

Supporting Information

Density Functional Theory Investigation on Pd-Catalyzed Cross-Coupling of Azoles with Aryl Thioethers

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1. The detailed isomerization processes of reactant-catalyst complexes

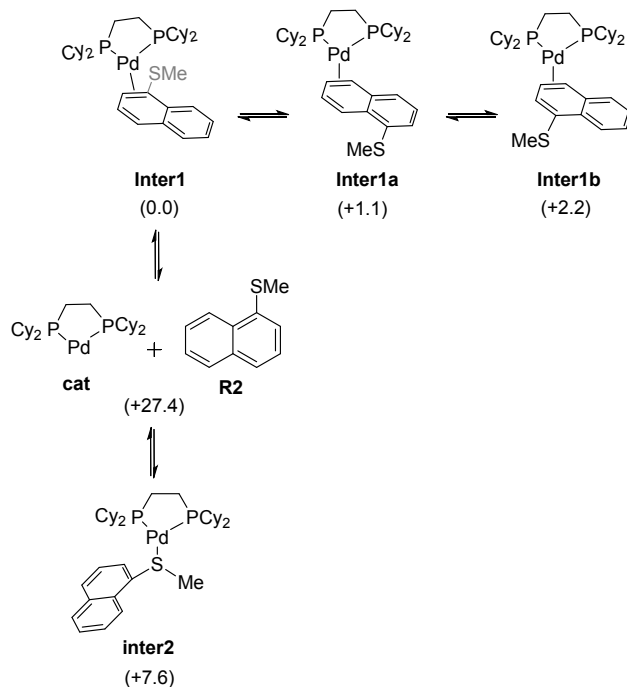


Figure S1. The isomerization processes among different types of reactant-catalyst complexes

2. C-H Palladation of R1 through syn or anti attack

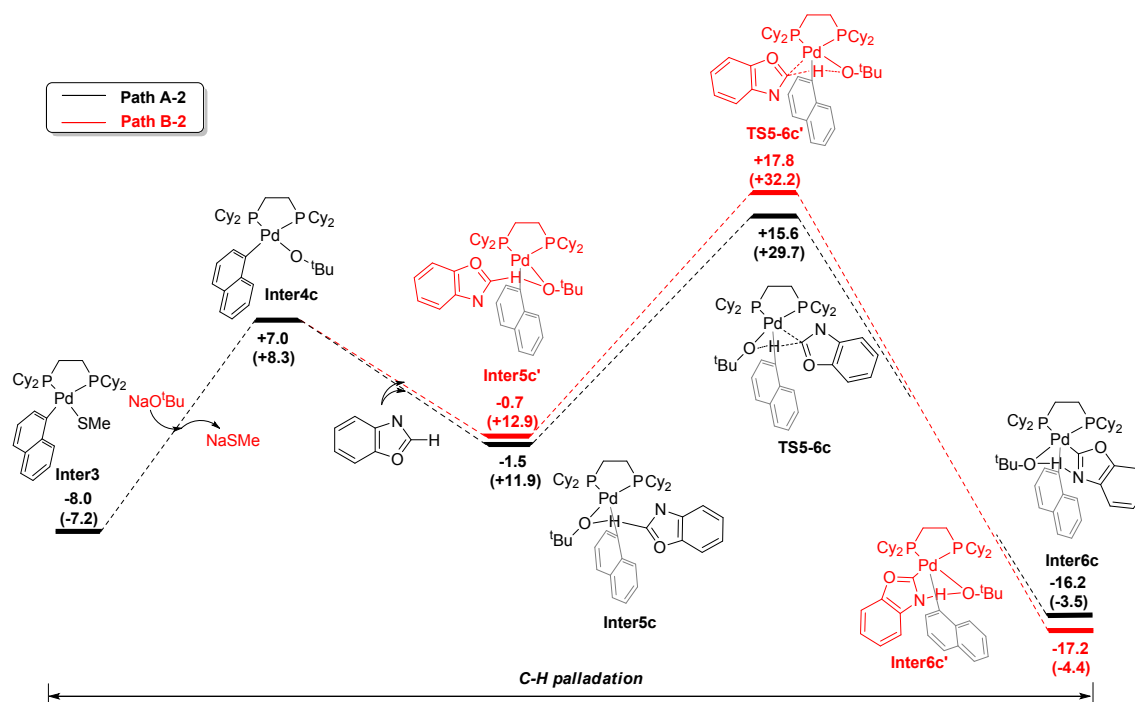
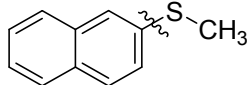
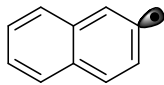
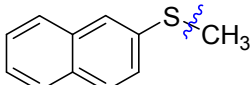
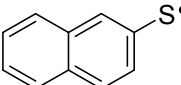


Figure S2. C-H palladation steps of R1-H through syn or anti attack.

3. The NBO charge on transition states of C-H palladation

	TS4-5a	TS4-5b		TS5-6c	TS5-6d
Pd atom	-0.17	0.02	Pd atom	0.01	0.19
-SMe	0.09	-0.13	-O ^t Bu	-0.51	-0.57
S atom of -SMe	0.09	-0.09	O atom of -O ^t Bu	-0.87	-0.89

4. Bond dissociation enthalpies of C_{Ar}-S/C_{alkyl}-S bond in R2

Compounds	TCE	E	Compounds	TCE	E	BDE (kcal/mol)
	0.187968	-823.155289		0.142585	-384.9950854	80.0
			•SMe	0.039962	-438.0272914	
	0.187968	-823.155289		0.146845	-783.2411199	61.9
			•CH ₃	0.033882	-39.80829566	

5. The overall pathway of C-H/C_{alkyl}-S activation between R1 and R2

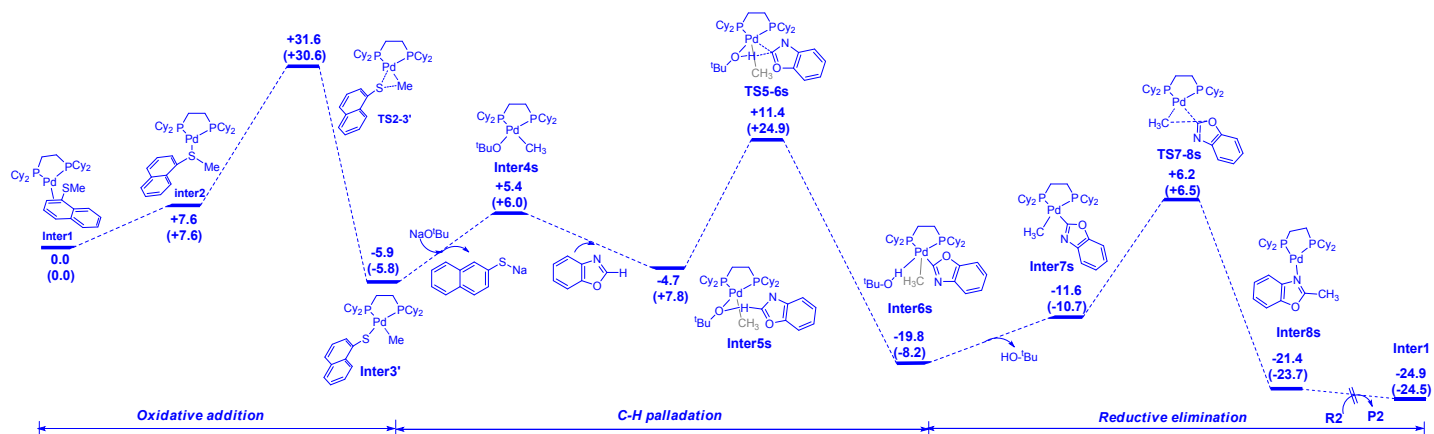


Figure S3. The overall pathway of C-H/C_{alkyl}-S activation between R1 and R2

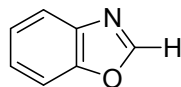
6. Thermal correction to Gibbs free energy (TCG) /Zero-point correction and electronic energies (au) in toluene solvent

Compounds	TCG	Zero-point correction	E	Compounds	TCG	Zero-point correction	E
R1	0.076137	0.106159	-399.5560384	TS5-6d	0.977661	1.072385	-2846.269999
R2	0.140575	0.176905	-823.155289	TS5-6s	0.891473	0.976208	-2501.104157
cat	0.642286	0.706735	-1828.684972	Inter6c	0.984959	1.078747	-2846.36042
Inter1	0.803945	0.883384	-2651.883644	Inter6c'	0.985432	1.079090	-2846.362322
Inter1a	0.803565	0.884093	-2651.882495	Inter6d	0.984055	1.078894	-2846.322362
Inter1b	0.803192	0.883776	-2651.880524	Inter6s	0.889658	0.977519	-2501.155129
Inter2	0.804010	0.884568	-2651.872649	TS6-7	0.987486	1.078201	-2846.336218
TS2-3	0.803925	0.882969	-2651.859267	Inter7	0.858624	0.941187	-2612.763292
TS2-3'	0.800658	0.881677	-2651.831550	Inter7'	0.985939	1.079453	-2846.385422
Inter3	0.806583	0.884855	-2651.897719	Inter7s	0.764101	0.839917	-2267.555054
Inter3'	0.804943	0.884227	-2651.893830	TS7-8	0.855427	0.938815	-2612.740025
Inter4a	0.901527	0.992592	-3051.464121	TS7-8s	0.761515	0.838260	-2267.525103
Inter4b	0.901992	0.991970	-3051.434768	Inter8	0.859290	0.941566	-2612.790632
Inter4c	0.889193	0.971165	-2446.765942	Inter8s	0.759535	0.840500	-2267.571301
Inter4s	0.794897	0.870144	-2101.557696	P1	0.193099	0.234066	-784.0513046
TS4-5a	0.899293	0.987832	-3051.392506	P2	0.101500	0.133779	-438.8605625
TS4-5b	0.894248	0.984601	-3051.379847	NaSMe	0.009431	0.038255	-600.4023693
Inter5c	0.987025	1.079612	-2846.337887	NaSnaph	0.101919	0.138538	-945.6123676
Inter5c'	0.987522	1.079943	-2846.336825	NaO^tBu	0.091135	0.124519	-395.2943828
Inter5a	0.898053	0.988888	-3051.442644	HSMe	0.022202	0.046421	-233.5855521
Inter5b	0.898339	0.988698	-3051.411673	HO^tBu	0.107168	0.136173	-233.5855521
Inter5d	0.985008	1.078524	-2846.310192	cat_dist	-	-	-1828.681764
Inter5s	0.891613	0.978012	-2501.131587	cat_dist	-	-	-1828.679356
TS5-6c	0.985533	1.077105	-2846.308082	sub_dist	-	-	-823.1101489
TS5-6c'	0.985491	1.076486	-2846.303949	sub_dist	-	-	-823.1134542

7. The explanation for Houk's distortion/interaction model

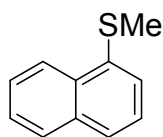
According to Houk's distortion/interaction model, the activation barrier is the sum of interaction energy and the distortion energy. The distortion energy is calculated from the distorted structural moieties with the free structures. For example, **TS2-3** can be formally divided into two fragments (i.e. cat: (dcype) Pd and sub: thioether). The single-point energy of the (dcype)Pd and the thioether moiety in **TS2-3** are named as E_{cat} and E_{sub} , respectively. The relative energy of the free (dcype)Pd and the thioether (after optimization) is named as $E_{\text{cat-opt}}$ and $E_{\text{sub-opt}}$, respectively. Therefore, the energy difference between the free structure and the distorted structure in transition state (i.e. $E_{\text{cat}} - E_{\text{cat-opt}}$; $E_{\text{sub}} - E_{\text{sub-opt}}$) corresponds to the distortion energies of cat and sub, respectively. For clarity reasons, they are named as $E_{\text{dist_cat}}$ and $E_{\text{dist_sub}}$ (Scheme 5). Meanwhile, the interaction energy (E_{int}) for each transition state equals to the $E_{\text{TS}} - E_{\text{dis_sub}} - E_{\text{dis_cat}}$, and E_{TS} is the electronic energy of the transition state.

Cartesian coordinates of all complexes.



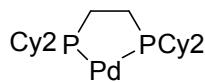
R1

H	-3.36103500	-0.04570200	-0.00005600
C	-2.28585600	0.06797900	-0.00007700
O	-1.56804000	-1.09938700	0.00000600
N	-1.60712600	1.16402900	-0.00002200
C	-0.26000800	-0.67192700	0.00009000
C	-0.27580900	0.72916200	0.00010100
C	0.89983300	-1.43289900	-0.00003300
C	0.92719100	1.43977900	-0.00002600
C	2.09474900	-0.71009500	-0.00002200
H	0.87818100	-2.51738100	0.00006600
C	2.10738500	0.69777500	-0.00001700
H	0.93181600	2.52494500	0.00015500
H	3.03790600	-1.24886300	-0.00003000
H	3.06242700	1.21524400	-0.00013300



R2

S	2.12047100	-1.17245500	-0.00009700
C	0.91414100	0.14731200	-0.00013200
C	-0.47434700	-0.22843700	-0.00007100
C	1.26161300	1.48538800	-0.00005300
C	-0.91403700	-1.57985900	0.00001000
C	-1.46660600	0.80788600	-0.00001100
C	0.27035900	2.49526200	0.00000600
H	2.30238300	1.78761400	-0.00001500
C	-2.25529400	-1.89494300	0.00004800
H	-0.18197500	-2.38138900	0.00001700
C	-2.84068700	0.44690300	0.00003900
C	-1.06341000	2.17007900	-0.00000500
H	0.58198500	3.53643400	0.00008500
C	-3.23137600	-0.87234100	0.00004900
H	-2.56497300	-2.93646100	0.00009500
H	-3.58323100	1.24148300	0.00007200
H	-1.82610800	2.94452000	0.00003000
H	-4.28678000	-1.13106500	0.00007000
C	3.71345300	-0.29016300	0.00019600
H	4.47733600	-1.07176300	0.00008900
H	3.83552700	0.32387200	-0.89622700
H	3.83544500	0.32351300	0.89688100



cat

Pd	-0.00382500	-0.31922400	-1.57910700
P	1.77540500	-0.17479600	-0.09942900
P	-1.73442700	0.08981000	-0.08996700
C	0.77398600	0.43787800	1.39223800
C	-0.69062300	-0.05759600	1.48844300
C	2.72900900	-1.64837800	0.60598400
C	1.77493100	-2.74131100	1.13105600
C	2.53655200	-3.97811300	1.64000600
C	3.47542800	-4.54980100	0.56925200
C	4.43783100	-3.47124400	0.05363200

C	3.67684400	-2.23718400	-0.46067100
C	3.13129700	1.14621600	-0.20754500
C	2.62668200	2.38588800	-0.97517900
C	3.75217100	3.40788100	-1.20749000
C	4.42978500	3.81825800	0.10812100
C	4.93011400	2.58901600	0.88041200
C	3.80235800	1.56746300	1.11681600
C	-3.12339700	-1.13334300	0.31477600
C	-2.61410900	-2.58577500	0.18928700
C	-3.72390000	-3.61483600	0.46387000
C	-4.93381300	-3.39747700	-0.45484700
C	-5.45254000	-1.95761000	-0.34570000
C	-4.34115600	-0.92683700	-0.61063500
C	-2.59658700	1.76857400	0.09174600
C	-1.61628100	2.93369200	-0.15906500
C	-2.34842100	4.28574600	-0.20287300
C	-3.16321000	4.52951700	1.07628700
C	-4.12732500	3.36684500	1.35194300
C	-3.39261200	2.01331000	1.39015000
H	1.29540500	0.19492300	2.32834200
H	0.77831800	1.53076700	1.31276800
H	-1.18335000	0.45277900	2.32644400
H	-0.69475600	-1.12383900	1.73711100
H	3.33409500	-1.29230500	1.45388900
H	1.09158800	-3.03788500	0.32220600
H	1.15072100	-2.34473100	1.94077100
H	1.82122400	-4.74290800	1.96976000
H	3.12681800	-3.69987600	2.52600000
H	2.87741800	-4.93279200	-0.27084000
H	4.03632800	-5.40388100	0.97019500
H	5.07210900	-3.87459500	-0.74640600
H	5.11457300	-3.17013400	0.86729300
H	3.08270900	-2.51748200	-1.34235000
H	4.39538000	-1.48051000	-0.79908400
H	3.89886000	0.67153000	-0.83745300
H	1.81665800	2.86791500	-0.40806400
H	2.18929500	2.07414000	-1.93120000
H	3.35324100	4.29128900	-1.72281500
H	4.50391900	2.96775600	-1.87955700
H	3.70801100	4.36755900	0.73123500
H	5.26051300	4.50824800	-0.08850400
H	5.36535400	2.89237000	1.84179800
H	5.73832500	2.10735600	0.31019700
H	3.05169300	2.01549500	1.78269300
H	4.20637000	0.69477600	1.64457300
H	-3.44196500	-0.96653100	1.35542100
H	-1.77486000	-2.76415500	0.87199800
H	-2.22038800	-2.73215700	-0.82683800
H	-4.04550100	-3.53379400	1.51307600
H	-3.32574100	-4.63011600	0.33766500
H	-5.73247700	-4.11046500	-0.21255900
H	-4.63835000	-3.59842600	-1.49523100
H	-5.86196100	-1.79589900	0.66276800
H	-6.28116300	-1.79530700	-1.04737600
H	-4.75212200	0.08236400	-0.49289600
H	-4.00857100	-1.00875800	-1.65616700
H	-3.31060100	1.77089700	-0.74537000
H	-1.06437400	2.76463900	-1.09136400
H	-0.86935200	2.96243400	0.64757400
H	-3.02289400	4.30041800	-1.07182300
H	-1.62570000	5.09796900	-0.35533800
H	-3.71735800	5.47412800	1.00255300
H	-2.47472900	4.63710300	1.92801700
H	-4.89430700	3.33685300	0.56387600
H	-4.65985100	3.52861500	2.29844800
H	-4.11803900	1.20980100	1.56491300
H	-2.70731800	2.00884000	2.24942500

