Electronic Supplementary Material (ESI) for Dalton Transactions.

Explicit account of solvation may be crucial for modeling Suzuki-Miyaura coupling in protic solvents.

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Supporting information

Simulation details

FEP

Energy minimization was performed with *steep* integrator to the energy tolerance of 100 kJ*mol^{-1}*nm^{-1}. Molecular dynamics was run with *sd* (Langevin dynamics) integrator with 2 fs timestep. Electrostatic interactions were treated by 6th order particle mesh Ewald (PME) with the cut-off radius 1.0 nm. Pressure was controlled by Parrinelo-Rahman barostat.

Transition free energies were calculated by Bennett acceptance ratio [1]. First, coulomb interactions of the solute with solvent were turned off. and then VdW component was decoupled (in order to avoid singularities).

An error estimate taking into account temporal correlations was made by splitting the data into blocks and determining the free energy differences over those blocks and assuming the blocks are independent. The final error estimate was determined from the average variance over 5 blocks.

Supporting tables 1-5. Phase space overlap measures

Phase space overlap at each λ window was estimated from relative entropies s_A and s_B by calculating parameter Π according to formula

$$\Pi_{A\to B} = \sqrt{\frac{s_A}{s_B} W_L\left[\frac{1}{2\pi}(M-1)^2\right]} - \sqrt{2s_A}.$$

$$\Pi_{B\to A} = \sqrt{\frac{s_B}{s_A} W_L\left[\frac{1}{2\pi}(M-1)^2\right]} - \sqrt{2s_B}.$$

, where s_A and s_B are an information theory entropy which reflects the "distance" between the distributions of phase space A and B. $W_L(x)$ is the Lambert W function. M is the number of work trials used in the free energy calculation. s_A and s_B are calculated as

$$s_A = \langle W \rangle_A - \Delta G.$$

$$s_A = -\langle W \rangle_B + \Delta G.$$

and represent the dissipated work. s_A and s_B are non-negative and equal to zero for identical distributions.

Maximum of $\Pi_{A\to B}$ and $\Pi_{B\to A}$ was selected [4].

Transitions with Π values < 0.5 (indicating poor phase space overlap) are denoted with asterisk * and were divided into two steps and re-calculated (see Table 8 below).

Supporting Table 1. Π values for benzene

λ	$Pd(PPh_3)_2Ph_2$		Transition state		$Pd(PPh_3)_2$		Ph_2	
	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW
0-0.1	4.48	3.98	4.48	4	4.42	4.1	4.48	5.62
0.1-0.2	4.42	3.39	4.42	3.41	4.42	3.45	4.42	4.47
0.2-0.3	4.42	3.54	6.33	3.54	4.42	3.55	4.48	4.45
0.3-0.4	4.48	3.53	6.33	3.56	4.38	3.52	4.48	4.49
0.4-0.5	4.34	3.43	4.42	3.46	4.42	3.4	4.42	4.39

0.5-0.6	4.38	3.27	4.48	3.25	4.38	3.19	4.42	4.33
0.6-0.7	4.38	2.92	4.48	2.95	4.42	2.87	4.42	4.16
0.7-0.8	4.38	2.12	4.42	2.2	4.38	2.09	4.48	3.74
0.8-0.9	4.42	0.21*	4.42	0.2*	4.38	1.01	4.42	2.81
0.9-1	4.38	2.16	4.42	2.24	4.34	2.16	4.48	3.53

