0.285 -0.286			-0.286 -0.285	
 **1**	-0.319 -0.319	0.022	 **2**	-0.319 -0.319	0.023

Table S9. Mulliken charge analyses of the palladium **3** and **4** complexes.

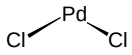
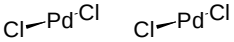
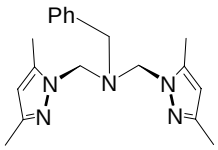
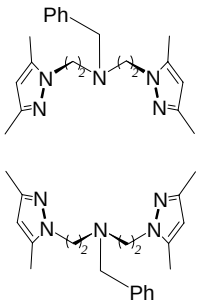
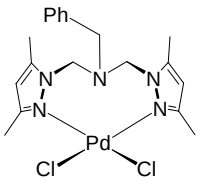
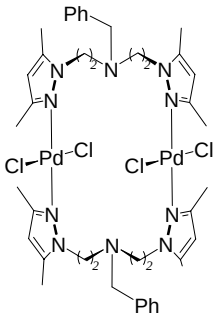
compound/specie	$N_{pyrazole}$	Pd	compound/specie	$N_{pyrazole}$	Pd
		0.269			0.448 0.448
	-0.286 -0.286			-0.315 -0.309 -0.315 -0.307	
	-0.320 -0.320	0.027		-0.306 -0.298 -0.306 -0.295	-0.006 -0.002
3			**4**		

Table S10. Electronic configuration of Pd in the palladium **1** and **2** complexes.

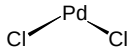
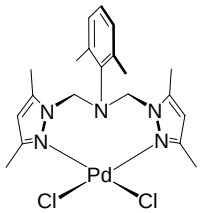
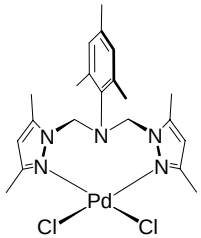
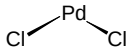
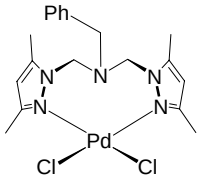
compound/specie	*5s*	*4d*	*5p*	*6p*	*6d*	*7p*	compound/specie	*5s*	*4d*	*5p*	*6p*	*6d*	*7p*
Pd^{2+}		8.00					Pd^{2+}		8.00				
	0.28	9.03	0.03					0.28	9.03	0.03			
 **1**	0.42	8.92		0.01	0.01	0.01	 **2**	0.42	8.92		0.01	0.01	0.01

Table S11. Electronic configuration of Pd in the palladium **3** and **4** complexes.

compound/specie	*5s*	*4d*	*5p*	*6p*	*6d*	*7p*
Pd^{2+}		8.00				
	0.28	9.03	0.03			
	0.42	8.92		0.01	0.01	0.01
3						

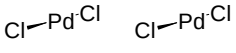
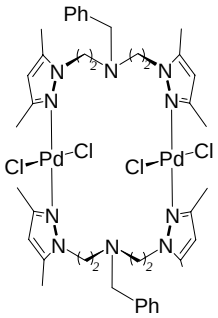
compound/specie	*5s*	*4d*	*5p*	*5d*	*6p*	*6d*
Pd^{2+}		8.00				
	0.06 0.06	8.91 8.91	0.04 0.04			
	0.41 0.41	8.91 8.90		 0.01	0.01 0.01	0.01 0.01
4						

Table S12. Bond distance & bond energy of Pd-$N_{pyrazole}$ in **1**–**4**.