H-O^tBu

O	0.01398900	-0.00020900	1.45238900
C	-0.00541200	-0.00006600	0.01378500
C	0.69588200	-1.26250900	-0.51027400

H	0.21909800	-2.15865300	-0.09974700
H	0.65939900	-1.31855500	-1.60452900
H	1.75323100	-1.27210100	-0.21349300
C	0.68508400	1.26851200	-0.50984200
H	0.64865500	1.32430000	-1.60411400
H	0.20015300	2.16039500	-0.09954500
H	1.74212700	1.28748700	-0.21242300
C	-1.49044700	-0.00617900	-0.35692700
H	-1.98738700	0.87786000	0.05589400
H	-1.62262000	-0.00594700	-1.44417400
H	-1.98000100	-0.89497900	0.05451700
H	0.94479300	0.00331700	1.72804700

Na-O^tBu

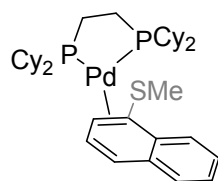
Na	2.69755300	-0.00014900	-0.00025000
O	0.75939100	0.00003700	0.00003000
C	-0.61950500	0.00016500	0.00023900
C	-1.14716900	-1.13382000	0.91236300
H	-0.77831700	-0.98686300	1.93520400
H	-2.24443300	-1.18197600	0.94491400
H	-0.77046900	-2.09991100	0.55362500
C	-1.14767000	-0.22327500	-1.43766300
H	-2.24494500	-0.23235400	-1.49472900
H	-0.77540000	0.57251200	-2.09502800
H	-0.77516600	-1.18052500	-1.82360700
C	-1.14694500	1.35717900	0.52564200
H	-0.77304800	2.16920900	-0.11053700
H	-2.24417900	1.41185200	0.54570700
H	-0.77453200	1.52790500	1.54346600

Na-SMe

Na	-1.91325000	0.35066800	0.00000000
S	0.35898600	-0.67875400	0.00000000
C	1.60745200	0.68766700	0.00000000
H	1.52628200	1.31960900	0.89040700
H	2.60491300	0.23726900	-0.00017700
H	1.52607500	1.31983300	-0.89022800

H-SMe

S	-0.66760900	-0.08719500	-0.00002600
C	1.16468100	0.01959100	0.00003200
H	1.53627400	0.52269700	0.89569200
H	1.53028200	-1.00998900	-0.00010600
H	1.53631800	0.52295400	-0.89546500
H	-0.90921400	1.24190400	0.00011000

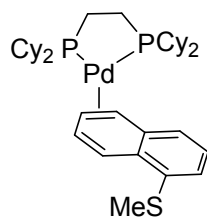


Inter1

P	-2.15328400	-0.37773300	0.49385000
P	0.85330000	0.95546700	1.18072000
C	-1.85994200	0.54540200	2.11621800
C	-3.78681600	0.37254600	-0.09068800
C	-2.67328600	-2.09643000	1.07848300
C	-0.38450500	0.62019000	2.56700900
C	2.44201100	0.21018300	1.87736100
C	1.15935800	2.81202100	1.31876100
H	-2.24039200	1.56016900	1.95383000
H	-2.46818200	0.11196100	2.92077200
C	-3.56217900	1.77786600	-0.68738200
C	-4.94153700	0.39240200	0.93271700
H	-4.08498200	-0.28005200	-0.92464300
C	-3.24946000	-2.93363000	-0.08386300

C	-1.48647100	-2.83692100	1.73132500
H	-3.45849900	-1.97154900	1.83972500
H	-0.28324700	1.36609200	3.36620300
H	-0.08989300	-0.34036600	3.00345400
C	2.39193200	-1.33284400	1.83217700
C	2.86657200	0.70216600	3.27620900
H	3.21098600	0.51903000	1.15452600
C	2.34207100	3.24338500	0.42459800
C	-0.10946700	3.61471800	0.96218300
H	1.41363700	3.03664000	2.36553100
C	-4.85373500	2.34970700	-1.29647700
H	-2.76965900	1.73259400	-1.44359400
H	-3.20686200	2.46295600	0.09626800
C	-6.23125500	0.96880600	0.31929300
H	-5.13884100	-0.61645100	1.31512800
H	-4.65443500	1.00519700	1.79928700
C	-3.63174500	-4.35425000	0.36555400
H	-2.49864100	-2.99564400	-0.88394200
H	-4.12966000	-2.44210300	-0.51543900
C	-1.86685000	-4.26086500	2.17276000
H	-0.65575000	-2.88142900	1.01356300
H	-1.12075100	-2.27581400	2.59982300
C	3.72838200	-1.95369400	2.27404700
H	2.13671000	-1.66629100	0.82074700
H	1.59605600	-1.69919000	2.49727200
C	4.20206800	0.07364300	3.71558600
H	2.95714700	1.79488000	3.29533900
H	2.08979400	0.43887000	4.00865100
C	2.57726600	4.76300200	0.47528300
H	2.14358600	2.93586400	-0.61184200
H	3.25958000	2.72633800	0.73019500
C	0.13488700	5.13282700	1.01388400
H	-0.44130000	3.33225200	-0.04692300
H	-0.92808600	3.35544200	1.64500800
C	-6.00268600	2.36449200	-0.27787800
H	-5.14523200	1.73738600	-2.16285200
H	-4.66872400	3.36203900	-1.67845900
H	-6.58766800	0.29105400	-0.47060800
H	-7.02189500	1.00299600	1.08017300
C	-2.44500700	-5.08111800	1.01127700
H	-4.00869100	-4.92435700	-0.49339400
H	-4.45881400	-4.29590600	1.08901000
H	-0.98700700	-4.76294700	2.59538800
H	-2.61195800	-4.20293900	2.98054100
C	4.15318500	-1.45985300	3.66411900
H	4.50174500	-1.69493900	1.53740400
H	3.64686200	-3.04820300	2.26562600
H	5.00186500	0.43254600	3.05115100
H	4.45879000	0.41632800	4.72667300
C	1.30793100	5.54687800	0.11515200
H	3.39725300	5.03116200	-0.20306000
H	2.90286700	5.04789100	1.48713800
H	-0.77974800	5.66492100	0.72122200
H	0.35078000	5.42985800	2.05108200
H	-6.92394500	2.73301000	-0.74684500
H	-5.76042400	3.06953800	0.53159000
H	-1.66247300	-5.24120100	0.25505000
H	-2.75074600	-6.07529900	1.36169300
H	5.12968700	-1.87992500	3.93777200
H	3.43524400	-1.82383100	4.41483400
H	1.04692700	5.35019800	-0.93512700
H	1.48850900	6.62640000	0.19688700
C	1.20893100	-0.23295700	-2.57976600
C	2.39399100	-1.04088000	-2.26624300
C	-0.03508900	-0.89722200	-2.82174800
C	3.66813800	-0.47192500	-2.04174200
C	2.26973000	-2.46518500	-2.19985700
C	-0.09655200	-2.33527100	-2.76252800
H	-0.81785100	-0.38847700	-3.37679300
C	4.77261100	-1.25920100	-1.75098800
H	3.77747300	0.60731300	-2.08453700
C	3.41102800	-3.24174800	-1.89763700
C	0.99961300	-3.08698500	-2.46145200
H	-1.04415000	-2.81677200	-2.99537600
C	4.64674000	-2.65733900	-1.67662400

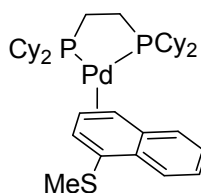
H	5.73852800	-0.78983600	-1.58169800
H	3.30200600	-4.32340100	-1.84955400
H	0.93918600	-4.17245400	-2.43465300
H	5.51262800	-3.27463300	-1.45199900
Pd	-0.12176700	-0.05657900	-0.77008400
S	1.58154100	1.36402800	-3.36746700
C	-0.00873500	2.25168100	-3.30480900
H	0.19547300	3.26301400	-3.66949500
H	-0.76331400	1.79476500	-3.95182100
H	-0.38190400	2.29592900	-2.27699200



Inter1a

P	-0.30806400	1.70292900	0.78565000
P	-2.10242300	-1.10055400	0.37723100
C	-1.39556300	1.05060800	2.18441400
C	1.33619300	2.01890700	1.65379200
C	-0.98827100	3.44024400	0.49636300
C	-2.55875000	0.14486700	1.72252900
C	-3.77570200	-1.42923600	-0.43955800
C	-1.79775500	-2.68810600	1.35159100
H	-0.72817400	0.47819000	2.83801600
H	-1.78970700	1.87762600	2.78935700
C	2.07786900	0.68597900	1.89388400
C	1.29215100	2.86109600	2.94484500
H	1.92004900	2.57152000	0.90290200
C	-0.08575200	4.22818400	-0.47730800
C	-2.43449900	3.38189900	-0.03952100
H	-1.00617800	3.97050500	1.46104700
H	-2.99643200	-0.36469500	2.59100100
H	-3.35388800	0.76545300	1.29473300
C	-4.16143900	-0.26819100	-1.38112000
C	-4.95012700	-1.77980200	0.49742100
H	-3.58048700	-2.30423200	-1.07790400
C	-1.53563700	-3.87133600	0.39483900
C	-0.62035900	-2.52453800	2.33628100
H	-2.70054900	-2.90805600	1.94145800
C	3.48549100	0.91848200	2.46697800
H	2.13801800	0.12321100	0.95635500
H	1.50568900	0.06535100	2.59939600
C	2.70386800	3.08694200	3.51899300
H	0.81349000	3.83078300	2.76117700
H	0.67948400	2.34606300	3.69878700
C	-0.65077600	5.62366800	-0.79328600
H	0.01360100	3.65570200	-1.41090700
H	0.92541600	4.32875100	-0.06522700
C	-2.99288900	4.77923400	-0.35968700
H	-2.45402300	2.76192400	-0.94716900
H	-3.08978500	2.89063400	0.69000500
C	-5.44302400	-0.58259500	-2.17124300
H	-3.33038100	-0.05406300	-2.06376200
H	-4.32373400	0.64700600	-0.79272600
C	-6.23389500	-2.08983000	-0.29494500
H	-4.69889400	-2.63797200	1.13208200
H	-5.14562800	-0.93603500	1.17435000
C	-1.23257600	-5.17337400	1.15584700
H	-0.68313500	-3.61992900	-0.25098200
H	-2.39576800	-4.02863300	-0.26775600
C	-0.31517200	-3.83043500	3.09069200
H	0.27241200	-2.20330300	1.78196100
H	-0.84255000	-1.73342200	3.06254600
C	3.44286700	1.76067600	3.74971600
H	4.09803700	1.42900600	1.71038800
H	3.97011800	-0.04715700	2.65917800
H	3.28203800	3.70485700	2.81603900
H	2.63758000	3.65772800	4.45469000

C	-2.08517100	5.54377100	-1.33255800
H	0.00217700	6.13170400	-1.51469100
H	-0.64125000	6.23536300	0.12121600
H	-4.00539900	4.68593300	-0.77361600
H	-3.08920100	5.35475100	0.57325400
C	-6.61030500	-0.93947100	-1.23959700
H	-5.24940700	-1.42620600	-2.85045000
H	-5.70901500	0.27297800	-2.80551300
H	-6.08061600	-3.00654300	-0.88342100
H	-7.05772000	-2.29992700	0.39972600
C	-0.05752400	-4.99676200	2.12691400
H	-1.01987600	-5.97806200	0.44024700
H	-2.12589400	-5.48366100	1.71854200
H	0.54876800	-3.68134800	3.75116600
H	-1.16718500	-4.08024700	3.74077000
H	4.45944600	1.95278400	4.11687000
H	2.92789300	1.19318900	4.53966900
H	-2.07877100	5.02771800	-2.30410600
H	-2.48234700	6.55058000	-1.51459700
H	-7.50012200	-1.20358100	-1.82536900
H	-6.88001800	-0.05522100	-0.64273900
H	0.85963700	-4.79753800	1.55384600
H	0.11722800	-5.92350100	2.68841400
C	4.48930200	-0.94031700	-1.43628800
C	3.12395400	-0.98685500	-1.85547800
C	5.16412700	0.27441700	-1.37959700
C	2.39018800	-2.21821400	-1.99417500
C	2.46546600	0.23878500	-2.18290300
C	4.51145600	1.46751500	-1.73949400
H	6.19962600	0.32070700	-1.06344300
C	1.09488500	-2.23150000	-2.42900700
H	2.88924000	-3.15857200	-1.78257800
C	1.07167500	0.21999800	-2.58804200
C	3.18690300	1.45148300	-2.13317800
H	5.06137500	2.40479500	-1.70370900
C	0.38740800	-1.01780800	-2.73693900
H	0.58357000	-3.18146300	-2.56834400
H	0.69806700	1.10696400	-3.09499000
H	2.68000200	2.37541200	-2.40240000
H	-0.50787800	-1.07852800	-3.35034200
Pd	-0.35928600	-0.02825100	-0.87509000
S	5.26655300	-2.49224300	-0.98787800
C	6.99871500	-2.02510600	-0.67510600
H	7.51518300	-2.96026800	-0.44292500
H	7.45961000	-1.57525600	-1.55897000
H	7.09187400	-1.34962700	0.18000400

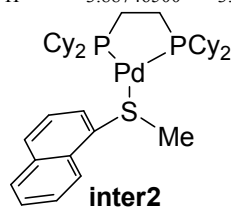


Inter1b

P	1.98831300	-0.82207000	0.42993500
P	0.00393300	1.85698500	0.78639600
C	2.10877900	0.25036100	1.97895700
C	1.96838100	-2.56219800	1.16561400
C	3.72307700	-0.70897200	-0.30772200
C	1.58248000	1.69222300	1.81321700
C	0.12153400	3.64137800	0.17822900
C	-1.35273000	1.94563100	2.09555800
H	1.51675900	-0.26503100	2.74345900
H	3.14056300	0.27589900	2.35292300
C	0.57523100	-2.88838500	1.74557700
C	3.07506400	-2.89264200	2.18882800
H	2.10810400	-3.21493300	0.29106600
C	3.87841000	-1.68030700	-1.49733900
C	4.05674400	0.73202700	-0.74853400
H	4.44251700	-0.99727600	0.47361900
H	1.44668400	2.15060200	2.80108400

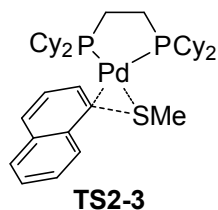
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C	1.13801200	3.76641900	-0.97661700
C	0.38238000	4.71756700	1.25231700
H	-0.87287400	3.82794900	-0.25311600
C	-2.68236500	2.44779300	1.49160100
C	-1.54948000	0.56415900	2.75743000
H	-1.03131100	2.65549700	2.87334700
C	0.48990900	-4.34661000	2.22777000
H	-0.19332600	-2.68798200	0.99009600
H	0.36142100	-2.22162100	2.59392400
C	2.98304600	-4.35244000	2.67050100
H	4.06846000	-2.71236000	1.76094700
H	2.98225600	-2.22646700	3.05828700
C	5.26961900	-1.58012900	-2.14610400
H	3.10753700	-1.44838600	-2.24625700
H	3.70091000	-2.71423600	-1.17769900
C	5.44847400	0.82823300	-1.39768200
H	3.29516700	1.07478300	-1.46324600
H	4.01032400	1.41261800	0.11024500
C	1.13373500	5.18069700	-1.58114100
H	0.91617100	3.01802400	-1.74651600
H	2.14992000	3.54338200	-0.60751000
C	0.38519600	6.13291200	0.64471100
H	-0.37067600	4.66158600	2.04760000
H	1.35553700	4.53258100	1.72891100
C	-3.82451000	2.44213100	2.52244400
H	-2.95881900	1.80991000	0.64109500
H	-2.56307900	3.46329000	1.09499400
C	-2.69579300	0.56724400	3.78294100
H	-1.76057100	-0.17690300	1.97371600
H	-0.62299700	0.24316300	3.24982800
C	1.59512400	-4.67492200	3.24196200
H	0.58185600	-5.01805500	1.36143400
H	-0.49835500	-4.53657500	2.66634900
H	3.19189700	-5.02454400	1.82510100
H	3.76059400	-4.54514600	3.42124600
C	5.59187300	-0.14297400	-2.57723800
H	5.32589500	-2.25972300	-3.00614300
H	6.02991600	-1.92185500	-1.42798900
H	5.63223900	1.85949700	-1.72597800
H	6.21674400	0.59879700	-0.64413700
C	1.38805300	6.25298800	-0.51208700
H	0.15943800	5.36621500	-2.05719700
H	1.88718500	5.24856600	-2.37650800
H	-0.62396500	6.36714100	0.27469200
H	0.61021000	6.87220300	1.42449000
C	-4.00860600	1.05838500	3.15888200
H	-4.75460400	2.76723600	2.03903300
H	-3.60747700	3.17802000	3.31159400
H	-2.82138100	-0.44156900	4.19728100
H	-2.42823100	1.22061600	4.62719400
H	1.54147900	-5.73053500	3.53728100
H	1.43436100	-4.08548000	4.15721400
H	4.90346900	0.15809200	-3.38080100
H	6.60484500	-0.08799800	-2.99597300
H	1.33713000	7.25518600	-0.95653000
H	2.40936700	6.13691500	-0.11916700
H	-4.33397900	0.34598500	2.38697300
H	-4.80324700	1.08874200	3.91544500
C	-2.37080500	-2.47380700	-1.99401600
C	-3.26617600	-1.32960600	-1.91358300
C	-1.05948600	-2.30085900	-2.35881800
C	-4.64560000	-1.45050800	-1.62950100
C	-2.73540600	-0.02628900	-2.16930200
C	-0.50543200	-1.00605200	-2.64771600
H	-0.41912400	-3.17339600	-2.45582000
C	-5.47672700	-0.34223800	-1.59139300
H	-5.05727000	-2.44146100	-1.46707800
C	-3.60875700	1.08308900	-2.14142700
C	-1.33281500	0.14058600	-2.50425500
H	0.40931200	-0.95806200	-3.23305800
C	-4.95523100	0.93722900	-1.85072400
H	-6.53486000	-0.46623000	-1.37593800
H	-3.19971800	2.06914900	-2.35319600
H	-1.05214900	1.07245100	-2.99001100