*Simulation was repeated with more λ steps, see Table 10

Supporting Table 2. Π values for DMF

λ	$Pd(PPh_3)_2Ph_2$		Transition state		$Pd(PPh_3)_2$		Ph_2	
	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW
0-0.1	4.27	3.48	4.3	3.48	4.3	3.58	4.38	5.38
0.1-0.2	4.22	3.1	4.34	3.12	4.27	3.14	4.38	4.28
0.2-0.3	4.15	3.24	4.34	3.26	4.27	3.22	4.34	4.27
0.3-0.4	4.38	3.18	4.34	3.2	4.34	3.13	4.34	4.23
0.4-0.5	4.17	2.99	4.3	3.04	4.25	2.95	4.38	4.15
0.5-0.6	4.27	2.69	4.38	2.72	4.27	2.61	4.34	3.99
0.6-0.7	4.27	2.16	4.3	2.15	4.3	2.06	4.34	3.66
0.7-0.8	4.2	0.9	4.3	1.02	4.62	1.19	4.34	3.04
0.8-0.9	4.25	-0.09*	4.34	-0.18*	4.48	0.65	4.34	2.7
0.9-1	4.22	2.27	4.3	2.3	4.15	2.26	4.34	3.56

*Simulation was repeated with more λ steps, see Table 10

Supporting Table 3. Π values for ethanol

λ	$Pd(PPh_3)_2Ph_2$		Transition state		$Pd(PPh_3)_2$		Ph_2	
	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW
0-0.1	4.25	4.12	4.34	4.17	3.99	4.26	4.34	5.73
0.1-0.2	4.54	3.55	4.38	3.57	3.97	3.58	4.38	4.52
0.2-0.3	4.2	3.66	4.38	3.67	4.15	3.67	4.38	4.57
0.3-0.4	5.41	3.62	4.38	3.68	4.37	3.62	4.42	4.48
0.4-0.5	4.62	3.55	4.38	3.57	4.46	3.5	4.42	4.49
0.5-0.6	4.34	3.36	4.38	3.4	4.34	3.32	4.42	4.4
0.6-0.7	4.3	3.1	4.42	3.05	4.27	2.98	4.42	4.26
0.7-0.8	4.34	2.35	5.41	2.41	4.34	2.41	4.42	3.79
0.8-0.9	4.34	0.82	4.38	0.9	4.3	1.4	4.42	3
0.9-1	4.27	2.63	4.38	2.66	4.34	2.62	4.42	3.82

Supporting Table 4. Π values for toluene

λ	$Pd(PPh_3)_2Ph_2$		Transition state		$Pd(PPh_3)_2$		Ph_2	
	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW
0-0.1	4.34	3.89	4.48	3.94	4.42	4.04	4.42	4.11
0.1-0.2	4.42	3.39	4.42	3.36	4.42	3.37	4.48	4.46
0.2-0.3	4.48	3.49	4.42	3.51	4.42	3.49	4.42	4.41
0.3-0.4	4.42	3.47	4.48	3.51	4.42	3.47	4.42	4.39
0.4-0.5	4.38	3.34	4.42	3.4	4.38	3.31	4.42	4.28
0.5-0.6	4.42	3.19	4.42	3.21	4.42	3.12	4.42	4.09
0.6-0.7	5.41	2.78	4.48	2.82	4.42	2.75	4.42	3.63
0.7-0.8	4.34	1.97	4.42	2.11	4.42	1.99	4.42	2.88
0.8-0.9	4.38	0.27*	4.42	0.26*	4.38	1.08	4.42	3.45
0.9-1	4.38	2.16	4.48	2.2	4.38	2.06	5.41	3.22

*Simulation was repeated with more λ steps, see Table 10

Supporting Table 5. Π values for water

λ	$Pd(PPh_3)_2Ph_2$		Transition state		$Pd(PPh_3)_2$		Ph_2	
	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW	Coulomb	VdW
0-0.1	4.23	3.83	4.13	3.83	4.15	3.85	4.38	4.61
0.1-0.2	4.11	3.73	4.22	3.76	3.99	3.74	4.17	4.58
0.2-0.3	4.09	3.6	4.2	3.59	4.07	3.56	4.2	4.49
0.3-0.4	4.04	3.41	4.22	3.43	4.37	3.39	4.22	4.31
0.4-0.5	4.3	3.24	4.54	3.27	3.91	3.17	4.25	4.24

