

Support information for
Role of Dissociation of Phenol in Its Selective Hydrogenation on Pt(111) and Pd(111)

Gaofeng Li,^{†,‡} Jinyu Han,[†] Hua Wang,[†] Xinli Zhu,^{,†} and Qingfeng Ge^{*,†,‡}*

[†]Collaborative Innovation Center of Chemical Science and Engineering, School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, China

[‡]Department of Chemistry and Biochemistry, Southern Illinois University, Carbondale, Illinois 62901, United States

Corresponding Authors

*Tel.:86-22-27890859 Email: xinlizhu@tju.edu.cn (X.Z.)

*Tel.:1-618-453-6406 Email: qge@chem.siu.edu (Q.G.)

I. Metastable adsorption configurations of phenol on Pt(111) and Pd(111)

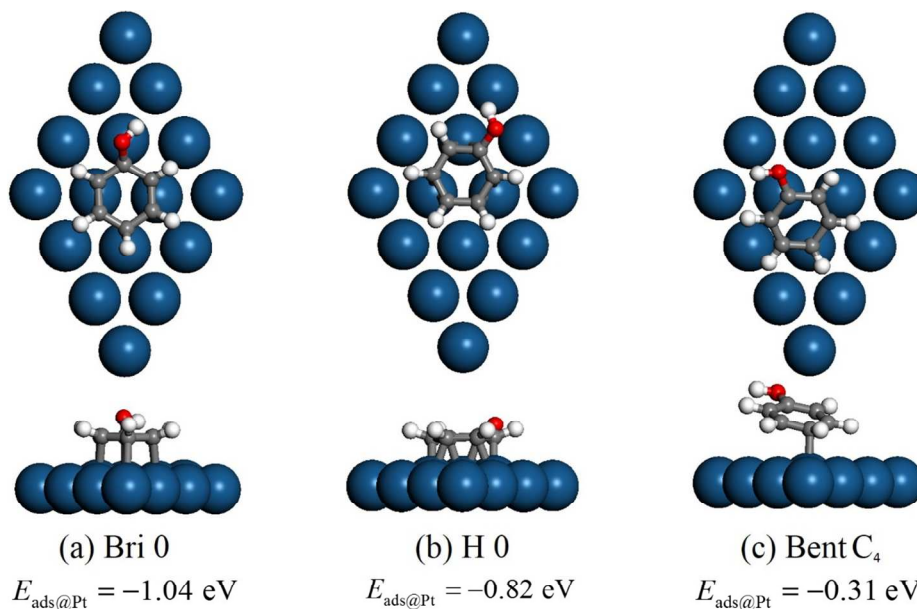


Figure S1. Schematic top view (upper) and side view (lower) of stable adsorption configurations of phenol on Pt (111). The Pt atoms is in blue; the O, H and C atoms are in red, white and gray, respectively.

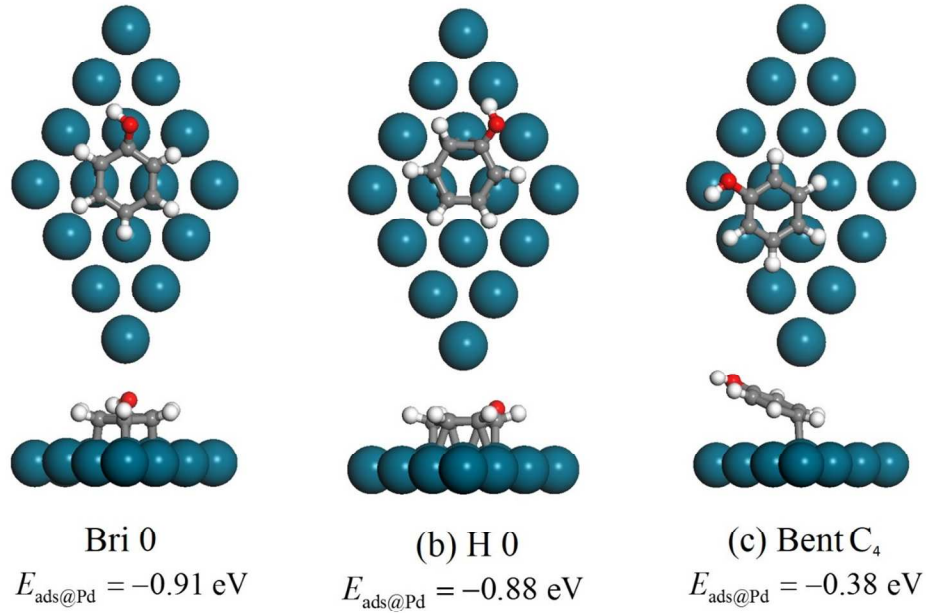
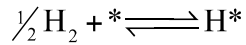
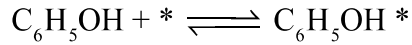