H	-5.60714700	1.80706500	-1.83405300
Pd	0.09907500	0.04542500	-0.77532700
S	-2.96694800	-4.14816900	-1.74526900
C	-3.18121100	-4.21074400	0.07754800
H	-3.58182100	-5.20130900	0.31315500
H	-2.22388000	-4.07972200	0.58843400
H	-3.88746500	-3.44923800	0.41916700



Pd	0.21293000	-0.21455200	-0.63704500
P	2.30329000	-0.77189500	0.28625700
P	-0.07913600	1.55690000	0.91068100
C	2.62311400	0.65027300	1.49783800
C	1.35696700	1.28229500	2.11648100
C	2.55416900	-2.30346300	1.36771900
C	1.52954600	-2.34379600	2.52029600
C	1.65907700	-3.61978900	3.37034100
C	1.55778400	-4.88779500	2.51209200
C	2.58717200	-4.86222800	1.37406800
C	2.45488500	-3.58927200	0.52045100
C	3.89961100	-0.75241900	-0.73573600
C	3.84744100	0.34926200	-1.81510600
C	5.06500200	0.28191700	-2.75242200
C	6.38703000	0.34371700	-1.97295300
C	6.44418200	-0.74405100	-0.89060100
C	5.22617000	-0.67556300	0.04873600
C	-1.51158100	1.72278500	2.14158100
C	-1.86643500	0.35007200	2.75361400
C	-3.05567700	0.44049000	3.72511600
C	-4.29109100	1.04769500	3.04676900
C	-3.95868800	2.41213800	2.42885100
C	-2.76039100	2.32893300	1.46714400
C	0.15528700	3.34168500	0.31878200
C	1.30342100	3.44250800	-0.70721000
C	1.38193100	4.84601100	-1.33152400
C	1.51592900	5.93550600	-0.25741600
C	0.38600500	5.83706800	0.77765500
C	0.30374300	4.43047800	1.40061900
H	3.30372000	0.33245000	2.29911300
H	3.16086700	1.41238000	0.92214500
H	1.62604800	2.21622300	2.62555300
H	0.96258500	0.61632100	2.89125400
H	3.56008400	-2.25332500	1.81111600
H	0.51620700	-2.28282500	2.09792500
H	1.65214500	-1.46690000	3.16702300
H	0.88810600	-3.62370300	4.15201500
H	2.62942200	-3.61213300	3.88910900
H	0.54664500	-4.95632100	2.08381500
H	1.69610800	-5.78216400	3.13331100
H	2.47451500	-5.74891000	0.73648500
H	3.60013100	-4.91195000	1.80085200
H	1.48397500	-3.59299000	0.00472100
H	3.22252800	-3.59454300	-0.26316700
H	3.87593800	-1.71663500	-1.26586300
H	3.82386200	1.33783900	-1.33307100
H	2.91555700	0.26137100	-2.38635000
H	5.01671500	1.09700900	-3.48625000
H	5.02639500	-0.65662700	-3.32544500
H	6.48025500	1.33156900	-1.49706700
H	7.23968800	0.24570200	-2.65739100
H	7.37066300	-0.65512500	-0.30791200
H	6.47216600	-1.73291000	-1.37219800
H	5.26517000	0.26715500	0.61270700
H	5.29097700	-1.48387000	0.78716800
H	-1.19358500	2.39171300	2.95636800
H	-1.00255200	-0.07805400	3.27637300

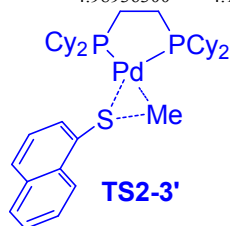
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H	-3.28823500	-0.55835000	4.11754700
H	-5.11394900	1.14561000	3.76715200
H	-4.64110600	0.36640500	2.25779100
H	-3.72851300	3.12759700	3.23292300
H	-4.83093100	2.81315000	1.89607500
H	-2.54350600	3.33088600	1.07917600
H	-3.02999100	1.70818300	0.60045400
H	-0.77556700	3.53972700	-0.23331100
H	1.17202700	2.68108800	-1.48529500
H	2.26014300	3.22355300	-0.21057000
H	0.47176300	5.02829300	-1.92202100
H	2.22450600	4.89659400	-2.03363500
H	1.52232000	6.93104800	-0.71995900
H	2.48424300	5.82218900	0.25316800
H	-0.57239600	6.07125600	0.29084700
H	0.52522400	6.58715700	1.56751500
H	-0.53101600	4.39341200	2.11098000
H	1.21834800	4.24983900	1.98299000
S	-1.04272200	-0.83860000	-2.61501900
C	-0.88739500	-2.57949400	-3.20263600
H	0.18097700	-2.75158800	-3.35327400
H	-1.26729100	-3.28464400	-2.45961800
H	-1.42164100	-2.70865900	-4.14829900
C	-2.84233400	-0.71450300	-2.52755800
C	-3.60967900	-1.35188500	-1.49609400
C	-3.47341700	0.05292700	-3.48807400
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C	1.22400200	3.17318300	1.59744200
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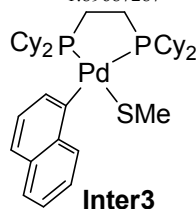
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H	-1.72468000	-1.43330000	2.13758200
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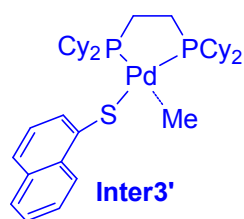
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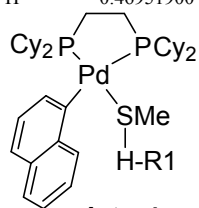
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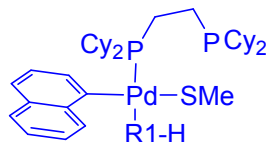
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H	-5.65312500	-1.94904000	-2.57641100
H	-3.85796900	-4.43037300	-2.39505100
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C	3.22598700	0.82591000	-3.17761800
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C	4.29293300	0.31028800	-3.94809700
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C	5.34199500	-0.33908300	-3.33968600
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H	5.42782300	-0.90553300	1.95218100
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H	6.16617800	-0.73926200	-3.92595500
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C	1.08374100	-1.65377500	-1.36746200
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H	-1.83196100	-0.88858300	1.39235200
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C	-0.90274000	-3.30923100	4.39343700
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H	0.20933900	-1.45816900	4.55310000
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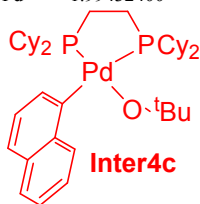
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Inter4b

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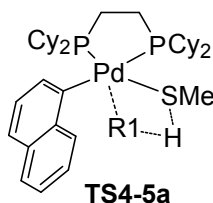
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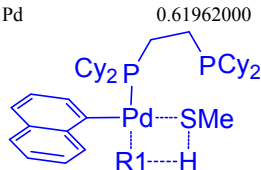
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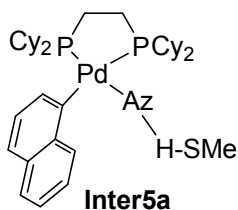
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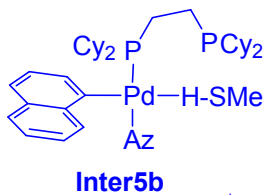
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C	-2.46545100	3.53487800	-2.57674100	C	1.99901500	5.30719900	-1.71455300
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H	-3.00759800	4.85145700	-0.97508600	H	3.38047500	5.27826700	-0.04857700
H	-2.00482500	4.79543300	1.27120900	H	-0.07623800	5.93833200	-1.52740900
H	-3.15790200	3.98179800	-3.28550100	H	0.89345000	6.19319400	-0.07928300
S	3.63308200	-0.99170000	-1.33174900	C	-5.57317000	3.09229300	-1.90724000
C	5.00051600	-0.71566500	-0.12777100	H	-4.39511600	1.80242500	-3.18827500
H	4.90274900	-1.38754200	0.72869900	H	-3.86234500	3.48127700	-3.19489400
H	5.95125300	-0.91133900	-0.63010600	H	-6.33507100	1.10777800	-1.50388400
H	4.97926400	0.32243900	0.21654500	H	-7.00587200	2.34717700	-0.44839800
Pd	1.60379200	0.34599300	-0.34643600	C	-3.52463700	-3.26365800	3.00912000
				H	-4.90868500	-3.56818500	1.35928300
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				H	-3.68547000	-1.59913300	4.38427300
				H	4.29281400	-0.03327700	5.36626300
				H	2.63686100	0.52175500	5.59397700
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				H	2.35928200	6.27774800	-2.07832700
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				H	-4.03532500	-3.95680100	3.68953100
				C	1.60318300	-0.20034700	-1.14192400
				O	1.84348900	0.27350100	-2.43662100
				N	2.64775800	-0.79643600	-0.62743600
				C	3.13788000	-0.07799000	-2.72329900
				C	3.64904400	-0.74504100	-1.60377800
				C	3.86891900	0.15386900	-3.87931000
				C	4.96511500	-1.21604700	-1.61355400
				C	5.18437500	-0.32306200	-3.88070500
				H	3.44263700	0.67063500	-4.73346100
				C	5.72071800	-0.99428400	-2.76784700
				H	5.37766900	-1.73295900	-0.75188100
				H	5.80273300	-0.17223500	-4.76141300
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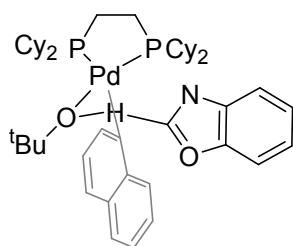
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C	2.07838700	1.22861600	2.31864700
C	1.29068800	3.45769000	0.52175600
C	-2.10403400	2.19060400	1.78654200
C	-3.69424700	1.23947400	-0.52167400
C	-3.19851800	-0.55483000	1.79376200
H	-0.61248800	1.58960400	3.24344300
H	-0.53070900	3.29252600	2.81483600
C	1.72724400	-0.11449600	2.99493300
C	2.57729700	2.25546100	3.35621800
H	2.88648100	1.01519100	1.60564800
C	2.58483100	3.27681100	-0.30225700
C	0.20608900	4.15491200	-0.32670100

S	3.50654900	-3.59842600	1.33841800
C	3.45228800	-4.65927900	-0.16050500
H	4.08540600	-4.24913200	-0.95087100
H	3.83553400	-5.64104100	0.12894300
H	2.42783100	-4.76586100	-0.52359500
C	-0.97532800	-1.21902000	-1.63872100
C	-0.97932600	-2.62347800	-1.34919000
C	-1.51205000	-0.80205300	-2.84544900
C	-0.39716700	-3.15727300	-0.16422100
C	-1.58371700	-3.54920700	-2.27214300
C	-2.09507300	-1.71267300	-3.76481900
H	-1.48522700	0.24990200	-3.11953500
C	-0.42299500	-4.50785900	0.11430900
H	0.09613000	-2.46811100	0.51509300
C	-1.60091800	-4.93551900	-1.95429000
C	-2.14247500	-3.05752400	-3.48142600
H	-2.50497700	-1.33693200	-4.70035100
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H	-2.06494100	-5.62285500	-2.65909100
H	-2.59377300	-3.76049700	-4.17832300
H	-1.05851000	-6.47188600	-0.56548100
Pd	-0.21503700	0.18707700	-0.30939600



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C	-0.09130400	2.97039200	-1.29752900
C	-0.60405700	3.24716100	1.62666400
C	2.26058600	0.51770300	-0.08644100
C	4.78675600	-0.24887900	-1.31621300
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H	2.04659400	2.46008300	0.86320400
H	1.40536600	1.12948300	1.80996400
C	-0.06692800	2.09554300	-2.57125000
C	1.06707100	3.98908800	-1.31321700
H	-1.03622500	3.53080700	-1.33094200
C	-1.63370500	4.33088400	1.24707800
C	-1.02574600	2.54315600	2.93665200
H	0.35621600	3.75312100	1.80867300
H	1.81963200	-0.47915200	-0.00993500
H	2.18886600	0.81366800	-1.13752500
C	4.82295500	0.82611400	-2.42497100
C	4.11443000	-1.53857500	-1.82610400
H	5.83498300	-0.48378900	-1.07614600
C	5.76282400	-1.32611600	1.69241100
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H	-0.91124100	1.39642100	-2.56132000
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C	1.02112400	4.85779900	-2.58352200
H	1.03567400	4.63108400	-0.42391100
H	2.02739300	3.45697400	-1.28050700
C	-1.84814800	5.33020200	2.39866500
H	-2.59246100	3.85872300	0.99535100
H	-1.31190800	4.87701300	0.35386100
C	-1.23778200	3.54513600	4.08323300
H	-1.95851500	1.98980500	2.75682000
H	-0.27866100	1.79769300	3.23256200
C	5.49015800	0.30045900	-3.70779400
H	5.34784600	1.71936300	-2.06379300
H	3.79753700	1.14370100	-2.66818900
C	4.78511700	-2.05911200	-3.11055200
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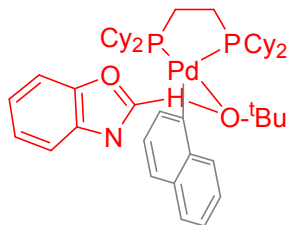
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H	2.57159500	-0.40218900	2.74941600
C	1.02493700	3.99948100	-3.85680600
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C	-2.25591800	4.62807500	3.70097700
H	-2.60555900	6.06884000	2.10689800
H	-0.91551200	5.88891300	2.56552000
H	-1.56620100	3.01083200	4.98363200
H	-0.27763800	4.01977500	4.33935300
C	4.81765300	-0.98632800	-4.20862300
H	6.55187700	0.09799700	-3.50267000
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H	5.81480500	-2.37209100	-2.88104100
H	4.25852100	-2.95407300	-3.46643700
C	5.33820900	-2.02658500	4.09844400
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H	5.87718700	-1.15786800	4.50541400
H	5.45600700	-2.83828400	4.82807900
H	-4.23541600	0.71128600	-1.53061500
C	-3.42751800	-1.18370500	-0.21818200
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N	-4.40235300	-1.08525000	-1.09715300
C	-4.55116700	3.06860300	-0.03290500
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H	-7.65233500	-4.35590800	-1.86885700
S	-3.67603000	1.86646500	-1.01063500
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C	-0.82895200	-1.20832700	0.87228000
C	-0.20215900	-2.20889500	0.06035300
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H	-0.86919700	-1.42904300	-1.83846200
C	1.17297400	-4.25094100	-0.12249300
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H	1.73511300	-5.04416600	0.36637500
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H	1.54003800	-4.98743600	-2.09888500
Pd	-1.98884300	0.25459500	0.06886200