0.5-0.6	4.25	2.92	4.22	2.92	4.03	2.79	4.25	4.1
0.6-0.7	4.07	1.91	4.25	1.96	4.07	1.74	4.27	3.53
0.7-0.8	4.17	-0.32*	4.25	-0.35*	4.09	0.55	4.3	2.41
0.8-0.9	4.2	1.98	4.27	1.97	4.21	2.03	4.3	3.86
0.9-1	4.17	3.45	4.27	3.46	4.21	3.5	4.3	4.27

*Simulation was repeated with more λ steps, see Table 10

Supporting table 6. Solvation free energy of reaction components calculated by MM FEP. kJ/mol

	$Pd(PPh_3)_2Ph_2$			TS			$Pd(PPh_3)_2$			PhPh		
	VdW	Q[1]	Total	VdW	Q	Total	VdW	Q	Total	VdW	Q	Total
Benzene	-122.7	-8.6	-131.3	-121.5	-5.6	-127.1	-127.2	-9.3	-136.5	-35.5	-3.7	-39.2
Toluene	-120.4	-9.3	-129.7	-120.2	-6.0	-126.3	-126.3	-10.1	-136.4	-36.3	-4.1	-40.3
Ethanol	-102.8	-13.8	-116.6	-102.5	-8.3	-110.7	-104.9	-23.8	-128.7	-29.3	-5.6	-34.9
DMF	-102.6	-22.6	-125.2	-102.7	-14.7	-117.4	-110.3	-23.6	-134.0	-28.5	-10.3	-38.8
Water	17.8	-26.1	-8.3	17.3	-16.0	1.2	8.7	-50.1	-41.4	6.6	-13.9	-7.3

[1] electrostatic interactions

Supporting table 7. Solvation free energy of reaction components calculated by PCM-SMD. kJ/mol (total energy)

	$Pd(PPh_3)_2Ph_2$	TS	$Pd(PPh_3)_2$	PhPh
Benzene	-111.5	-107.0	-77.8	-37.8
Toluene	-109.2	-104.5	-80.7	-37.3
Ethanol	-98.3	-86.1	-54.0	-35.1
DMF	-192.7	-180.7	-136.0	-64.2
Water	-18.8	-6.1	14.4	-11.4

[1] sum of cavitation. dispersion and repulsion components
[2] electrostatic interactions

Supporting table 8. Results of re-run for Π values < 0.5.