Figure S2. The top view (upper) and bottom view (lower) of adsorption structures of phenol on Pd (111). The Pt atoms is in dark blue; the O, H and C atoms are in red, white and gray, respectively.

II. Microkinetics analysis

The elementary steps likely involve phenol and hydrogen (dissociative) adsorption as well as hydrogenation of the adsorbed species. The adsorption phenol and hydrogen can be written,



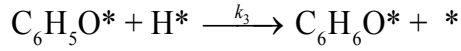
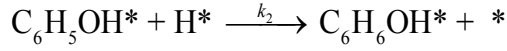
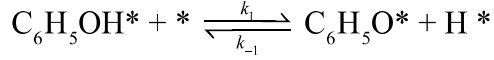
For simplicity, we neglect the size difference of the surface species and assume the adsorption of phenol and hydrogen (dissociative) competes for the same type of surface sites. As adsorption of phenol and hydrogen are highly exothermic, the processes are assumed to be in quasi-equilibrium and expected to strongly favor adsorption,

$$K_{\text{ph}} = \frac{\theta_{\text{ph}}}{p_{\text{ph}} \theta_*} \quad (\text{S1})$$

$$K_{\text{H}_2} = \frac{\theta_{\text{H}}}{p_{\text{H}_2}^{\frac{1}{2}} \theta_*} \quad (\text{S2})$$

where θ is the surface coverage of adsorbates.

The adsorbed phenol may undergo dissociation by breaking its OH bond, forming surface phenoxy and hydrogen, or hydrogenation. The surface phenoxy can recombine with a surface hydrogen to form surface phenol species or undergo hydrogenation at different carbon positions. These steps can be expressed as,



Under steady state,

$$\frac{d\theta_{\text{phox}}}{dt} = k_1\theta_{\text{ph}}\theta_* - k_{-1}\theta_{\text{phox}}\theta_{\text{H}} - k_2\theta_{\text{phox}}\theta_{\text{H}} \quad (\text{S3})$$

$$\frac{d\theta_{\text{Hph}}}{dt} = k_2\theta_{\text{ph}}\theta_{\text{H}} \quad (\text{S4})$$

$$\frac{d\theta_{\text{Hphox}}}{dt} = k_3\theta_{\text{phox}}\theta_{\text{H}} \quad (\text{S5})$$

where we used Hph to represent surface $\text{C}_6\text{H}_6\text{OH}$, and phox and Hphox as surface $\text{C}_6\text{H}_5\text{O}$ and $\text{C}_6\text{H}_6\text{O}$ species, respectively. At steady state, the surface coverage is constant and the coverage of the hydrogenated species is low, i.e.

$$\theta_{\text{ph}} + \theta_{\text{phox}} + \theta_{\text{H}} + \theta_* \approx 1 \quad (\text{S6})$$

The coverage ratio of phenol/phenoxy ($\theta_{\text{phenol}}/\theta_{\text{phenoxy}}$) can be obtained as,

$$\frac{\theta_{\text{ph}}}{\theta_{\text{phox}}} = \frac{(k_{-1} + k_3)K_{\text{H}_2}p_{\text{H}_2}^{1/2}}{k_1} \quad (\text{S7})$$