Inter5c

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C	1.24853200	0.45098000	3.02101500
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C	3.05866100	-1.53062900	1.82337300
H	2.51709000	2.07760700	2.34093500
H	1.15464100	2.60244200	3.32085300
C	2.91452400	3.06760500	-0.37992200
C	1.73436100	4.88929500	0.93856500
H	0.95914000	3.84099600	-0.78373200
C	-1.79516600	3.69957100	0.26504900
C	-1.94386800	2.16730200	2.28971700
H	-0.73050800	3.93954800	2.13555600
H	1.97957000	0.20005500	3.79937600
H	0.25890500	0.35794900	3.47883000
C	-1.26516700	-1.77987900	2.38686800
C	0.64974900	-2.83259700	3.66418700
H	0.28377200	-2.99455500	1.53835100
C	3.25951500	-2.88181600	1.10427700
C	4.11986100	-0.50468700	1.37190500
H	3.19466300	-1.69669500	2.90333500
C	3.68509100	4.14071800	-1.16778400
H	2.76307600	2.17856000	-1.00155700
H	3.52515700	2.75581700	0.48012300
C	2.51322100	5.95777200	0.14932700
H	0.76434600	5.29826200	1.24352900
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C	-3.11062900	4.37252600	0.69314500
H	-1.98837500	2.89677300	-0.45505600
H	-1.16972500	4.43415100	-0.25703300
C	-3.24767300	2.86394000	2.71574200
H	-2.19200400	1.28426200	1.68774600
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C	-2.17407900	-2.96098800	2.76256000
H	-1.59344700	-1.34142200	1.44045700
H	-1.38252300	-0.99621900	3.14906300
C	-0.26390700	-4.00955300	4.05549200
H	1.68843800	-3.17894900	3.62564200
H	0.60195100	-2.06398100	4.44969100
C	4.69029500	-3.41231800	1.30368600
H	3.06492300	-2.75900300	0.03433800
H	2.54168800	-3.62427200	1.47102600
C	5.54813600	-1.04802600	1.55539100
H	3.95520400	-0.26188500	0.31537800
H	4.01290700	0.43151100	1.93356900
C	3.86459300	5.42676700	-0.34858100
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H	4.51358600	5.21971300	0.51582600
H	-4.32491700	2.58836100	0.86741700
H	-4.91378900	3.94402600	1.82962300
H	-2.37012700	-4.47538600	4.31552500
H	-1.90273200	-2.88387300	4.90748100
H	5.64158800	-2.24497800	-0.24467800
H	6.75138100	-2.77645300	1.01896900
C	-3.43210600	-0.05477700	-1.02898400
O	-4.31171300	0.22748300	-2.06968100
N	-3.87295200	-0.41768300	0.13541000
C	-5.43069400	-0.76321600	-1.48354200
C	-5.16869000	-0.88562900	-0.11212600
C	-6.62759000	-1.13747800	-2.07749500
C	-6.14609800	-1.40932700	0.73848100
C	-7.59563800	-1.66035400	-1.21618500
H	-6.79768000	-1.03095700	-3.14361200
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H	-5.96175400	-1.50969400	1.80372500
H	-8.55350800	-1.97187400	-1.62305700
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H	-2.45329200	0.36322200	-1.28912500
C	-0.52628100	1.29463000	-3.13629600
C	0.57335600	-1.67119500	-1.29680700
C	1.68999500	-2.04708100	-2.11678900
C	-0.50753400	-2.53538500	-1.23507500
C	2.85049900	-1.23154500	-2.25355900
C	1.66466200	-3.28948700	-2.84557600
C	-0.53816800	-3.75674400	-1.95693700
H	-1.38017700	-2.27675300	-0.64082400
C	3.91726200	-1.60426700	-3.04333600
H	2.87192700	-0.28850900	-1.71480000
C	2.78079100	-3.64747700	-3.65178900
C	0.52498000	-4.13023500	-2.74511500
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C	3.88323800	-2.82961900	-3.75228500
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H	0.50820500	-5.06499000	-3.30124300
H	4.72529900	-3.11880300	-4.37591400
Pd	0.48662700	0.13117000	-0.29007000
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C	-0.87857300	0.02694400	-3.94500900
H	-0.17798900	-0.78343500	-3.73205300
H	-1.88684100	-0.31981900	-3.69294100
H	-0.85080200	0.22759100	-5.02445200
C	-1.52089700	2.41533000	-3.52405300
H	-1.29530200	3.33307400	-2.96869900
H	-1.47508900	2.64118600	-4.59728800
H	-2.54762300	2.11561100	-3.28437700
C	0.89719300	1.75431600	-3.50437500
H	1.62745700	0.98328300	-3.24070800
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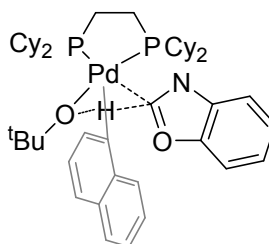


Inter5c'

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H	-5.93056600	-0.67548400	-0.96932800
C	-5.91246200	1.19174600	1.26794600
C	-3.65236700	1.26550400	2.41529200
H	-4.01958900	1.66709400	0.33147300
C	0.39568900	-3.76308300	-2.93278500
H	1.10076700	-1.87221800	-2.14266000
H	-0.66471700	-2.07002400	-2.10399200
C	-0.48662000	-5.35108800	-1.16940100
H	-0.47900500	-4.55896100	0.84988500
H	-1.62420700	-3.77502600	-0.23142300
C	2.33600100	-4.21413300	3.67060100
H	3.00628300	-3.00486200	2.00414200
H	1.89646800	-4.29211900	1.55564400
C	1.44964000	-2.17208900	4.86831600
H	2.09873000	-0.90564500	3.23568500
H	0.38222400	-0.77652200	3.59937100
C	-5.52944600	-2.40538400	-3.09759100
H	-5.15623700	-3.01263100	-1.04111900
H	-3.71580200	-2.54492200	-1.93781700
C	-5.15870100	0.06089100	-3.53683100
H	-4.52202900	1.20383900	-1.80599400
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C	-6.23887100	2.58761700	1.82659600
H	-6.31108700	0.42868600	1.95336300
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C	-3.99098600	2.65889300	2.97232800
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H	-2.56895100	1.19905100	2.26580800
C	-0.62204500	-4.86918100	-2.62053700
H	1.41218800	-4.17909700	-2.87961700
H	0.26135100	-3.39963600	-3.95992700
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C	-1.24837300	-6.10821500	-0.94253700
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H	3.18278400	-4.90662100	3.58342700
H	1.45796900	-4.82530700	3.92789300
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O	3.90507400	2.33054600	-2.94578700
N	2.98944100	1.60145700	-1.03997600
C	3.96856200	3.37012100	-2.04012800
C	3.39181700	2.93051600	-0.84324700
C	4.49863800	4.63781700	-2.22595600
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C	4.42652600	5.48695200	-1.12021500
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C	-1.56641300	4.32932800	-0.23288400
C	-0.51951500	3.81453800	1.95442800
H	0.44771900	3.23132200	3.77207400
C	-1.77904100	4.03165600	-1.56000900
H	-1.34509600	2.65080400	-3.17829900
H	-2.02288400	5.21125800	0.21211400
H	-0.98278000	4.70280400	2.37778100
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O	3.06727900	-1.32280800	-1.10674600
C	4.94853800	-1.15974900	0.47052500
H	5.97615900	-1.49893400	0.65744500
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C	4.41816400	-3.29125700	-0.77513000
H	4.02949400	-3.70911100	-1.71150400
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H	3.79212700	-3.65892400	0.04327600
C	5.31556500	-1.31402800	-2.00329300
H	6.31686900	-1.75327400	-1.90707400
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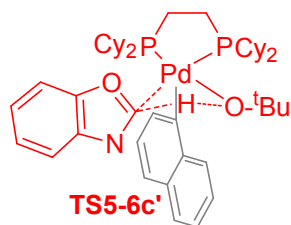


TS5-6c

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C	-0.56763500	-2.78721600	-2.01399800
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C	-1.02144400	2.79322200	-1.49922500
C	1.93418700	2.93020000	-1.75137200
H	2.24382600	-0.47228600	-3.02820800
H	0.89898800	-1.19476400	-3.90305900
C	3.47409400	-1.78297000	-0.72852600
C	2.61469500	-3.62972100	-2.24842600
H	1.95839100	-3.20600300	-0.22824600
C	-0.96507900	-3.75830800	-0.88086200
C	-1.81096100	-2.08766700	-2.60410800
H	-0.10230800	-3.36889500	-2.82418700
H	0.85109600	1.37168200	-3.86505400
H	-0.61447500	0.60462500	-3.26374600
C	-2.30514200	1.94689700	-1.35928300
C	-1.12199800	3.72571200	-2.72689800
H	-0.93592800	3.41095200	-0.59499600
C	1.96305200	4.11233200	-0.76023900
C	3.30573400	2.22576500	-1.81699600
H	1.72083000	3.33263600	-2.75385500
C	4.68417700	-2.65665300	-0.35746000
H	3.20882500	-1.13537000	0.11249600
H	3.75752100	-1.12502800	-1.56313900
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H	1.76754800	-4.28465200	-2.47919900
H	2.84303400	-3.07247200	-3.16931000
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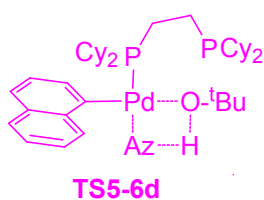
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C	-3.55133900	2.84256000	-1.26551100
H	-2.24112000	1.29033700	-0.48776700
H	-2.41280500	1.28820000	-2.23311300
C	-2.37769600	4.61420300	-2.64216800
H	-0.23470900	4.36275900	-2.81532500
H	-1.17210000	3.12233600	-3.64496300
C	3.09874000	5.09478800	-1.09725100
H	2.10216000	3.73278600	0.25635300
H	1.00507000	4.64421100	-0.76863700
C	4.43638700	3.22033600	-2.13697700
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C	5.04355200	-3.63645300	-1.48257100
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H	3.56064300	-5.14226300	-1.02424400
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H	-1.57130100	-5.43087500	-2.12421300
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H	-7.46877100	-0.45903700	0.77862500
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H	2.89230400	-2.91061700	2.53366100
C	0.53752000	-0.92354600	4.15889500
H	0.74311000	-1.21927900	5.19555900
H	1.05057800	0.02221700	3.96456000
H	-0.53832000	-0.75633500	4.04614200



P	0.98365500	-1.74533700	-1.57109400
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C	2.48915100	-2.85254500	-1.72994000
C	-0.48637800	-2.88748800	-1.80620400
C	0.41735600	0.66133900	-3.01311500
C	-0.67405300	2.67580400	-1.17826800
C	2.23073100	2.67152900	-1.82972800
H	2.08499900	-0.65433100	-3.44122000
H	0.53184000	-1.28106400	-3.96855300
C	3.79808900	-2.03751700	-1.64114200
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C	-0.48420700	-4.03583700	-0.77450300
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H	-0.39060800	-3.31767700	-2.81514600
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H	3.86442100	-1.32073700	-2.47337700
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H	1.58224100	-4.37365900	-3.01651300
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C	-2.06810400	4.62487900	-2.02920900
H	0.01323000	4.27963100	-2.50641000
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C	3.61996700	4.71581700	-1.22922200
H	2.69957300	3.35147200	0.17514000
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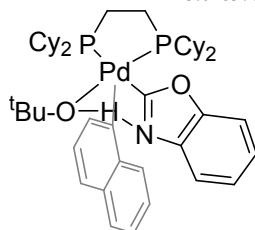
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C	-3.01965000	-4.19227500	-0.92325400
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H	-1.60891100	-5.47406100	-1.94681500
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C	-3.35865200	3.85185500	-1.72393800
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H	-2.21974100	5.30488000	-2.87703200
C	4.91185300	3.92403100	-1.47278600
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H	3.34003400	5.25045300	-2.14982100
H	5.59700200	2.21983200	-2.64144300
H	4.45376600	3.26286500	-3.48230800
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H	5.12821700	-3.22909800	-3.83367500
H	-3.16214800	-3.78563600	0.08826900
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C	2.38082000	-2.31751700	1.91841700
O	3.04112600	-1.84867200	3.09113900
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C	4.11428900	-2.66523200	3.27902100
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C	4.96498600	2.37197000	3.31712900
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H	1.48537300	4.10995900	4.51014000
H	5.93895400	2.61147000	3.73599700
C	-0.99856300	-1.71335600	2.90300800
Pd	0.95227500	-0.06969400	0.24513100
O	-0.20746600	-1.64314600	1.70074700
C	-1.23139600	-3.20046100	3.23038900
H	-0.27580300	-3.71035000	3.39364000
H	-1.83887700	-3.31340500	4.13700200
H	-1.74969100	-3.70201700	2.40536200
C	-0.28445200	-1.02564400	4.07818600
H	-0.11438800	0.03197900	3.86261300
H	-0.88766000	-1.10262900	4.99169200
H	0.68758800	-1.49085300	4.26800600
C	-2.33565000	-1.02714500	2.60254300
H	-3.00577300	-1.08033700	3.46887400
H	-2.18015700	0.02837000	2.35673000
H	-2.83399700	-1.51022200	1.75385200



P	-0.25544500	-1.73430500	-0.59195000
P	4.18388600	-0.55692400	-0.22421500
C	1.51873400	-1.24555700	-0.93156000
C	-0.21337900	-3.02690900	0.77065300
C	-0.58098000	-2.71147100	-2.17999500
C	2.33873900	-0.60877700	0.20205000
C	4.94976500	-0.52327200	1.50847600
C	4.42975000	1.22254200	-0.81518700
H	2.02014200	-2.15764100	-1.27702100
H	1.48049300	-0.56994800	-1.79127300
C	-0.24803400	-2.41304100	2.19006800
C	0.92266100	-4.06265400	0.62293100
H	-1.17087800	-3.54805300	0.64476700
C	-1.69717800	-0.56994800	-2.08878700
C	-0.84930800	-1.77071100	-3.37464500
H	0.36439100	-3.24145100	-2.37295900
H	1.95098500	0.38069500	0.45767100
H	2.26469300	-1.22239100	1.10502300
C	4.91592800	-1.93682600	2.13062300
C	4.40451600	0.52420900	2.49961900
H	6.00899900	-0.29082700	1.31997900
C	5.93691900	1.51730200	-0.98188900
C	3.68673600	1.45382100	-2.14960800
H	4.01344800	1.91896600	-0.07303300
C	-0.32473600	-3.51675000	3.26008900
H	-1.11771900	-1.75411400	2.27600700
H	0.64886300	-1.80450000	2.36492900
C	0.82307500	-5.15252300	1.70555200
H	0.90119500	-4.52770600	-0.37092600
H	1.89674000	-3.56379000	0.71308800
C	-1.82568800	-4.55614200	-3.40716300
H	-2.65142500	-3.27753500	-1.86572100
H	-1.50469500	-4.47310100	-1.27122900
C	-0.96579900	-2.55393200	-4.69269700
H	-1.78944400	-1.23361000	-3.19027900
H	-0.06652200	-1.00942500	-3.46204400
C	5.65126400	-1.98569600	3.48113700
H	5.35371700	-2.66251800	1.43390500
H	3.87197900	-2.24785400	2.28925600
C	5.14337600	0.46870200	3.84949300
H	4.48398100	1.53230300	2.07656200
H	3.33366700	0.34687500	2.67143500
C	6.19810700	2.91622300	-1.56587600
H	6.37843400	0.76113200	-1.64834400
H	6.45525700	1.42443900	-0.01980100
C	3.95887400	2.85184400	-2.73118700
H	4.00268300	0.69147100	-2.87781300
H	2.60652200	1.33453100	-2.00834800
C	0.80577000	-4.54482900	3.11517900
H	-1.29429600	-4.02840000	3.17425800
H	-0.30235300	-3.06016500	4.25752400
H	-0.09688500	-5.73472500	1.54942100
H	1.66014200	-5.85422600	1.59834400
C	-2.05681300	-3.62982900	-4.60906800
H	-2.64389100	-5.28198300	-3.32002100
H	-0.90697600	-5.13921700	-3.56919600
H	-1.17556600	-1.85885800	-5.51538500
H	0.00043600	-3.02722000	-4.92166900
C	5.10296400	-0.93881400	4.46159100
H	6.72250900	-1.79948800	3.31373600
H	5.57352600	-2.99209800	3.91286000
H	6.19174900	0.76735000	3.69967500
H	4.70765600	1.19941900	4.54335400
C	5.46052300	3.11855200	-2.89607700
H	7.27768800	3.06598600	-1.69799100

H	5.86218200	3.67741600	-0.84629300	C	1.02971200	3.49809500	0.91412700
H	3.44011200	2.95739400	-3.69264900	C	-2.19869400	1.83651300	2.16926100
H	3.52702700	3.60661900	-2.05916700	C	-3.86067700	1.05651200	-0.14333600
H	0.70030600	-5.33680100	3.86743800	C	-3.06685500	-0.97304600	1.87732700
H	1.77222300	-4.05567900	3.31007600	H	-0.58791000	1.24037600	3.49592200
H	-3.03750500	-3.14251500	-4.50757300	H	-0.65618800	2.97056600	3.20275700
H	-2.09147000	-4.21360200	-5.53742800	C	1.80761500	-0.23623200	3.04317700
H	5.67028200	-0.96264200	5.40087000	C	2.56052400	2.15100300	3.49881200
H	4.06330600	-1.19213400	4.71814200	H	2.84631200	1.03329500	1.66814400
H	5.87361000	2.42963300	-3.64808600	C	2.30372800	3.53284400	0.04212000
H	5.62964900	4.13458000	-3.27570800	C	-0.13705000	4.19614200	0.18360700
N	-3.24467100	2.25217000	1.58717600	H	1.22685700	4.05542900	1.84195300
C	-3.86062100	3.39480100	1.10219500	H	-2.90314300	1.67889900	2.99555900
C	-3.55244300	1.29417400	0.74965800	H	-2.50218400	2.76430900	1.67453900
C	-4.55997300	3.06307900	-0.07130500	C	-3.51760900	2.32739200	-0.95032100
C	-3.88131900	4.71122000	1.58355100	C	-5.17908200	1.25420100	0.63486600
O	-4.37629200	1.73641700	-0.30245700	H	-3.99827000	0.24413500	-0.87073000
C	-5.29719500	3.98426700	-0.80867100	C	-3.69659200	-2.06621800	0.98683400
C	-4.61198900	5.64676600	0.85810500	C	-1.96896700	-1.57388300	2.78228900
H	-3.34337100	4.97833500	2.48759600	H	-3.85395300	-0.55845700	2.52573800
C	-5.30798200	5.28914700	-0.31674300	C	3.05555500	-0.75723900	3.77481100
H	-5.83022000	3.70204900	-1.71067300	H	1.52947200	-0.95336900	2.26582400
H	-4.65096000	6.67766700	1.19874500	H	0.97697400	-0.17995900	3.76226600
H	-5.86672400	6.05186000	-0.85221300	C	3.80691300	1.61407800	4.22602100
O	-3.37660000	-1.26727500	1.19108100	H	2.79491100	3.12463200	3.05359200
C	-0.80387000	1.35456600	-0.84772500	H	1.76403900	2.32596700	4.23751900
C	-0.04757700	2.25201600	-0.02440500	C	2.66978900	4.97198500	-0.36008900
C	-0.97007500	1.64363900	-2.18988600	H	2.13420600	2.93738400	-0.86285000
C	0.14943200	2.04593900	1.37078200	H	3.14799300	3.07390600	0.56953500
C	0.52592000	3.43135300	-0.61852500	C	0.23124200	5.63297500	-0.22638000
C	-0.41287000	2.81419400	-2.76772400	H	-0.39843000	3.61517800	-0.71135700
H	-1.55322900	0.98364100	-2.82425900	H	-1.03024600	4.21932700	0.82023600
C	0.88328200	2.92908300	2.13257300	C	-4.66543700	2.70858500	-1.90005100
H	-0.30962300	1.17757800	1.83311400	H	-2.59209300	2.17372100	-1.51361900
C	1.27807500	4.32207500	0.19661400	H	-3.33681700	3.16840000	-0.26558200
C	0.32266900	3.68667000	-2.00128200	C	-6.32942000	1.64947900	-0.30954100
H	-0.57580400	3.01450100	-3.82416500	H	-5.45364700	0.34429900	1.18010500
C	1.45883900	4.07861700	1.53949500	H	-5.04445000	2.04367700	1.38873800
H	1.01059300	2.75015500	3.19685300	C	-4.22209400	-3.24238100	1.82858100
H	1.70277400	5.21164200	-0.26392900	H	-2.94640700	-2.43486100	0.27889800
H	0.75341200	4.58420300	-2.43872600	H	-4.51730800	-1.65215800	0.38989700
H	2.03254100	4.77236800	2.14862700	C	-2.49768300	-2.75705100	3.61113400
C	-4.53490800	-2.05246600	0.92294500	H	-1.13322400	-1.91134500	2.15590800
C	-4.16450600	-3.53877600	1.05734600	H	-1.56754200	-0.80912100	3.45845700
H	-3.74687300	-3.73420200	2.05138500	C	3.55513800	0.22949800	4.83752300
H	-5.04115400	-4.18425100	0.91907000	H	3.84361900	-0.94054700	3.03319100
H	-3.41784900	-3.82156600	0.30828800	H	2.82848700	-1.73022800	4.22776100
C	-5.59566400	-1.69554300	1.98452600	H	4.63782800	1.54795500	3.50845800
H	-5.88332700	-0.64116100	1.90168900	H	4.11743000	2.32852700	4.99954800
H	-6.50103800	-2.30530300	1.87194400	C	1.50699000	5.66985600	-1.07901600
H	-5.18942200	-1.85700100	2.98876700	H	3.56066400	4.95669800	-1.00000700
C	-5.09603700	-1.77146800	-0.48446900	H	2.93912700	5.54584400	0.53947700
H	-5.98063600	-2.38640200	-0.69273400	H	-0.60734800	6.08589400	-0.77068900
H	-5.38106900	-0.71929200	-0.58844100	H	0.38123600	6.24035300	0.67878500
H	-4.34052500	-1.99150400	-1.24786500	C	-5.98667700	2.89415000	-1.14009300
Pd	-1.86426800	-0.14427300	-0.03224400	H	-4.78330100	1.91869900	-2.65555500
H		-3.62837800	0.04162300	H	-4.40596000	3.62585600	-2.44389700