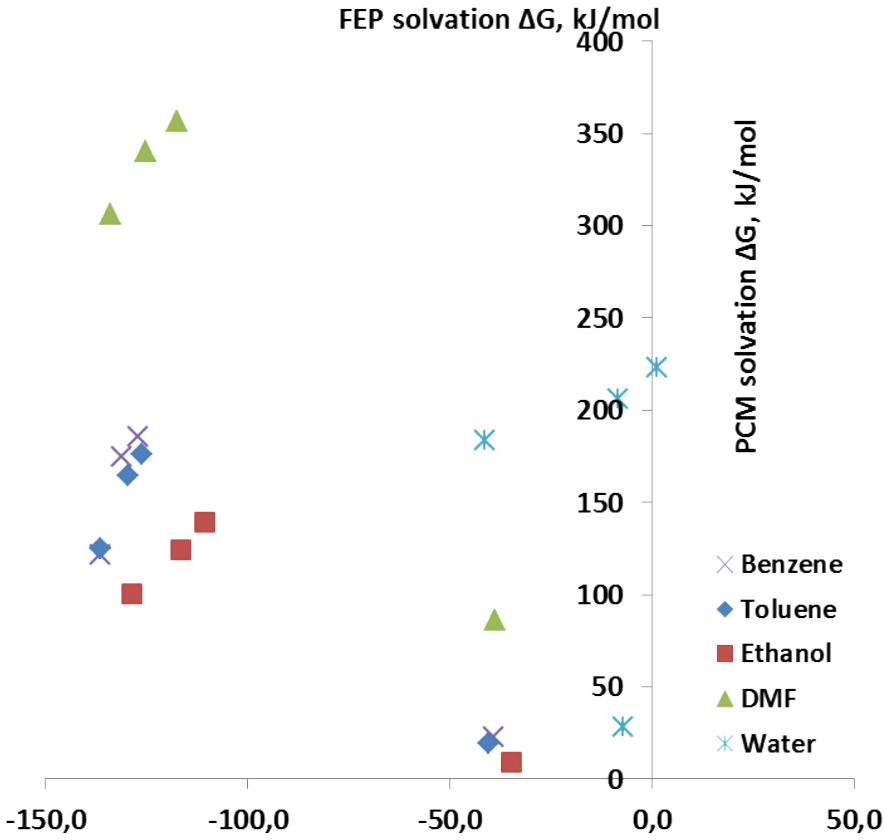
	Π value		ΔG. kJ/mol	
	Δλ=0.1	Δλ=0.05	Δλ=0.1	Δλ=0.05
Benzene				
$Pd(PPh_3)_2Ph_2$. VdW. λ=0.8-0.9	0.21	2.44	-13.00±0.33	-12.77±0.18
TS. VdW. λ=0.8-0.9	0.2	2.39	-12.87±0.11	-12.66±0.09
DMF				
$Pd(PPh_3)_2Ph_2$. VdW. λ=0.8-0.9	-0.09	1.99	-24.87±0.37	-24.58±0.30
TS. VdW. λ=0.8-0.9	-0.18	2.03	-23.87±0.73	-24.11±0.16
Toluene				
$Pd(PPh_3)_2Ph_2$. VdW. λ=0.8-0.9	0.27	2.39	-12.63±0.47	-13.28±0.27
TS. VdW. λ=0.8-0.9	0.26	2.32	-12.44±0.42	-12.72±0.31
Water				
$Pd(PPh_3)_2Ph_2$. VdW. λ=0.7-0.8	-0.32	2.17	-33.80±0.59	-33.55±0.04
TS. VdW. λ=0.7-0.8	-0.35	2.15	-33.40±0.89	-32.89±0.30

(1) Bennett. C. H. *Journal of Computational Physics* **1976**. *22*. 245.

(2) Marenich. A. V.; Cramer. C. J.; Truhlar. D. G. *The Journal of Physical Chemistry B* **2009**. *113*. 6378.
(3) Vreven. T.; Mennucci. B.; da Silva. C. O.; Morokuma. K.; Tomasi. J. *J. Chem. Phys.* **2001**. *115*. 62.
(4) Wu. D.; Kofke. D. A. *J Chem Phys* **2005**. *123*. 054103.

Supporting Figure 1.

Correlation between electrostatic + non-electrostatic PCM (g09) and FEP solvation free energies for reactant. products and transition state.



XYZ coordinates of vacuum-optimized compounds

$Pd(PPh_3)_2Ph_2$

91

Pd	-0.077670	0.944093	0.069027
C	-1.452570	2.489654	0.245520
C	1.228360	2.580016	-0.007657
C	-1.973755	3.167138	-0.863894
C	-2.903267	4.197949	-0.716189
C	-3.332869	4.582442	0.552293
C	-2.819803	3.926097	1.667881
C	-1.890448	2.894917	1.513292
C	1.583959	3.086192	-1.266800