If we assume dissociation of surface phenol is in equilibrium with an equilibrium constant of K_1 , eq. (S7) becomes

$$\frac{\theta_{\text{ph}}}{\theta_{\text{phox}}} = \frac{(1 + k_3/k_{-1})K_{\text{H}_2}p_{\text{H}_2}^{1/2}}{K_1} \quad (\text{S8})$$

Clearly, the coverage ratio of surface phenol and phenoxy species depends on the rates of phenol

dissociation, recombination as well as hydrogenation. It can also be regulated by hydrogen partial pressure. Using this ratio and equations S4 and 5, we get the relative rate of phenol vs phenoxy hydrogenation as,

$$\frac{d\theta_{\text{Hph}}}{d\theta_{\text{Hphox}}} = \frac{k_2}{k_3} \frac{(k_{-1} + k_3)K_{\text{H}_2}p_{\text{H}_2}^{1/2}}{k_1} \quad \text{or} \quad \frac{d\theta_{\text{Hph}}}{d\theta_{\text{Hphox}}} = \frac{(1/k_{-1} + 1/k_3)k_2K_{\text{H}_2}p_{\text{H}_2}^{1/2}}{K_1} \quad (\text{S9})$$

Using the DFT calculated energetics, we estimated the rate and equilibrium constants in eqs. (S8) and (S9). Our results indicate that $K_1 \ll 1$ on Pt and $K > 1$ on Pd. Furthermore, k_2 and k_3 are comparable on Pt whereas k_3 is many orders of magnitude larger than k_2 on Pd. Table S1 shows the coverage ratio of surface phenol and phenoxy on Pt(111) and Pd(111) at different temperature. Clearly, phenol is the dominant surface species in the temperature range of 373-523 K on both surfaces. Even on Pd, the coverage of surface phenoxy species only becomes comparable to that of surface phenol at high temperatures.

Table S1 The surface coverage ratio of phenol/phenoxy on Pt(111) and Pd(111) at different temperatures under 1 bar hydrogen partial pressure.

Temperature (K)	$\theta_{\text{ph}} / \theta_{\text{phox}}$	
	Pt (111)	Pd (111)
373	4.42×10^6	181
423	1.95×10^5	32.1
473	1.65×10^4	8.22
523	2.23×10^3	2.72

We then compared the reaction rates of phenol and phenoxy hydrogenation on both surfaces and calculated the ratio of the hydrogenation rate at different temperatures. The results are shown in Table S2.

Table S2. The ratio of hydrogenation rates of phenol and phenoxy on Pt(111) and Pd(111) at different temperatures under 1 bar hydrogen partial pressure.

Temperature (K)	$d\theta_{\text{Hph}} / d\theta_{\text{Hphox}}$	
	Pt (111)	Pd (111)
373	1.46×10^7	1.59×10^{-5}
423	5.83×10^5	2.37×10^{-5}
473	4.59×10^4	3.28×10^{-5}
523	5.87×10^3	4.27×10^{-5}

The data in Table S2 demonstrate that the hydrogenation of phenol is dominant on Pt whereas the hydrogenation of phenoxy is dominant of Pd. The kinetics analysis showed that although phenol is the majority species on both the Pt and Pd surfaces, the hydrogenation of the surface phenoxy is much faster on Pd than on Pt, making Pd a selective catalyst for cyclohexanone formation.