1.05330700

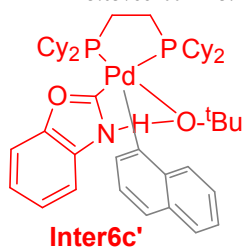


Inter6c

P	0.58153900	1.74717900	1.43159400
P	-2.39942500	0.47432100	0.88246100
C	-0.76755700	1.99152600	2.72044300
C	2.06114500	1.15775400	2.42742600

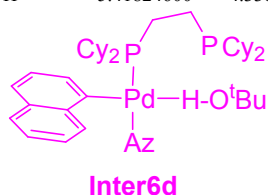
C	1.02971200	3.49809500	0.91412700
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C	-3.86067700	1.05651200	-0.14333600
C	-3.06685500	-0.97304600	1.87732700
H	-0.58791000	1.24037600	3.49592200
H	-0.65618800	2.97056600	3.20275700
C	1.80761500	-0.23623200	3.04317700
C	2.56052400	2.15100300	3.49881200
H	2.84631200	1.03329500	1.66814400
C	2.30372800	3.53284400	0.04212000
C	-0.13705000	4.19614200	0.18360700
H	1.22685700	4.05542900	1.84195300
H	-2.90314300	1.67889900	2.99555900
H	-2.50218400	2.76430900	1.67453900
C	-3.51760900	2.32739200	-0.95032100
C	-5.17908200	1.25420100	0.63486600
H	-3.99827000	0.24413500	-0.87073000
C	-3.69659200	-2.06621800	0.98683400
C	-1.96896700	-1.57388300	2.78228900
H	-3.85395300	-0.55845700	2.52573800
C	3.05555500	-0.75723900	3.77481100
H	1.52947200	-0.95336900	2.26582400
H	0.97697400	-0.17995900	3.76226600
C	3.80691300	1.61407800	4.22602100
H	2.79491100	3.12463200	3.05359200
H	1.76403900	2.32596700	4.23751900
C	2.66978900	4.97198500	-0.36008900
H	2.13420600	2.93738400	-0.86285000
H	3.14799300	3.07390600	0.56953500
C	0.23124200	5.63297500	-0.22638000
H	-0.39843000	3.61517800	-0.71135700
H	-1.03024600	4.21932700	0.82023600
C	-4.66543700	2.70858500	-1.90005100
H	-2.59209300	2.17372100	-1.51361900
H	-3.33681700	3.16840000	-0.26558200
C	-6.32942000	1.64947900	-0.30954100
H	-5.45364700	0.34429900	1.18010500
H	-5.04445000	2.04367700	1.38873800
C	-4.22209400	-3.24238100	1.82858100
H	-2.94640700	-2.43486100	0.27889800
H	-4.51730800	-1.65215800	0.38989700
C	-2.49768300	-2.75705100	3.61113400
H	-1.13322400	-1.91134500	2.15590800
H	-1.56754200	-0.80912100	3.45845700
C	3.55513800	0.22949800	4.83752300
H	3.84361900	-0.94054700	3.03319100
H	2.82848700	-1.73022800	4.22776100
H	4.63782800	1.54795500	3.50845800
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C	1.50699000	5.66985600	-1.07901600
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H	2.93912700	5.54584400	0.53947700
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H	0.38123600	6.24035300	0.67878500
C	-5.98667700	2.89415000	-1.14009300
H	-4.78330100	1.91869900	-2.65555500
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C	-3.12224000	-3.83725200	2.71834100
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H	-5.05567900	-2.89815000	2.45996100
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H	-3.25230300	-2.39295700	4.32484700
H	4.47104000	-0.14731900	5.31052700
H	2.80437600	0.31897700	5.63764600
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H	1.77321200	6.70695400	-1.31935800
H	-6.80129300	3.11866200	-1.84006800
H	-5.90065300	3.76382100	-0.47125500
H	-2.34332000	-4.27725000	2.08006100
H	-3.52709700	-4.65118000	3.33313600
C	1.42928100	0.22636200	-1.36408300
O	1.47806300	1.02857600	-2.50858500
N	2.55296600	-0.41656100	-1.16535000

C	2.72818700	0.84520000	-3.04084300	C	-4.54235100	-0.35071000	0.30207200
C	3.40926900	-0.05323800	-2.21165900	C	-3.82160900	1.69275600	-1.02200100
C	3.28073700	1.41444700	-4.17865200	H	-4.47332500	-0.18404500	-1.85189600
C	4.72354400	-0.41689000	-2.51721500	C	0.12420500	5.22955400	-0.83445800
C	4.59577600	1.04155200	-4.47645500	H	-0.41008500	3.26190800	-0.08303000
H	2.72190700	2.10469600	-4.80272400	H	-1.17576000	3.69120700	-1.61472800
C	5.30237400	0.14296200	-3.65889700	C	1.55996600	5.19352300	-2.92013900
H	5.27469200	-1.11000800	-1.88908600	H	2.03890400	3.21169200	-3.65588600
H	5.07871600	1.45386100	-5.35809800	H	0.33904200	3.64512700	-3.81104300
H	6.32253100	-0.12254700	-3.92294600	C	4.55757800	0.24043400	-2.89818200
H	2.68965000	-1.84922500	0.11508700	H	3.34095200	0.48079300	-1.12316200
C	-1.09264200	-0.86476400	-1.82770300	C	3.46345800	1.93397700	-2.11365400
C	-1.13842900	-2.29716900	-1.79146500	C	3.12197800	-1.67364400	-3.70587500
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C	-0.51504000	-3.05689200	-0.75982600	H	0.98889200	-1.34629000	-3.51065000
C	-1.83017800	-3.01811700	-2.82996300	C	-1.37544700	-4.74272500	-1.41211400
C	-2.30454200	-0.92970500	-3.95950000	H	-0.36205600	-2.89309700	-0.87581300
H	-1.57361400	0.86051100	-3.01016700	H	-0.81229100	-3.01346600	-2.57239600
C	-0.60587000	-4.43304800	-0.72379100	C	-3.80660700	-4.45141200	-2.06337800
H	0.07953500	-2.53668700	-0.01452900	H	-4.53447400	-2.41460400	-1.96081000
C	-1.90983300	-4.43635000	-2.75803900	H	-3.34558100	-2.68743200	-3.23171500
C	-2.41191800	-2.29963400	-3.90756300	C	-5.93810900	0.27009800	0.48428100
H	-2.72693300	-0.37913600	-4.79785600	H	-3.91338500	-0.09149800	1.16130200
C	-1.32202800	-5.13176200	-1.72612200	H	-4.62912100	-1.44344400	0.29452900
H	-0.11235200	-4.98585200	0.07158200	C	-5.21839900	2.30707800	-0.82688700
H	-2.44352300	-4.96571200	-3.54510100	H	-3.15412000	2.04540400	-0.22550600
H	-2.92658900	-2.85075000	-4.69176400	H	-3.39947400	2.04643000	-1.97083900
H	-1.39067100	-6.21612400	-1.68735700	C	0.45066800	5.93316600	-2.15938300
Pd	-0.30091800	0.29253500	-0.29079700	H	0.99263400	5.29350000	-0.16331400
O	2.61617100	-2.53930500	0.81747100	H	-0.70291700	5.73886700	-0.32381600
C	3.52728600	-3.60868300	0.54310500	H	2.49746300	5.25769800	-2.34878200
C	4.97018900	-3.14271100	0.81337300	H	1.75018000	5.67648400	-3.88717200
H	5.07731100	-2.81977700	1.85488600	C	4.43922400	-1.28444500	-3.02088600
H	5.69555200	-3.94374600	0.62373500	H	5.47799700	0.50858600	-2.36516700
H	5.22738600	-2.29389100	0.16882900	H	4.63175100	0.68920700	-3.90117700
C	3.14794800	-4.73379000	1.51268200	H	3.01778300	-2.76568800	-3.74559800
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H	3.20784100	-4.37905800	2.54778600	H	-1.61784500	-4.97649700	-0.36546200
C	3.37834300	-4.07914500	-0.91359800	H	-0.44261700	-5.27189500	-1.64305100
H	4.03398400	-4.93327500	-1.12365500	H	-4.17089600	-4.67838800	-1.05093600
H	2.34392100	-4.37440900	-1.11455700	H	-4.59348100	-4.77270500	-2.75778200
H	3.63788400	-3.27522700	-1.61194300	C	-5.88251000	1.80362800	0.46207400



P	0.52800800	1.16862300	-1.94712900	H	-6.89156000	2.22406000	0.55840200
P	-2.16156300	-0.59561900	-1.24674200	C	1.34946600	0.61680300	1.17712700
C	-0.86858000	1.06470600	-3.20477400	O	1.33311000	1.80692600	1.90638600
C	0.88507100	3.00570500	-1.80863600	N	2.49051100	-0.01356900	1.28528800
C	2.02104400	0.46107200	-2.84384400	C	2.56712900	1.89474400	2.50452800
C	-1.75925500	-0.18197700	-3.03831900	C	3.29860600	0.76749000	2.11965300
C	-2.45951500	-2.44814700	-1.26186700	C	3.06930500	2.88463500	3.33679700
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H	-1.47132300	1.96814400	-3.06469100	C	4.38336100	2.70180000	3.78210800
H	-0.46801800	1.10873000	-4.22500800	H	2.47716200	3.74677100	3.62708800
C	-0.23456000	3.74885100	-1.04824000	C	5.13971500	1.57981200	3.39804400
C	1.20919400	3.71101900	-3.14207300	H	5.18539000	-0.27242100	2.24583400
H	1.77831000	3.04062600	-1.16923800	H	4.82826300	3.44483700	4.43844300
C	3.35156600	0.84407800	-2.15726900	H	6.15858900	1.48014200	3.76287700
C	1.90774500	-1.07376700	-2.97567000	H	3.45419900	-1.56837800	0.70662900
H	2.01220800	0.89519500	-3.85594800	C	-1.00131200	-0.73466100	1.83389000
H	-2.68592200	-0.06381400	-3.61368200	C	-1.73015600	0.03070000	2.80339800
H	-1.24685300	-1.05813800	-3.44850400	C	-0.77941600	-2.07598200	2.09659300
C	-1.15739200	-3.22671100	-1.55065000	C	-1.98033600	1.42388900	2.64326000
C	-3.59511100	-2.93122400	-2.18853000	C	-2.24385600	-0.60699000	3.98779400
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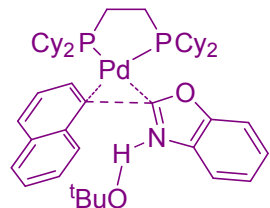
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C	-2.98511400	0.16300500	4.92627700
C	-1.99784400	-1.99028500	4.19316000
H	-1.07198600	-3.76240500	3.43160500
C	-3.21461500	1.50530000	4.72621700
H	-2.86862100	3.20865500	3.42462600
H	-3.36832400	-0.33341100	5.81566500
H	-2.38264100	-2.46692800	5.09211000
H	-3.78154100	2.07842800	5.45556200
Pd	-0.28843200	0.11446000	0.07553600
O	4.18765100	-2.18536000	0.47361400
C	3.90817500	-3.48509200	1.00095100
C	3.59483100	-3.39323500	2.50421000
H	2.70342100	-2.77981400	2.67878900
H	3.41461100	-4.38595100	2.93489700
H	4.43293800	-2.93361700	3.03940000
C	2.72102800	-4.10861500	0.24438000
H	2.94071100	-4.15903800	-0.82821500
H	2.49942200	-5.12253300	0.60066200
H	1.82137900	-3.49666500	0.38188900
C	5.18093600	-4.30539100	0.76454000
H	6.02799700	-3.84594800	1.28523100
H	5.06356600	-5.33294800	1.12744100
H	5.41824600	-4.33882600	-0.30467000



P	-0.22846800	-1.75620500	-0.69045400
P	4.21570700	-0.67703800	-0.12099500
C	1.56231000	-1.28808300	-0.99741700
C	-0.17901100	-3.06708300	0.66366400
C	-0.50759800	-2.76217200	-2.27449000
C	2.34260200	-0.62497900	0.15108000
C	4.83105700	-0.41201200	1.65314100
C	4.57174100	0.99942100	-0.92605100
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C	-0.26266400	-2.46342200	2.08526800
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H	-1.11791700	-3.61646200	0.51456100
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C	-0.68063100	-1.83852200	-3.50009000
H	0.41636100	-3.34306400	-2.41645200
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C	4.68686600	-1.71122300	2.47652800
C	4.25189200	0.78895800	2.42663900
H	5.91172200	-0.24399900	1.52914200
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C	4.04612600	1.01953800	-2.37887000
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C	-0.35787800	-3.57223700	3.14858000
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C	0.86691700	-5.17973900	1.62162600
H	0.99785900	-4.54050400	-0.44721100
H	1.94009400	-3.56436500	0.67199100
C	-1.80084000	-4.56877300	-3.51783500
H	-2.61705900	-3.21073100	-2.04261000
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C	-0.79103600	-2.64200100	-4.80676300
H	-1.59424400	-1.24452900	-3.36295600
H	0.14556400	-1.12364300	-3.57544600
C	5.31917700	-1.57271200	3.87247600
H	5.14235200	-2.55045000	1.93601800
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C	4.88528800	0.92325900	3.82335700
H	4.40030400	1.71828500	1.86476600
H	3.16536700	0.66883500	2.53699400
C	6.43853600	2.60048200	-1.64118400
H	6.62329700	0.45930900	-1.38291100
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C	4.40410100	2.32467500	-3.10971900
H	4.47134200	0.16664400	-2.92879200
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C	0.79239300	-4.58244400	3.03402500
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H	-0.03582400	-5.77958500	1.43283400
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H	5.95261700	1.16735100	3.71393700
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C	5.91302700	2.59872500	-3.08278700
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C	-5.63098400	3.07122900	2.29337700
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C	-4.58081800	4.80562700	0.26642200
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H	-6.88246000	4.74477400	2.79375800
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H	2.27940700	4.99076300	-0.79846000
H	1.34686300	4.25206000	-2.94621400
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C	-4.55294700	-1.98190400	0.86115300
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H	-3.70508900	-3.72249000	1.84014300
H	-4.97707000	-4.10028300	0.65802800
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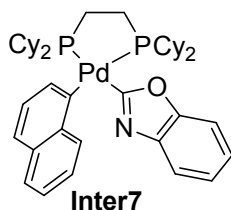
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H	-4.35531300	-1.70816600	-1.28726900
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TS6-7