C	2.439831	4.179709	-1.403415
C	2.964444	4.805732	-0.274894
C	2.610106	4.331629	0.984743
C	1.749237	3.239012	1.112491
H	1.181224	2.631835	-2.167575
H	2.691189	4.546234	-2.395292
H	3.628871	5.658354	-0.376162
H	2.995152	4.818869	1.876738
H	1.470031	2.923605	2.111643
H	-1.643375	2.904726	-1.864955
H	-3.285817	4.707672	-1.596618
H	-4.051206	5.387978	0.669496
H	-3.137677	4.219117	2.665163
H	-1.500874	2.411527	2.405410
P	1.885599	-0.445865	0.080177
P	-1.897071	-0.588263	-0.101520
C	-1.595111	-1.958499	-1.399573
C	-3.570336	0.138738	-0.686250
C	-2.451917	-1.494052	1.476339
C	2.800440	-0.477662	1.752074
C	3.173125	0.176958	-1.173440
C	1.876462	-2.350083	-0.221382
C	-1.002629	-1.575056	-2.598758
C	-0.764115	-2.512391	-3.591583
C	-1.107452	-3.841001	-3.389990
C	-1.689885	-4.226747	-2.193068
C	-1.935618	-3.289801	-1.199806
C	-3.956146	0.087115	-2.017967
C	-5.163482	0.646040	-2.411896
C	-5.985705	1.259624	-1.481113
C	-5.597164	1.315434	-0.150365
C	-4.391873	0.760386	0.247747
C	-1.669509	-1.404557	2.619372
C	-2.064195	-2.039033	3.789515
C	-3.245135	-2.762368	3.822802
C	-4.036587	-2.845775	2.685407
C	-3.645131	-2.212347	1.517575
C	3.988898	-1.192255	1.889095
C	4.629427	-1.246929	3.114844
C	4.086129	-0.595523	4.214564
C	2.899463	0.105688	4.083783
C	2.255350	0.163493	2.854177
C	2.864730	0.093044	-2.528101
C	3.758039	0.566725	-3.474945
C	4.956548	1.140385	-3.075249
C	5.255603	1.240795	-1.726198
C	4.366618	0.762018	-0.774002
C	2.625796	-2.962743	-1.216039
C	2.604980	-4.343767	-1.354601
C	1.844833	-5.121175	-0.496954
C	1.101019	-4.511892	0.503277
C	1.114090	-3.133562	0.638308
H	4.606244	0.856190	0.275861
H	6.184069	1.697326	-1.407249

H	5.652361	1.515114	-3.815410
H	3.513896	0.492596	-4.527033
H	1.926189	-0.343476	-2.843397
H	4.412774	-1.710125	1.038974
H	5.553844	-1.801530	3.213429
H	4.588550	-0.640000	5.172975
H	2.467582	0.611437	4.937963
H	1.326834	0.710548	2.758427
H	3.234749	-2.372325	-1.885444
H	3.192925	-4.810691	-2.134771
H	1.833202	-6.198424	-0.604284
H	0.507457	-5.111461	1.181819
H	0.533533	-2.667478	1.422440
H	-4.275756	-2.270220	0.640438
H	-4.964398	-3.403114	2.708458
H	-3.554310	-3.256516	4.735609
H	-1.446752	-1.962151	4.675387
H	-0.751584	-0.831530	2.601606
H	-3.325188	-0.390861	-2.753633
H	-5.458883	0.599502	-3.452401
H	-6.926827	1.696078	-1.791000
H	-6.231888	1.797028	0.582643
H	-4.092333	0.814367	1.285596
H	-2.387035	-3.606685	-0.270493
H	-1.956991	-5.262915	-2.028028
H	-0.919111	-4.574477	-4.163930
H	-0.308976	-2.202670	-4.523828
H	-0.733520	-0.538108	-2.759523