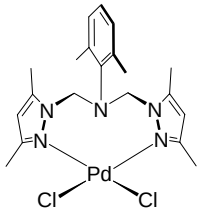
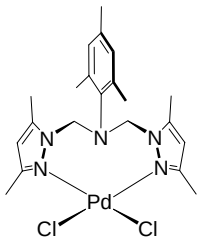
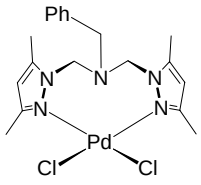
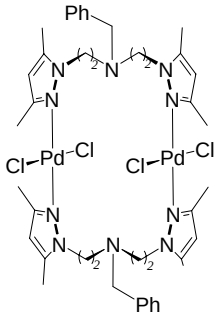
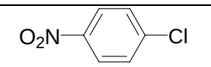
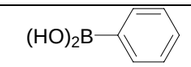
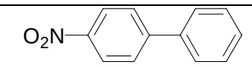
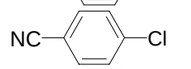
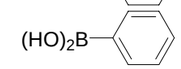
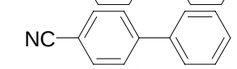
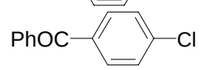
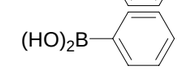
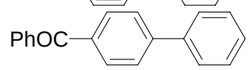
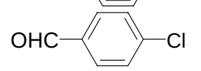
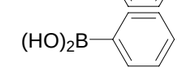
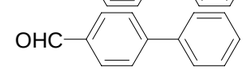
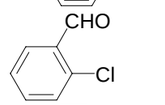
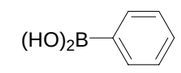
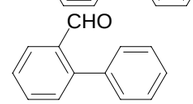
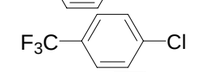
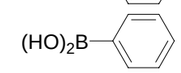
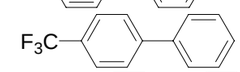
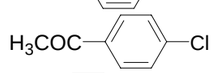
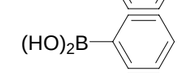
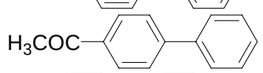
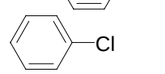
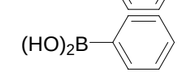
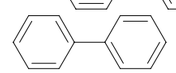
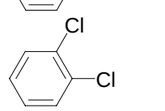
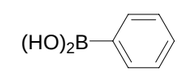
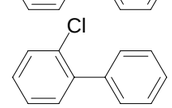
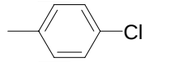
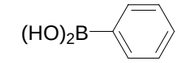
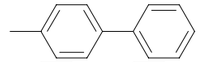
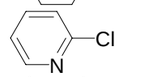
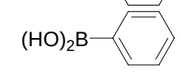
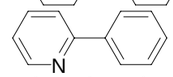
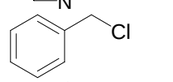
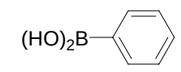
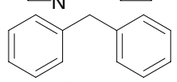
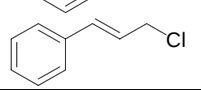
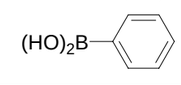
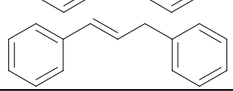
compound	d(Pd-$N_{pyrazole}$) (Å)	D_e(Pd-$N_{pyrazole}$) (kcal/mol)
 **1**	2.09	41.98
 **2**	2.09	42.05
 **3**	2.09	41.87
 **4**	2.06	50.20

Table S13. Selected results for Suzuki–Miyaura cross-coupling reaction of chlorides catalyzed by $PdCl_2$ and by **3** under Hg(0) conditions.

entry	Reagent[a]	reagent[a]	cross-coupled product	yield[b] $PdCl_2$	yield[b] $(COD)PdCl_2$	yield[b] Hg(0) drop
1				>99	91	>99
2				77	51	>99
3				78	86	>99
4				26	39	>99
5				67	49	>99
6				62	24	>99
7				15	15	69
8				41	12	70
9				11	10	29
10				4	2	10
11				14	13	15
12				32	49	>99
13				0	0	15

[a] Reaction conditions: 1.00 mmol of aryl chloride, 1.20 mmol of boronic acid, 1.50 mmol of Cs_2CO_3, 1.50 mmol of TBAB, 2 mol % of $PdCl_2$ or $(COD)PdCl_2$ or **3** in 8 mL of DMF:H_2O (9:1), at 120 °C for 5 hours. [b] The yields (%) were determined by GC using diethylene glycol di-n-butyl ether as an internal standard.

References

[1]. GAUSSIAN 03: Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.