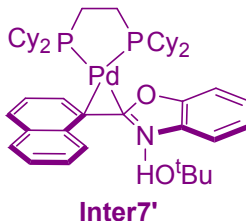
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C	2.25923900	-0.46995100	2.83100900
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H	-1.80865100	2.02720700	1.78414100
H	-2.60931100	0.80649300	2.76084700
C	-2.62202900	2.28830200	-1.02937100
C	-4.55497900	1.31921800	0.30746100
H	-3.49546700	0.35678100	-1.30756000
C	-3.55254700	-2.28015600	-0.16886800
C	-2.02609300	-2.50010300	1.84581600
H	-3.74297300	-1.20156700	1.69318100
H	-0.26734700	1.52326300	3.56713400
H	-0.52023800	-0.20735400	3.41735600
C	1.78391200	-1.92713100	3.01892400
C	2.58872100	0.18009900	4.19214600
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C	1.87258600	-0.78315900	-1.59089800
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C	3.96138600	-0.41008700	-2.21686500
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C	-1.76286600	-2.58003400	-5.02025100
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H	2.31265600	-6.81969500	-1.40424800
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H	2.49198800	-5.14812600	-1.97474400
C	3.30849900	-5.28352500	0.68822500
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H	3.76514200	-6.28082800	0.66661000
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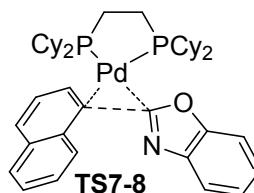
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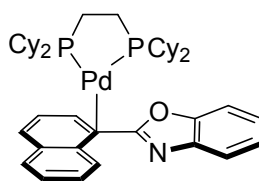
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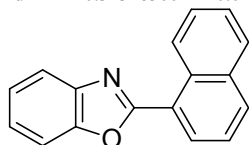
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H	-2.06799100	-1.74671400	-5.73776100
H	-2.04277900	-5.83204900	-3.28391500
Pd	0.10586700	-0.21478900	-0.46715900



Inter8

P	2.14209400	-1.26231700	0.42137100
P	-0.19597100	0.78134400	1.68138500
C	1.92294000	-1.08887700	2.28910500
C	2.13755400	-3.13406400	0.18502300
C	3.95130300	-0.80314000	0.15209200
C	1.26962000	0.23512800	2.74075700
C	-0.21846000	2.64990600	1.91782600
C	-1.68967000	0.19611200	2.67099600
H	1.28843100	-1.92855500	2.59398200
H	2.88331900	-1.22377100	2.80340700
C	0.70792200	-3.70306000	0.31443900
C	3.12500100	-3.93503000	1.05909900
H	2.43425200	-3.25889700	-0.86670100
C	4.40496000	-1.16255900	-1.27883800
C	4.19262000	0.69707200	0.42792100
H	4.55653800	-1.38211700	0.86598800
H	0.97560000	0.16058600	3.79573000
H	2.00626100	1.04441900	2.67968800
C	0.94260400	3.32021300	1.15164900
C	-0.27433200	3.15461300	3.37475100
H	-1.14476500	2.95492100	1.40974700
C	-2.99212200	0.84982600	2.15902900
C	-1.80837200	-1.34282400	2.62906500
H	-1.53562400	0.49653500	3.71867200
C	0.66842500	-5.20474500	-0.01629600
H	0.02617600	-3.14770400	-0.34039900
H	0.34291900	-3.55679400	1.34137800
C	3.07878900	-5.43812300	0.72783900
H	4.14920500	-3.56438700	0.93074300
H	2.87171800	-3.79654900	2.12001700
C	5.86381900	-0.75278100	-1.54235700
H	3.74735300	-0.65279200	-1.99655800
H	4.29547500	-2.23822400	-1.46147800
C	5.65379900	1.10110700	0.16342000
H	3.52548400	1.28998400	-0.21314800
H	3.92989900	0.94010000	1.46482800
C	0.84522000	4.85387400	1.21550300
H	0.93994000	2.98660200	0.10820500
H	1.90428100	3.00696800	1.58429100
C	-0.37102300	4.69040600	3.43233200
H	-1.12601500	2.71629000	3.90887700
H	0.63092200	2.83202600	3.90959700
C	-4.22773000	0.33772200	2.92021800
H	-3.11042900	0.63997100	1.08738800
H	-2.93718100	1.94025000	2.25828700
C	-3.04710600	-1.84622700	3.39015600
H	-1.86775100	-1.66731000	1.58091500
H	-0.90842300	-1.80683200	3.05256600
C	1.65590100	-6.00268500	0.84772200
H	0.91930500	-5.34599700	-1.07818100
H	-0.35158600	-5.58721600	0.11713000
H	3.44345000	-5.59104900	-0.29869500
H	3.76504700	-5.98518600	1.38732600
C	6.09264900	0.73845200	-1.26165800
H	6.13309300	-0.99333000	-2.57889500
H	6.52958600	-1.34914300	-0.90060000
H	5.77571000	2.17763000	0.33933100
H	6.30843200	0.59012700	0.88526600
C	0.77558000	5.36176800	2.66309600
H	-0.05162600	5.17548800	0.66780400
H	1.70262600	5.30023300	0.69555200
H	-1.33124800	5.00392400	2.99693600
H	-0.37859100	5.02357000	4.47849900
C	-4.33446900	-1.19214500	2.87024700

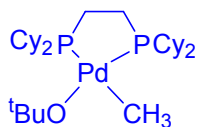
H	-5.13165400	0.79779500	2.50102300
H	-4.16879700	0.66308600	3.97007400
H	-3.11142200	-2.93887000	3.30596800
H	-2.93134100	-1.62095200	4.46119600
H	1.64276000	-7.06263100	0.56346800
H	1.33566300	-5.95699400	1.89948100
H	5.51429600	1.33596200	-1.98150000
H	7.14798200	0.99857700	-1.41354100
H	0.65558400	6.45272100	2.67994800
H	1.72717300	5.14466000	3.17187400
H	-4.51274300	-1.50959800	1.83321900
H	-5.19727500	-1.53351900	3.45685700
C	-2.18481600	-0.11244200	-2.00349200
O	-2.08319200	-1.48226300	-2.24175800
N	-3.37541200	0.26312000	-1.61493200
C	-3.32674400	-1.98020600	-1.95944100
C	-4.13386600	-0.90097900	-1.57261700
C	-3.77010600	-3.29122000	-2.02981900
C	-5.47044300	-1.12475700	-1.22918400
C	-5.10947000	-3.50262900	-1.68179300
H	-3.11937600	-4.10237000	-2.34006300
C	-5.94086100	-2.43915600	-1.28945500
H	-6.11362800	-0.30173400	-0.93357300
H	-5.51390000	-4.51014000	-1.71895400
H	-6.97559300	-2.64610900	-1.03046200
C	-0.96873500	0.67001200	-2.24071000
C	-1.00368400	2.13864800	-2.36096800
C	0.18256000	-0.04334400	-2.73028100
C	-2.09186200	2.93196500	-1.93277500
C	0.12108000	2.80245800	-2.94542700
C	1.26110100	0.68388200	-3.34388900
H	0.08291500	-1.09599900	-2.96973700
C	-2.06810200	4.31492300	-2.05606300
H	-2.95851000	2.44178100	-1.50946200
C	0.11649100	4.21039400	-3.05609400
C	1.24051100	2.04147300	-3.43627500
H	2.09440200	0.11687500	-3.75208600
C	-0.95742900	4.96576600	-2.61651600
H	-2.92349700	4.89465400	-1.71762700
H	0.98088800	4.69606100	-3.50443100
H	2.06212500	2.57883300	-3.90443800
H	-0.94356300	6.04836800	-2.71254700
Pd	0.34328300	-0.01156000	-0.52206500



P1

C	0.60228000	0.54266300	-0.02741400
O	1.06889400	-0.72555100	0.26726200
N	1.53843400	1.41020000	-0.29083800
C	2.43411600	-0.62204800	0.17137400
C	2.72879100	0.70403100	-0.17224100
C	3.39223400	-1.60484700	0.36542900
C	4.06020500	1.09820400	-0.33912800
C	4.71809100	-1.19671200	0.19683200
H	3.12926300	-2.62300800	0.63198200
C	5.04355700	0.12855900	-0.14874200
H	4.30770300	2.12056100	-0.60599300
H	5.51573800	-1.92064800	0.33610300
H	6.08872200	0.39906500	-0.26933200
C	-0.83734200	0.82143700	0.02295300
C	-1.87717800	-0.17519000	-0.03076500
C	-1.17544800	2.16669300	0.11833200
C	-1.65328400	-1.57354100	-0.17739300
C	-3.24178700	0.27537100	0.04299500
C	-2.51521200	2.58934300	0.18246700
H	-0.37312600	2.89544900	0.14859300
C	-2.70369300	-2.46401200	-0.22942200
H	-0.64135400	-1.94565700	-0.24852400

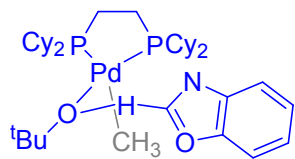
C	-4.29849800	-0.67380400	-0.00712300
C	-3.52912700	1.66013000	0.15322800
H	-2.73858600	3.64916900	0.26327000
C	-4.04138000	-2.01741500	-0.13832400
H	-2.49808100	-3.52497300	-0.34396800
H	-5.32139000	-0.31001200	0.05510300
H	-4.56902100	1.97284800	0.21001000
H	-4.85802000	-2.73295700	-0.17781800



Inter4s

P	-1.29897900	0.08138500	-0.98772400
P	1.88433500	-0.11679600	-0.40047400
C	-0.16038100	-0.26736000	-2.44037400
C	-2.65403100	-1.20325500	-1.08988700
C	-2.15268100	1.69814600	-1.42452900
C	1.29181700	0.18043800	-2.16671100
C	3.21368800	1.18775400	-0.15742000
C	2.84354000	-1.73020700	-0.52893600
H	-0.19023400	-1.35011000	-2.60343700
H	-0.52750400	0.19898900	-3.36327300
C	-2.13269900	-2.59623300	-0.67691400
C	-3.41406900	-1.26651500	-2.43021500
H	-3.34199000	-0.88284900	-0.29621200
C	-3.29533000	2.00452600	-0.43074700
C	-1.13864100	2.86209100	-1.46504900
H	-2.57959300	1.58519300	-2.43318200
H	1.98015500	-0.29697600	-2.87550600
H	1.37768300	1.25990300	-2.33052700
C	2.58912900	2.58345300	0.05316300
C	4.30784800	1.22889700	-1.24494900
H	3.68805600	0.90428300	0.79243000
C	3.67258000	-2.02543600	0.73958100
C	1.90777600	-2.91644100	-0.84472800
H	3.53642100	-1.60977900	-1.37631600
C	-3.27336900	-3.62795900	-0.63882600
H	-1.65276300	-2.52153300	0.30451400
H	-1.36860300	-2.94034200	-1.39023300
C	-4.54696800	-2.30853500	-2.38547200
H	-3.83163100	-0.28628000	-2.69033800
H	-2.71506400	-1.53435900	-3.23687100
C	-3.95532400	3.36460800	-0.71439600
H	-2.89358300	1.97110000	0.58913900
H	-4.05852700	1.21928400	-0.48087800
C	-1.81834600	4.20946700	-1.75973400
H	-0.62410900	2.91979200	-0.49633900
H	-0.36887200	2.67194700	-2.22403900
C	3.66524000	3.63362200	0.37508400
H	1.84434900	2.53446900	0.85546400
H	2.05278100	2.89233200	-0.85586100
C	5.37774800	2.28754600	-0.91997300
H	4.78505800	0.24778400	-1.35494200
H	3.85287100	1.46858200	-2.21670800
C	4.44556000	-3.35007900	0.61685500
H	2.99754500	-2.07285200	1.60279500
H	4.38032100	-1.21197700	0.93892500
C	2.68393000	-4.23963700	-0.96229500
H	1.15638300	-2.99882900	-0.04797600
H	1.35998800	-2.73468600	-1.77722300
C	-4.02835700	-3.69373800	-1.97423500
H	-3.97435400	-3.35462300	0.16286300
H	-2.87120900	-4.61548100	-0.37825100
H	-5.30805800	-1.97780700	-1.66383400
H	-5.04356900	-2.35880700	-3.36329700
C	-2.93128700	4.50709800	-0.74692200
H	-4.72361000	3.56117800	0.04411700
H	-4.47701800	3.32242600	-1.68286500
H	-1.06681200	5.00964100	-1.75246400

H	-2.24483400	4.18959600	-2.77393900
C	4.75759300	3.67526500	-0.70366400
H	4.12169100	3.39520800	1.34686600
H	3.19794500	4.62041400	0.48423800
H	5.91729400	1.98511800	-0.01045400
H	6.12088200	2.32099300	-1.72700000
C	3.51171700	-4.52490900	0.29790900
H	4.99556800	-3.53969400	1.54719000
H	5.20007700	-3.25883300	-0.17905400
H	1.98141600	-5.06061200	-1.15421700
H	3.35409800	-4.19110900	-1.83375200
H	-4.86084000	-4.40583800	-1.90804100
H	-3.35293400	-4.07421400	-2.75557800
H	-2.48865900	4.62731500	0.25254200
H	-3.42487600	5.45686100	-0.98971700
H	5.53559600	4.39980800	-0.43211500
H	4.31906500	4.02654300	-1.64978600
H	2.83328200	-4.69026900	1.14752900
H	4.08966200	-5.44927500	0.17282100
O	-1.77187800	-0.00558900	1.94553800
C	-2.22285000	0.10721700	3.26755500
C	-3.76423300	-0.03132100	3.20608200
H	-4.22466300	0.04914800	4.19981000
H	-4.18889400	0.75025600	2.56553100
H	-4.03408500	-1.00425800	2.77862200
C	-1.67764400	-1.01804900	4.17534200
H	-1.89248000	-1.99178300	3.71882700
H	-0.59610100	-0.93612800	4.30608900
H	-2.14177300	-0.99581700	5.17076200
C	-1.88230300	1.49051900	3.86636700
H	-2.31772100	2.28102100	3.24298700
H	-2.27062800	1.60678400	4.88733400
H	-0.79964300	1.64690700	3.89403800
Pd	0.07427400	-0.01483200	1.00130500
C	1.31646500	-0.08722400	2.68736600
H	0.88934000	0.59089900	3.42853300
H	1.28952200	-1.11093600	3.07661600
H	2.35959600	0.19793400	2.51628600

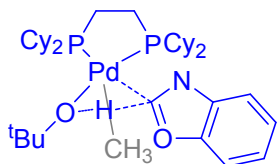


Inter5s

P	1.48479300	-1.16417800	-1.03113900
P	0.91863700	1.99830700	-0.50486500
C	2.15273100	0.07922500	-2.27634300
C	2.96846700	-2.24770000	-0.63195400
C	0.36045900	-2.27551300	-2.04439800
C	1.41896600	1.43495600	-2.22958500
C	-0.53216200	3.14294800	-0.83142000
C	2.30643200	3.14606300	0.03421500
H	3.21239600	0.22320000	-2.04252100
H	2.10995800	-0.32949900	-3.29333400
C	4.03972400	-1.47060500	0.16254700
C	3.60965300	-2.97728200	-1.83116800
H	2.54857300	-3.00438600	0.04562500
C	-0.08177200	-3.50862700	-1.22554200
C	-0.86825400	-1.50092300	-2.56989400
H	0.93837500	-2.61838900	-2.91691600
H	2.01908000	2.21216300	-2.71927000
H	0.48217300	1.36076200	-2.79202700
C	-1.78897200	2.34685700	-1.24429600
C	-0.25646300	4.29011600	-1.82706800
H	-0.74289900	3.58868000	0.15016600
C	1.96518200	3.88918500	1.34406900
C	3.64617000	2.39340200	0.17676500
H	2.42025700	3.89006600	-0.76877800
C	5.18229900	-2.39451900	0.61661700

H	3.58067100	-0.98062000	1.02789700
H	4.46253100	-0.67399800	-0.46630400
C	4.76045200	-3.89515600	-1.37910200
H	2.86277100	-3.57156200	-2.36900600
H	3.99852500	-2.23708000	-2.54590100
C	-1.03735600	-4.40608600	-2.03081700
H	-0.55693000	-3.16658800	-0.29824900
H	0.79300300	-4.09849700	-0.92344800
C	-1.80026000	-2.41233700	-3.38668900
H	-1.43535500	-1.08799300	-1.72697500
H	-0.54700500	-0.65527600	-3.19304900
C	-3.01025600	3.27095500	-1.38652500
H	-1.98930500	1.55494200	-0.51565100
H	-1.61319400	1.84644700	-2.20760400
C	-1.48563800	5.20635300	-1.97402800
H	0.60594600	4.88881400	-1.50987000
H	-0.00484400	3.87081200	-2.81183600
C	3.10682400	4.82335700	1.78076400
H	1.77345400	3.15095200	2.13308300
H	1.04332100	4.47160900	1.22980200
C	4.78336200	3.33028600	0.61990600
H	3.52704000	1.58830100	0.91408800
H	3.91975700	1.91568500	-0.77162600
C	5.81888200	-3.13168200	-0.57036500
H	4.78737500	-3.12881600	1.33348200
H	5.93959300	-1.80990600	1.15453500
H	4.34795900	-4.70584300	-0.76090900
H	5.21821200	-4.37307100	-2.25486900
C	-2.24818900	-3.62732400	-2.56285800
H	-1.36736800	-5.24275100	-1.40172100
H	-0.49104300	-4.84931600	-2.87800400
H	-2.67284800	-1.83492900	-3.71698400
H	-1.28155500	-2.75191100	-4.29664800
C	-2.74085200	4.41737400	-2.37198300
H	-3.26281900	3.68888100	-0.40097700
H	-3.87895900	2.68247800	-1.70577100
H	-1.66691500	5.71814000	-1.01744200
H	-1.27407900	5.99065400	-2.71226300
C	4.43529700	4.06803300	1.91942900
H	2.84067400	5.30774800	2.72857700
H	3.22275700	5.62832200	1.03954500
H	5.70770100	2.75157900	0.74274600
H	4.97829500	4.06596700	-0.17474600
H	6.59786100	-3.82018900	-0.21911700
H	6.31852000	-2.40186100	-1.22514900
H	-2.85784800	-3.27385000	-1.72133400
H	-2.88513600	-4.28486600	-3.16898100
H	-3.60770300	5.08800900	-2.42598300
H	-2.60229500	4.00264900	-3.38177800
H	4.35510600	3.34002000	2.73995600
H	5.24171500	4.76048600	2.19181800
C	-3.16019000	-1.15734300	1.02129700
O	-4.03040100	-0.95350200	2.06604900
N	-3.66820400	-0.99637600	-0.16070500
C	-5.21774500	-0.62832000	1.46086500
C	-5.00358800	-0.65324900	0.07583600
C	-6.43707700	-0.32147700	2.04783000
C	-6.05524700	-0.35772600	-0.79603400
C	-7.47973100	-0.02699500	1.16522700
H	-6.56983700	-0.31139000	3.12453800
C	-7.29150500	-0.04515300	-0.22959200
H	-5.90815100	-0.37651900	-1.87154700
H	-8.45858800	0.22089100	1.56597300
H	-8.13152600	0.18884700	-0.87781800
H	-2.13039100	-1.41373500	1.29520100
C	0.17077800	-2.14853900	2.94361700
Pd	0.44417800	0.14422100	0.76089800
O	-0.21360900	-1.61862900	1.69658900
C	-0.77736500	-1.68438000	4.07562300
H	-0.70414100	-0.60415600	4.22942400
H	-1.81725400	-1.91959600	3.82121500
H	-0.54197200	-2.18015300	5.02715300
C	0.07725800	-3.68781800	2.82672000
H	0.74859200	-4.04871100	2.03868100
H	0.34540200	-4.18856500	3.76641500