$Pd(PPh_3)_2Ph_2$

91

Pd	0.065211	-0.857043	0.038035
C	1.008372	-2.752458	0.263620
C	-0.924068	-2.739976	-0.171627
C	1.785343	-3.369384	-0.733007
C	2.824766	-4.235794	-0.409773
C	3.128664	-4.515278	0.922864
C	2.372054	-3.912366	1.926247
C	1.324788	-3.054189	1.602306
C	-1.237096	-3.046284	-1.509666
C	-2.303706	-3.879314	-1.834884
C	-3.089203	-4.447151	-0.832797
C	-2.787254	-4.166357	0.499336
C	-1.721195	-3.332611	0.823360
H	-0.633738	-2.632913	-2.311959
H	-2.518094	-4.090155	-2.878974
H	-3.913053	-5.106912	-1.084536
H	-3.380348	-4.607652	1.295573
H	-1.491059	-3.165795	1.869602
H	1.560393	-3.190004	-1.779152
H	3.399868	-4.699300	-1.206633
H	3.933310	-5.198605	1.173665
H	2.591052	-4.117853	2.970521
H	0.739319	-2.619963	2.406727
P	-1.911418	0.502864	0.134112
P	1.967407	0.571893	-0.128553
C	1.750422	2.060764	-1.312066
C	3.584392	-0.215685	-0.799821
C	2.624975	1.348042	1.485460
C	-2.844930	0.477846	1.802751
C	-3.198532	-0.130475	-1.121269
C	-1.951824	2.405362	-0.159084
C	1.084243	1.829055	-2.511292
C	0.892872	2.860808	-3.416820
C	1.357145	4.135132	-3.126692
C	2.014261	4.371174	-1.929614
C	2.213085	3.338531	-1.024816
C	4.016288	-0.008957	-2.102759
C	5.177454	-0.618604	-2.555224
C	5.911226	-1.436588	-1.711589
C	5.477680	-1.648280	-0.410984
C	4.315794	-1.045393	0.043371
C	1.817338	1.332541	2.614688
C	2.270703	1.876225	3.808848
C	3.536370	2.434735	3.881267
C	4.351028	2.445911	2.757727
C	3.899656	1.904209	1.565339
C	-4.016260	1.211231	1.979588
C	-4.664747	1.203944	3.202840
C	-4.147982	0.468420	4.261082
C	-2.980073	-0.255955	4.091394

C	-2.328582	-0.249834	2.864700
C	-2.902544	-0.013443	-2.476949
C	-3.789544	-0.490968	-3.427650
C	-4.970993	-1.102107	-3.032457
C	-5.258856	-1.234859	-1.684019
C	-4.375740	-0.752183	-0.728165
C	-2.822921	3.017302	-1.050925
C	-2.820278	4.397595	-1.193644
C	-1.956051	5.176234	-0.441586
C	-1.089978	4.568909	0.455767
C	-1.085215	3.190335	0.593389
H	-4.609674	-0.866628	0.321064
H	-6.175047	-1.717903	-1.368662
H	-5.662528	-1.478627	-3.775569
H	-3.555082	-0.388681	-4.479591
H	-1.979822	0.458417	-2.789005
H	-4.422250	1.791978	1.161953
H	-5.575265	1.775134	3.331643
H	-4.656221	0.464472	5.217357
H	-2.569299	-0.828143	4.913448
H	-1.412946	-0.812910	2.736919
H	-3.510028	2.424607	-1.638066
H	-3.502405	4.863733	-1.893429
H	-1.957628	6.253187	-0.552294
H	-0.413513	5.169770	1.050326
H	-0.406607	2.723740	1.294621
H	4.546025	1.909097	0.697821
H	5.342905	2.876500	2.810081
H	3.891742	2.857411	4.812838
H	1.632230	1.858420	4.682886
H	0.831116	0.888903	2.564484
H	3.455732	0.631071	-2.769416
H	5.508419	-0.449343	-3.572056
H	6.817822	-1.910175	-2.066268
H	6.042794	-2.289343	0.253692
H	3.980167	-1.220707	1.057024
H	2.725428	3.538694	-0.094458
H	2.376716	5.364223	-1.695787
H	1.204792	4.942785	-3.831524
H	0.378453	2.668123	-4.349740
H	0.718667	0.835058	-2.738706