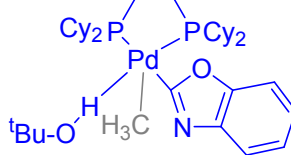
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C	1.61889200	-1.76797700	3.31310200
H	1.72319300	-0.67806400	3.37099600
H	1.92013700	-2.19490300	4.27901200
H	2.31189100	-2.13629400	2.54808700
C	-0.46787500	1.30688800	2.23659600
H	-1.41614000	0.80920100	2.45112000
H	0.17273700	1.26544500	3.12450200
H	-0.65733500	2.35428600	1.98481200



TS5-6s

P	0.74125900	-1.58815700	-1.50916800
P	0.44174400	1.68301200	-1.45517100
C	1.10670200	-0.61092600	-3.07435500
C	2.28355800	-2.62070300	-1.21621000
C	-0.54864800	-2.83730800	-2.05872400
C	0.39450700	0.75500800	-3.09010400
C	-1.07408900	2.78805800	-1.52457100
C	1.89988200	2.85913500	-1.64914200
H	2.19073500	-0.46678300	-3.11976300
H	0.82753900	-1.18481000	-3.96632100
C	3.48861500	-1.73486300	-0.83319100
C	2.65973200	-3.59605300	-2.35142900
H	2.01836900	-3.20213400	-0.32268300
C	-0.86261000	-3.85121000	-0.93665100
C	-1.83895800	-2.14564000	-2.54947900
H	-0.11407200	-3.38157900	-2.91120700
H	0.80004400	1.39258800	-3.88581500
H	-0.66798200	0.60978300	-3.31218400
C	-2.36516500	1.97690200	-1.28114800
C	-1.18732500	3.65055200	-2.80030200
H	-0.95186300	3.46235400	-0.66609400
C	1.94108900	3.96294500	-0.57099000
C	3.24333500	2.10218500	-1.69275800
H	1.75155500	3.34176000	-2.62771200
C	4.72054200	-2.58169400	-0.47173400
H	3.21685000	-1.08367700	0.00460000
H	3.75147100	-1.07824300	-1.67522900
C	3.89973700	-4.43331800	-1.98809700
H	1.82492200	-4.26793400	-2.57942900
H	2.86648100	-3.02754400	-3.27043800
C	-1.92325000	-4.87184800	-1.38476900
H	-1.22501700	-3.30903400	-0.05588700
H	0.04784100	-4.38214800	-0.63203400
C	-2.89437400	-3.17657800	-2.98964600
H	-2.24859500	-1.53662800	-1.73624800
H	-1.61635800	-1.47658600	-3.39158600
C	-3.59947600	2.89231400	-1.23879000
H	-2.27890900	1.41417700	-0.34704400
H	-2.49723400	1.23639500	-2.08332600
C	-2.43019000	4.55827100	-2.74648600
H	-0.28972800	4.26586800	-2.93827800
H	-1.26235900	2.99852300	-3.68213200
C	3.12497900	4.92022300	-0.79441000
H	2.03337700	3.49803400	0.41775200
H	1.00612900	4.53484000	-0.56511400
C	4.43112100	3.05876200	-1.89833500
H	3.37049800	1.55056100	-0.75202300
H	3.23838300	1.35696500	-2.49647300
C	5.09405600	-3.54994900	-1.60281900
H	4.50811800	-3.15408700	0.44251100
H	5.56599300	-1.92231000	-0.23684500
H	3.65010100	-5.09346300	-1.14461000
H	4.16217800	-5.08811900	-2.82904500
C	-3.20383200	-4.17859700	-1.86876800
H	-2.14864600	-5.55168300	-0.55344400

H	-1.51467300	-5.49372700	-2.19635500
H	-3.80859200	-2.65299700	-3.29812100
H	-2.53058500	-3.71910900	-3.87583700
C	-3.71464500	3.75225900	-2.50513100
H	-3.53056800	3.54708700	-0.35802600
H	-4.49907500	2.28146500	-1.10003700
H	-2.30391300	5.29178000	-1.93660500
H	-2.50443300	5.13274900	-3.67884300
C	4.46072100	4.16615400	-0.83632300
H	3.13693400	5.67718200	-0.00045700
H	2.98241900	5.46162000	-1.74151000
H	5.36767300	2.48708000	-1.88357700
H	4.35925000	3.51530600	-2.89672500
H	5.94738300	-4.17309400	-1.30658400
H	5.41802000	-2.97361300	-2.48260200
H	-3.66152300	-3.64517300	-1.02567200
H	-3.93268900	-4.92278000	-2.21498000
H	-4.57553100	4.42861800	-2.43201300
H	-3.90156300	3.10131700	-3.37260200
H	4.65567800	3.71912300	0.14944700
H	5.28608800	4.86127500	-1.03452100
C	-1.95910200	-0.87184100	1.45421100
O	-2.97671800	-1.33420800	0.54570600
N	-2.50044500	-0.12236200	2.38460300
C	-4.15363500	-0.81157200	0.99349300
C	-3.87138600	-0.05742600	2.14269200
C	-5.43309500	-0.94413400	0.46618300
C	-4.90659500	0.59909100	2.81565400
C	-6.46033700	-0.28064000	1.14679100
H	-5.62670800	-1.53433600	-0.42498400
C	-6.20007100	0.47700800	2.30267900
H	-4.70239500	1.18362200	3.70829800
H	-7.47943700	-0.35545600	0.77586600
H	-7.02495700	0.97608600	2.80507000
H	-0.37911500	-1.54605600	1.75526700
C	1.09662400	-1.94320600	3.14482300
Pd	0.37306600	0.13608700	0.19749900
O	0.64237800	-1.67637000	1.80092500
C	0.53996400	-3.31602600	3.56015000
H	0.84820500	-4.08539400	2.84344300
H	0.89875900	-3.60464900	4.55572600
H	-0.55510800	-3.29126500	3.58728900
C	2.62601100	-1.97872300	3.08659400
H	3.01559000	-1.01533100	2.73803600
H	3.05025500	-2.18301300	4.07656200
H	2.96934400	-2.75958300	2.39841100
C	0.61814900	-0.85633800	4.11958300
H	0.89927000	-1.11443800	5.14830100
H	1.07133800	0.10891300	3.87460800
H	-0.46909200	-0.73944400	4.07237700
C	0.26647300	1.67197500	1.60298100
H	-0.47533400	1.29288300	2.30712100
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H	-0.03330000	2.66200500	1.25239700

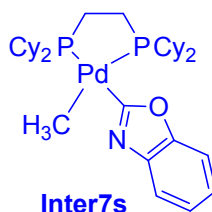


Inter6s

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C	-1.50611400	-0.48017400	2.51924800
C	-0.13859800	-2.96083300	1.64406200
C	2.75650000	-0.44497700	1.76100800
C	3.97030800	-0.20497200	-0.92213600
C	2.85192400	2.20078600	0.41370700
H	1.20042100	0.28750100	3.08621700
H	1.61509300	-1.39896000	3.34965600
C	-1.56644000	1.06266900	2.56356100
C	-1.62075800	-1.07633500	3.93890600

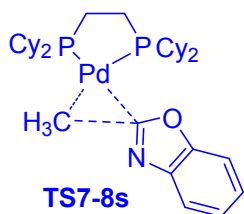
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C	-1.47013600	-3.49731200	1.07468300
C	1.05805500	-3.63947700	0.94280000
H	-0.08983200	-3.21039800	2.71474200
H	3.49111200	0.11313300	2.35466200
H	3.20600600	-1.42028000	1.54504100
C	3.78080900	-1.66930400	-1.37408700
C	5.35090900	-0.00316300	-0.26244100
H	3.92975700	0.41539800	-1.82853300
C	2.96597300	3.00643900	-0.89928700
C	1.77440200	2.82749500	1.32608300
H	3.81859300	2.24957300	0.93892200
C	-2.83407400	1.54664300	3.28901600
H	-1.53986700	1.48551100	1.55430700
H	-0.68850200	1.45221100	3.10027100
C	-2.88737200	-0.57875500	4.65920100
H	-1.63184700	-2.17211700	3.90584700
H	-0.73812500	-0.78783700	4.52869600
C	-1.54658800	-5.03122300	1.16539100
H	-1.56237700	-3.18868500	0.02624300
H	-2.32159300	-3.05970000	1.60904100
C	0.97314500	-5.17382300	1.02561400
H	1.07980000	-3.32795000	-0.11044200
H	2.00277600	-3.30704600	1.39097000
C	4.92432300	-2.12180700	-2.29793700
H	2.81434300	-1.77620700	-1.87964200
H	3.75208800	-2.32996100	-0.49505000
C	6.48962400	-0.46763600	-1.18884100
H	5.50335500	1.04894400	0.00656300
H	5.39714400	-0.57781000	0.67370000
C	3.25521000	4.49229200	-0.62282800
H	2.02475700	2.91262000	-1.45555700
H	3.75652100	2.59730400	-1.53974000
C	2.06708500	4.31263600	1.60261400
H	0.79220000	2.73307800	0.84477900
H	1.71980100	2.28927200	2.28012600
C	-2.95332300	0.95400700	4.69958400
H	-3.71556600	1.26146200	2.69689300
H	-2.83156800	2.64300900	3.33226100
H	-3.77245000	-0.96587400	4.13335800
H	-2.92100800	-0.99379500	5.67496700
C	-0.35547300	-5.69897600	0.46520800
H	-2.49097100	-5.37656300	0.72642100
H	-1.56311700	-5.33469000	2.22315600
H	1.81979300	-5.61784800	0.48634800
H	1.07297300	-5.48592600	2.07609600
C	6.29782900	-1.92223200	-1.64103500
H	4.88096100	-1.54379900	-3.23249500
H	4.78151900	-3.17390100	-2.57499500
H	6.52318000	0.18600400	-2.07276300
H	7.45320200	-0.34901500	-0.67678800
C	2.19862700	5.11362300	0.30037700
H	3.30222700	5.03833600	-1.57350300
H	4.24789800	4.58795200	-0.15729100
H	1.26870800	4.73083000	2.22833500
H	2.99942400	4.40044300	2.18111200
H	-3.88672600	1.28064300	5.17561700
H	-2.13261100	1.33530200	5.32596500
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H	-0.40962400	-6.78966400	0.57427000
H	7.09802800	-2.21216900	-2.33357500
H	6.38306100	-2.58739800	-0.76852700
H	1.22795600	5.12314500	-0.21416500
H	2.45176200	6.15884100	0.51947400
C	-1.52895400	-0.54909400	-1.41378700
O	-1.80485300	-1.76245500	-2.05714000
N	-2.57306900	0.24271500	-1.39460200
C	-3.11568400	-1.68501000	-2.45533900
C	-3.60610800	-0.43866400	-2.04709100
C	-3.87480300	-2.62535000	-3.13579000
C	-4.93012600	-0.09067700	-2.32699500
C	-5.19913500	-2.26650200	-3.41079200
H	-3.46248100	-3.58215800	-3.44071400
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H	-5.33306700	0.87097100	-2.02317300

H	-5.83934800	-2.96406500	-3.94388300
H	-6.74813800	-0.77790500	-3.24578800
H	-2.13573400	2.01052800	-0.78146200
Pd	0.34526700	-0.18080100	-0.69550700
O	-1.81323500	2.87480300	-0.42728400
C	-2.74291600	3.89764700	-0.79486900
C	-4.10946600	3.62219000	-0.14166100
H	-4.00600700	3.57848800	0.94830000
H	-4.84051800	4.40190700	-0.38929800
H	-4.51008000	2.66007500	-0.48091300
C	-2.15479700	5.20756000	-0.26010900
H	-1.17795300	5.39957500	-0.71782800
H	-2.81253700	6.05646500	-0.47956200
H	-2.01742600	5.14570500	0.82529300
C	-2.87731000	3.95440000	-2.32677900
H	-3.55821400	4.75499400	-2.64177600
H	-1.89751900	4.13285200	-2.78345700
H	-3.26341100	3.00555600	-2.71618100
C	0.71020100	0.52357300	-2.64396900
H	0.40454800	-0.24962000	-3.35556900
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H	1.76034100	0.77563100	-2.82036700



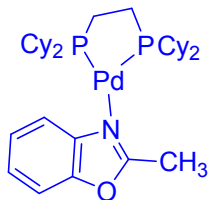
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C	0.88311400	0.61049100	2.48320100
C	-1.84776100	1.54103400	1.76978700
C	-1.35754800	-1.33637700	2.29245000
C	2.21026600	0.04940300	1.92902900
C	3.52523800	-1.29024400	-0.36834700
C	3.31698800	1.66683500	-0.29361000
H	0.92389300	1.70467700	2.50003100
H	0.74342200	0.28735400	3.52217800
C	-1.42313800	2.84655000	1.06414900
C	-2.18386100	1.79423200	3.25373400
H	-2.74776400	1.19363600	1.24541200
C	-2.66464100	-1.78739100	1.60284100
C	-0.35678600	-2.50961300	2.36165300
H	-1.59321200	-1.03662100	3.32478200
H	3.06170400	0.57216500	2.38278500
H	2.30833600	-1.00514700	2.20773800
C	2.85560000	-2.66956700	-0.18746100
C	4.89164700	-1.24228000	0.34626900
H	3.69770500	-1.16065100	-1.44652000
C	3.78398500	1.74380300	-1.76385400
C	2.50300700	2.92586200	0.07588100
H	4.20678000	1.63388600	0.35361200
C	-2.49782600	3.93482300	1.22481000
H	-1.25555100	2.64202000	0.00220700
H	-0.47657700	3.21630100	1.48716000
C	-3.25360400	2.89132000	3.40479600
H	-2.53644900	0.87617800	3.73886600
H	-1.27583500	2.10593200	3.79152200
C	-3.27469700	-3.01677800	2.29709600
H	-2.44955600	-2.02793000	0.55379000
H	-3.39640300	-0.97196600	1.58862200
C	-0.97119500	-3.73958100	3.05186400
H	-0.04785600	-2.78075000	1.34271800
H	0.54992200	-2.21015000	2.90211800
C	3.77881500	-3.80463800	-0.66247600
H	1.90543400	-2.69225000	-0.73371600
H	2.61594400	-2.83044300	0.87386700
C	5.80865400	-2.38484700	-0.12768800
H	5.38901000	-0.28005500	0.17524300

H	4.74150600	-1.32992900	1.43206100	C	4.09267100	-3.05075800	-0.65293200
C	4.56767200	3.03811300	-2.04247700	H	3.61737600	-1.11366300	-1.46406700
H	2.90624600	1.69696000	-2.42125200	C	3.98651400	0.58801200	0.91802500
H	4.41127100	0.88064100	-2.01602200	C	2.47500800	-0.15515900	2.80984600
C	3.28709800	4.21803400	-0.21074700	H	3.89731500	-1.39651600	1.77266600
H	1.56859700	2.92675200	-0.50120200	H	-0.50801700	-3.58118100	2.08095800
H	2.21996900	2.90308800	1.13516800	H	0.11288300	-2.09436800	2.78371300
C	-2.83889500	4.19015100	2.70002800	C	-1.65401900	0.31429400	3.00304200
H	-3.40215000	3.61637900	0.68776300	C	-2.96483000	-1.85579700	3.26419900
H	-2.15932500	4.86228300	0.74527400	H	-3.22144200	-0.36952400	1.72279000
H	-4.19829600	2.53014900	2.97310900	C	-3.60231200	-2.04404100	-0.65910100
H	-3.44625100	3.07593300	4.46977900	C	-1.61527900	-3.57515800	-1.02789500
C	-2.27497300	-4.17916100	2.37156500	H	-2.80639500	-3.46754400	0.76633300
H	-4.18093900	-3.32576700	1.76165500	C	3.10051300	-2.96204400	-3.44850500
H	-3.59028400	-2.74294000	3.31514500	H	1.51125700	-1.73732300	-2.60133400
H	-0.24375000	-4.56166900	3.05457800	H	1.60507600	-3.36537700	-1.94337400
H	-1.17441500	-3.49844800	4.10601300	C	4.97480200	-3.50312800	-1.83136000
C	5.14304800	-3.75772400	0.04155400	H	4.72808000	-2.66518300	0.15332200
H	3.92557600	-3.71764500	-1.74887000	H	3.56495000	-3.92545100	-0.24645900
H	3.29242600	-4.77310500	-0.49061900	C	4.96566300	1.19138200	1.93984600
H	6.05472000	-2.22954500	-1.18837600	H	3.27896800	1.36270300	0.58985600
H	6.75836200	-2.34902700	0.42135100	H	4.54039000	0.27056900	0.02622400
C	3.75404300	4.28497000	-1.67092500	C	3.45497100	0.45176400	3.82846900
H	4.85712600	3.07024000	-3.10032700	H	1.69939300	0.58268400	2.56079400
H	5.50244200	3.02860400	-1.46191200	H	1.96265700	-1.00901000	3.26913100
H	2.66236600	5.08675600	0.03267700	C	-2.56194200	0.97627900	4.05355400
H	4.16290600	4.26639500	0.45371000	H	-1.31832300	1.06071500	2.27538800
H	-3.63784800	4.93796700	2.78426100	H	-0.75813600	-0.07983800	3.50643400
H	-1.95982600	4.61367800	3.20958100	C	-3.86897800	-1.17580000	4.30951800
H	-2.05181500	-4.52965200	1.35332400	H	-3.53294500	-2.63225300	2.73732100
H	-2.71536400	-5.02964100	2.90738100	H	-2.14294200	-2.36718000	3.78594500
H	5.79953800	-4.54712800	-0.34559600	C	-4.49298200	-3.02091500	-1.44645400
H	5.00533500	-3.96361500	1.11372800	H	-3.21552000	-1.27121900	-1.33691600
H	2.87637600	4.35489400	-2.32968600	H	-4.21059200	-1.52442300	0.09037100
H	4.34738400	5.19242500	-1.83985100	C	-2.51209000	-4.54542400	-1.81604700
C	-1.76265800	-0.18100300	-1.57693700	H	-1.13258600	-2.87613400	-1.72549800
O	-2.14416600	-1.24217700	-2.41525000	H	-0.81291500	-4.14199400	-0.53923800
N	-2.74520300	0.65843200	-1.36375900	C	4.13235800	-4.01154700	-3.00993500
C	-3.45393400	-1.00720800	-2.73308200	H	3.62476000	-2.08667700	-3.85939100
C	-3.83763100	0.17541600	-2.08617700	H	2.47245900	-3.35727100	-4.25695800
C	-4.30531700	-1.75383900	-3.53544300	H	5.59171600	-2.65559700	-2.16444900
C	-5.14065800	0.65765400	-2.23791700	H	5.67153000	-4.28194300	-1.49499100
C	-5.60693100	-1.26108400	-3.67995500	C	4.24737700	1.62031600	3.22676700
H	-3.97770800	-2.66553200	-4.02548700	H	5.48769300	2.04530900	1.48987700
C	-6.01578600	-0.07676100	-3.04160300	H	5.73738800	0.44660500	2.18515200
H	-5.45436200	1.57459900	-1.74697800	H	2.90320800	0.78083300	4.71823300
H	-6.31499400	-1.80427000	-4.30016100	H	4.15564500	-0.32696600	4.16486500
H	-7.03537200	0.27369500	-3.18023300	C	-3.13289900	-0.04728800	5.04496100
Pd	0.14268900	-0.08703500	-0.83517800	H	-3.38868700	1.48672800	3.53907300
C	0.79146400	-0.33694100	-2.81746700	H	-2.00102200	1.75435600	4.58686800
H	0.21685900	-1.15588900	-3.25626800	H	-4.75395300	-0.76177100	3.80433000
H	0.57302500	0.58566100	-3.36785900	H	-4.23777400	-1.92452300	5.02279400
H	1.86092800	-0.55787900	-2.89748500	C	-3.68613900	-3.81559700	-2.48169600



P	1.96114900	-1.27693700	0.25931700
P	-1.30054600	-1.53348700	0.90095600
C	1.28161800	-2.81847300	1.10478300
C	3.06317300	-1.98958300	-1.09373400
C	3.19024000	-0.59361300	1.51353900
C	-0.06557100	-2.60825800	1.83264000
C	-2.38515200	-0.83059100	2.26764500
C	-2.41371600	-2.76505200	0.01509500
H	1.15698500	-3.56533900	0.31344900
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C	2.21496200	-2.51213700	-2.27420700

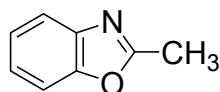
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H	-5.90614600	4.52121600	-0.59654100
Pd	-0.01925300	0.05365700	-0.35144700
C	0.44560300	1.86738500	-1.63183800
H	-0.06954400	2.51777200	-2.33842900
H	1.00955400	2.47758700	-0.92523500
H	1.10429600	1.21887900	-2.22267200



Inter8s

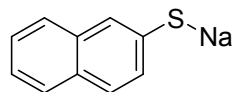
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C	0.67170100	2.02606500	1.68268100
C	-1.56061800	3.04768400	0.09090700
C	-2.07218000	1.16925900	2.29681700
C	1.75726400	0.94783900	1.89298700
C	2.77404500	-1.73012800	1.28873400
C	3.57062300	0.54501000	-0.38592400
H	1.07375600	2.82014000	1.04278800
H	0.43203100	2.49705700	2.64538300
C	-0.80124400	3.40096300	-1.20479200
C	-1.62173400	4.26970300	1.03039900
H	-2.59055400	2.79906800	-0.20629200
C	-3.52324300	0.93563000	1.82775500
C	-1.59661600	-0.01228800	3.16738600
H	-2.04834000	2.07787600	2.91767400
H	2.69964200	1.42835300	2.18811700
H	1.46627100	0.30199300	2.72938600
C	1.65733400	-2.60661000	1.89258300
C	3.88104300	-1.47312600	2.33251800
H	3.21752900	-2.30697900	0.46315400
C	4.10136800	-0.35392500	-1.52117000
C	3.28110400	1.96200100	-0.92236400
H	4.35194900	0.62878800	0.38505600
C	-1.41106800	4.62611400	-1.90707100
H	-0.79900500	2.53273900	-1.87517900
H	0.25204600	3.61554700	-0.97118200
C	-2.23134400	5.49664800	0.32590800
H	-2.20365900	4.03944800	1.93120300
H	-0.60749100	4.52335700	1.36983000
C	-4.47645800	0.65026600	3.00182200
H	-3.53881200	0.08599100	1.12955000
H	-3.89003900	1.80322600	1.26608700
C	-2.55235300	-0.29815800	4.33887400
H	-1.51313000	-0.90775700	2.53446900
H	-0.59199000	0.18497600	3.56058600
C	2.21241700	-3.92322900	2.46170900
H	0.89615200	-2.80595600	1.12849900
H	1.15031100	-2.05622200	2.69936000
C	4.43667900	-2.79220500	2.90234100
H	4.70126200	-0.88871300	1.89719900
H	3.47445900	-0.87340400	3.15909300
C	5.32073000	0.26008800	-2.22999100
H	3.29399700	-0.51197000	-2.25145200
H	4.36593800	-1.34614800	-1.13617600
C	4.49965600	2.57546700	-1.63443800
H	2.43465900	1.91228200	-1.62260900
H	2.97049500	2.62251300	-0.10400900
C	-1.47999200	5.83972500	-0.96826000
H	-2.42608700	4.37653800	-2.25089500
H	-0.82900700	4.87181300	-2.80529300
H	-3.28510400	5.28822500	0.08777400
H	-2.23071600	6.35760200	1.00769000
C	-3.98932300	-0.52990300	3.85303600

H	-5.48713900	0.45514600	2.61975600
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H	-2.19469800	-1.16779200	4.90594900
H	-2.53939000	0.55450300	5.03429400
C	3.32338600	-3.67035800	3.49156200
H	2.61452200	-4.53030700	1.63674800
H	1.40037500	-4.50884900	2.91257900
H	4.94622300	-3.34474100	2.09871100
H	5.19816400	-2.57872000	3.66433900
C	5.01670700	1.66830500	-2.75881400
H	5.64329000	-0.39523800	-3.04989900
H	6.16290200	0.31311600	-1.52378700
H	4.23781400	3.56527000	-2.03131000
H	5.30454600	2.73666500	-0.90162800
H	-1.95910600	6.68842600	-1.47360300
H	-0.45771600	6.16140900	-0.71810500
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H	-4.66111000	-0.68943500	4.70648000
H	3.73833600	-4.62170500	3.84935600
H	2.89316400	-3.16674000	4.37042300
H	4.25450900	1.60100000	-3.54970400
H	5.91083700	2.10498100	-3.22247600
C	-1.01657300	-1.50106400	-3.42297700
O	-1.90997800	-2.26978600	-4.12953200
N	-1.16553500	-1.54640600	-2.13029900
C	-2.69489800	-2.86012700	-3.16728000
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C	-3.75303800	-3.74105700	-3.33397500
C	-2.86132200	-2.85938400	-0.75067500
C	-4.36706800	-4.17931900	-2.15741000
H	-4.08124700	-4.06677900	-4.31522200
C	-3.92919600	-3.74637400	-0.89190400
H	-2.51541500	-2.51640000	0.21897200
H	-5.20246300	-4.87042800	-2.22308300
H	-4.43759500	-4.11322800	-0.00478500
Pd	-0.09399100	-0.31249200	-0.55042800
C	-0.02201900	-0.71966500	-4.19817100
H	-0.46665700	0.20442400	-4.58907600
H	0.80302800	-0.45089500	-3.53312800
H	0.34966400	-1.30104300	-5.04798500



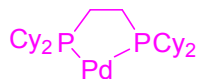
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C	0.18647100	-0.66360100	0.00001500
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C	1.33666700	-1.43773400	0.00007000
C	1.39960900	1.43203000	-0.00011100
C	2.54227900	-0.73061800	0.00005700
H	1.30160200	-2.52200800	0.00008400
C	2.57204000	0.67581000	-0.00001800
H	1.41807600	2.51716200	-0.00007500
H	3.47820900	-1.28194600	0.00006300
H	3.53298600	1.18247000	-0.00002200
C	-3.32542500	-0.02547100	-0.00000900
H	-3.66856700	-0.57631200	0.88317600
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S	2.08168700	-1.39933100	-0.57027200
C	0.93095000	-0.04381700	-0.42290800
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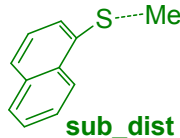
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H	2.40481700	1.46919100	-0.80319100
C	-2.38297100	-1.75107500	0.14769100
H	-0.36913100	-2.40628600	-0.21271100
C	-2.73764700	0.63717900	0.23309700
C	-0.83775900	2.19073400	-0.08779600
H	0.89673200	3.39645400	-0.43170500
C	-3.24336500	-0.64102400	0.30930900
H	-2.78625300	-2.75876400	0.20568900
H	-3.39311000	1.49685400	0.35494200
H	-1.51415200	3.03228500	0.03953500
H	-4.30323600	-0.79869800	0.49283500



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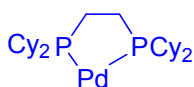
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C	-1.86868600	-0.34755600	2.10037900
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C	-3.57845700	-3.86616400	-0.87143600
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C	3.28272400	1.76739300	1.18626900
C	1.79936100	-1.13799000	1.38128400
C	1.07132400	-2.39876000	0.86990600
C	1.99638100	-3.62715700	0.89747800
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C	3.28527300	-2.60957300	2.82929200
C	2.35837300	-1.37983100	2.79822200
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H	-4.10294100	-2.12135400	1.96979400
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H	1.97153000	1.62177700	2.89807400
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H	2.64812500	-0.97065500	0.70201500
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H	0.19441300	-2.60019800	1.50263100
H	2.81591700	-3.47103400	0.18105100
H	1.44808500	-4.51516300	0.55673100
H	3.27859300	-4.71350400	2.28041200
H	1.76902600	-4.14425500	2.98615000
H	4.17369600	-2.40329400	2.21456100
H	3.64599300	-2.77812800	3.85240300
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sub_dist

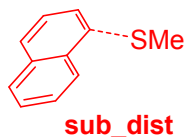
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C	0.99851000	0.56740200	-2.55256800
C	2.06835000	1.54703200	-2.62374400
C	1.30030800	-0.76966300	-2.85523800
C	1.84585500	2.92573300	-2.39658000
C	3.39824300	1.11345100	-2.94273700
C	2.62223900	-1.17375300	-3.14662100
H	0.51490500	-1.51968400	-2.83710400
C	2.87143600	3.84982000	-2.47857400
H	0.83909100	3.25716600	-2.15715000
C	4.43346100	2.08483100	-3.00691800
C	3.65683400	-0.26590000	-3.19168400
H	2.81474200	-2.22684100	-3.34344300
C	4.18223800	3.42257100	-2.78377600
H	2.66817700	4.90462000	-2.31231600
H	5.44032500	1.74976100	-3.24794100
H	4.66871500	-0.57925700	-3.43497800
H	4.98936300	4.14811600	-2.84753400



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Pd	-0.23910400	0.18957500	-0.97941500
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C	-1.82107000	-0.42776900	1.99611000
C	-0.55239200	0.36082400	2.38886900
C	-3.67589800	1.06154400	0.23691000
C	-3.06984500	2.43320500	0.60537100
C	-4.12287100	3.55457300	0.58345500
C	-4.83861800	3.63110900	-0.77167900
C	-5.45777100	2.27600300	-1.13850000
C	-4.41120300	1.14856500	-1.11856900
C	-3.33519000	-1.85495000	-0.07391800

C	-2.40039800	-3.07439300	-0.22012400	C	-2.02370900	1.26297300	-5.29894200
C	-3.18206800	-4.34421500	-0.59574000	C	-1.88013500	-0.79102800	-3.98436700
C	-4.30178700	-4.63706900	0.41366000	C	-1.67983500	2.61362900	-5.57715300
C	-5.23214600	-3.42611500	0.57723200	C	-2.95036800	0.60505000	-6.17748600
C	-4.45067000	-2.15215600	0.94962300	C	-2.77706700	-1.42994600	-4.86999600
C	1.90122700	1.75318300	1.64214200	H	-1.48319600	-1.33288600	-3.13092400
C	1.19422800	3.05800500	1.21487400	C	-2.21920800	3.28273100	-6.65483100
C	2.03457800	4.30394600	1.54476000	H	-0.97393600	3.12024000	-4.92723900
C	3.43162900	4.22638000	0.91442500	C	-3.48977600	1.32649300	-7.27699000
C	4.14806900	2.93541300	1.33094600	C	-3.30862700	-0.74999300	-5.94066000
C	3.30746200	1.68836100	1.00667000	H	-3.04769600	-2.46794500	-4.69139400
C	1.92203100	-1.20010700	1.80457900	C	-3.13743000	2.63577800	-7.51400200
C	1.20605100	-2.55109300	1.59163200	H	-1.93601500	4.31435200	-6.84673300
C	2.11667700	-3.73842900	1.94648700	H	-4.19208300	0.81759100	-7.93362400
C	2.64588200	-3.63107900	3.38397600	H	-4.00393000	-1.23593600	-6.62081600
C	3.34781500	-2.28568000	3.61695400	H	-3.55950000	3.17229000	-8.35975800
C	2.44120100	-1.09463700	3.25345300	C	1.25478100	-0.17298500	-2.78949400
H	-2.64737200	-0.14257500	2.66032700	H	1.06799200	-0.57463800	-3.78395000
H	-1.64509100	-1.49664000	2.16128500	H	2.13006400	0.47194900	-2.76299800
H	-0.22686900	0.05643500	3.39160500	H	1.34696900	-1.00851300	-2.07832100
H	-0.79351100	1.42657200	2.45607600				
H	-4.40507900	0.79105300	1.01639600				
H	-2.26775800	2.66903900	-0.10723600				
H	-2.60801100	2.38985700	1.59959900				
H	-3.64366400	4.51393100	0.81862600				
H	-4.86506400	3.37352800	1.37573100				
H	-4.11566500	3.92123500	-1.54783500				
H	-5.61023400	4.41157300	-0.75226500				
H	-5.92581600	2.32442200	-2.12989100				
H	-6.26079400	2.04030100	-0.42362900				
H	-3.67422500	1.31957100	-1.91500900				
H	-4.90431700	0.19693700	-1.35037300				
H	-3.80707400	-1.69834000	-1.05509200				
H	-1.87170200	-3.25223500	0.72777600				
H	-1.62806400	-2.86471700	-0.97032100				
H	-2.49646900	-5.19882400	-0.66395700				
H	-3.62085800	-4.21401700	-1.59612500				
H	-3.85434000	-4.88365600	1.38838500				
H	-4.87646500	-5.51883900	0.10239200				
H	-5.99555100	-3.63080600	1.33930900				
H	-5.77113200	-3.25348800	-0.36599500				
H	-4.00826000	-2.28513200	1.94731600				
H	-5.14409000	-1.30611200	1.02420900				
H	2.01153900	1.76422200	2.73719200				
H	0.21366800	3.14409800	1.69793400				
H	1.00203300	3.01825000	0.13359000				
H	2.13436600	4.39890500	2.63652700				
H	1.50889500	5.20361100	1.19984200				
H	4.02874500	5.10294200	1.19698700				
H	3.33638700	4.25056400	-0.18108900				
H	4.34959000	2.96425000	2.41229200				
H	5.12423700	2.86135300	0.83422800				
H	3.84635100	0.79447300	1.34169100				
H	3.19705000	1.59889300	-0.08395700				
H	2.79447900	-1.19364500	1.13343700				
H	0.85506700	-2.63249000	0.55628000				
H	0.31151500	-2.59338400	2.22984900				
H	2.96522500	-3.76472900	1.24680200				
H	1.57058600	-4.68085800	1.81002500				
H	3.33090400	-4.46020000	3.60256000				
H	1.80467400	-3.72688900	4.08692800				
H	4.25950800	-2.24274400	3.00279000				
H	3.67265100	-2.19998700	4.66211200				
H	2.99273000	-0.15946100	3.40361500				
H	1.58987700	-1.07023900	3.94901600				



S	-0.34440300	1.32219600	-3.07679200
C	-1.49893400	0.52999000	-4.17336400