$Pd(PPh_3)_2$

69

Pd	0.000088	-0.000547	-0.001181
P	-2.294863	0.000372	-0.000868
P	2.295048	-0.000025	-0.001307
C	3.127984	1.696031	-0.259134
C	3.128978	-1.072079	-1.339878
C	3.126536	-0.623880	1.597844
C	-3.125959	-0.438480	1.658413
C	-3.129316	-1.216882	-1.208909
C	-3.128101	1.655991	-0.449933
C	2.544360	2.576058	-1.163946
C	3.113072	3.819955	-1.392159
C	4.262159	4.194918	-0.712017
C	4.842715	3.321606	0.194516
C	4.280055	2.074154	0.419941
C	4.281232	-0.673312	-2.006679
C	4.844426	-1.492848	-2.973501
C	4.264218	-2.714889	-3.275928
C	3.114944	-3.116185	-2.611278
C	2.545694	-2.296017	-1.648969
C	2.544586	-0.274780	2.811682
C	3.111973	-0.698164	4.003932
C	4.257997	-1.479317	3.990300
C	4.836784	-1.833170	2.781519
C	4.275459	-1.405562	1.587466
C	-4.274078	0.199804	2.111818
C	-4.835009	-0.158771	3.328572
C	-4.256650	-1.158032	4.095594
C	-3.111419	-1.797813	3.645164
C	-2.544431	-1.436878	2.432371
C	-2.547053	-1.393692	-2.459291
C	-3.116893	-2.263318	-3.376800
C	-4.265710	-2.967207	-3.047598
C	-4.844884	-2.796836	-1.799785
C	-4.281107	-1.922679	-0.882423
C	-4.281642	1.727391	-1.221683
C	-4.844396	2.959577	-1.519296
C	-4.262457	4.124827	-1.044902
C	-3.111899	4.056747	-0.273420
C	-2.543106	2.826685	0.020189
H	-4.741455	-1.795314	0.087898
H	-5.741081	-3.344556	-1.537373
H	-4.708261	-3.649604	-3.762407
H	-2.659412	-2.392717	-4.349386
H	-1.646379	-0.847894	-2.713736
H	-4.733890	0.979425	1.519862
H	-5.728378	0.344494	3.675910
H	-4.696957	-1.436793	5.044744
H	-2.654573	-2.578436	4.240040
H	-1.646564	-1.932284	2.082718
H	-4.744199	0.823875	-1.594977

H	-5.741981	3.007140	-2.122705
H	-4.704227	5.085572	-1.277878
H	-2.652258	4.963263	0.099292
H	-1.641095	2.773172	0.617992
H	4.735609	-1.685394	0.649588
H	5.730797	-2.443498	2.765165
H	4.698624	-1.813636	4.921183
H	2.654828	-0.419166	4.944749
H	1.646144	0.330654	2.821522
H	4.742419	0.277496	-1.776620
H	5.740983	-1.174375	-3.490012
H	4.706314	-3.353327	-4.030525
H	2.656645	-4.069044	-2.843609
H	1.644654	-2.606354	-1.133533
H	4.741491	1.399196	1.127871
H	5.739140	3.609696	0.728791
H	4.703854	5.167942	-0.886945
H	2.654515	4.497889	-2.100742
H	1.643483	2.284811	-1.690679

PhPh

22

C	0.000011	-0.742617	-0.000063
C	-0.000011	0.742617	-0.000063
C	-1.125644	1.464019	0.424205
C	1.125644	-1.464019	0.424205
C	-1.125982	2.855815	0.424622
C	1.125982	-2.855815	0.424622
C	0.000000	3.558282	0.000027
C	0.000000	-3.558282	0.000027
C	1.125658	1.464042	-0.424226
C	-1.125658	-1.464042	-0.424226
C	1.125995	2.855829	-0.424585
C	-1.125995	-2.855829	-0.424585
H	-1.998647	0.928037	0.782343
H	1.998647	-0.928037	0.782343
H	-2.005604	3.392816	0.765679
H	2.005604	-3.392816	0.765679
H	0.000005	4.643542	0.000059
H	-0.000005	-4.643542	0.000059
H	1.998663	0.928063	-0.782364
H	-1.998663	-0.928063	-0.782364
H	2.005616	3.392859	-0.765598
H	-2.005616	-3.392859	-0.765598