III. Relaxed Atomic Coordinates

Notes: Only relaxed atoms were included for systems with adsorbates

Pt (111) Slab			
Pt	8.438750107	0.000000092	0.000000000
Pt	9.845208563	2.436057698	0.000000000
Pt	1.406458456	2.436057606	0.000000000
Pt	-0.000000702	4.872114938	0.000000000
Pt	1.406457254	7.308171678	0.000000000
Pt	4.219374867	7.308171953	0.000000000
Pt	2.812916747	0.000000775	0.000000000
Pt	4.219374703	2.436057515	0.000000000
Pt	7.032291816	2.436056923	0.000000000
Pt	5.625833158	4.872115121	0.000000000
Pt	7.032291114	7.308171861	0.000000000
Pt	-1.406458127	7.308171270	0.000000000
Pt	0.000000000	0.000000000	0.000001000
Pt	2.812916411	4.872114347	0.000001000
Pt	-0.000000537	9.744229376	0.000001000
Pt	-2.812916949	4.872115030	0.000001000
Pt	0.000000276	3.248076581	2.296737000
Pt	8.438750383	3.248076672	2.296737000
Pt	7.032291928	0.812019066	2.296737000
Pt	9.845209541	0.812019340	2.296737000
Pt	2.812916688	8.120190927	2.296737000
Pt	-0.000000425	8.120191519	2.296737000
Pt	-1.406458881	5.684133913	2.296737000
Pt	1.406458232	5.684133321	2.296737000
Pt	5.625833636	3.248075898	2.296737000
Pt	2.812916523	3.248076489	2.296737000
Pt	1.406458068	0.812018883	2.296737000
Pt	4.219375681	0.812019157	2.296737000
Pt	-2.812917172	8.120190744	2.296737000
Pt	5.625833435	8.120191702	2.296737000
Pt	4.219374979	5.684134096	2.296737000
Pt	7.032292092	5.684133504	2.296737000

Pt	4.219390474	4.060068882	4.573112000
Pt	2.812922377	1.624074577	4.573125000
Pt	1.406549133	4.060010715	4.573161000
Pt	5.625781906	6.496144400	4.573171000
Pt	0.000031153	1.623984011	4.573173000
Pt	7.032194546	4.060058499	4.573176000
Pt	5.625800787	1.624100949	4.573180000
Pt	-4.219435902	8.932260843	4.573186000
Pt	2.813021768	6.496132881	4.573206000
Pt	-1.406467396	4.059997113	4.573211000
Pt	4.219413236	8.932216461	4.573221000
Pt	8.438746156	1.624011298	4.573222000
Pt	-2.813021297	6.496170344	4.573226000
Pt	-1.406496547	8.932324775	4.573234000
Pt	0.000051890	6.496150080	4.573251000
Pt	1.406519597	8.932279710	4.573268000
Pt	4.219387337	2.436081397	6.882321000
Pt	5.625777250	4.872094284	6.882344000
Pt	7.032239371	2.436034086	6.882399000
Pt	4.219417250	7.308191362	6.882423000
Pt	-0.000020026	-0.000012687	6.882430000
Pt	2.813017576	4.872075569	6.882451000
Pt	1.406501711	2.435994527	6.882460000
Pt	2.812870197	0.000076148	6.882464000
Pt	8.438798052	0.000015134	6.882473000
Pt	7.032181753	7.308208443	6.882477000
Pt	5.625850817	0.000103554	6.882492000
Pt	9.845204730	2.435949059	6.882541000
Pt	-2.813018142	4.872063757	6.882593000
Pt	1.406562778	7.308220451	6.882630000
Pt	-1.406496383	7.308243009	6.882683000
Pt	0.000057143	4.872041127	6.882695000

Phenol on Pt Bri30

Pt	4.238993837	4.062096904	4.546524000
Pt	2.793424234	6.502628956	4.599903000
Pt	5.642475500	6.496972554	4.548383000
Pt	7.049764395	4.068394369	4.544454000
Pt	1.413091731	4.052728828	4.559437000

Pt	-1.408301429	4.046840474	4.555100000
Pt	2.818590079	1.621317324	4.559345000
Pt	-4.226458544	8.923603269	4.555091000
Pt	5.628270581	1.593010757	4.596337000
Pt	-0.003875027	1.612080307	4.566111000
Pt	0.018426431	6.503777720	4.624301000
Pt	1.392282268	8.916989933	4.634027000
Pt	-1.387859611	8.927290896	4.610508000
Pt	8.433244187	1.583595607	4.601032000
Pt	4.185697070	8.934118348	4.606627000
Pt	-2.755087682	6.520046310	4.614736000
Pt	4.304800580	7.264779629	6.851365000
Pt	2.857934554	4.797912055	6.866481000
Pt	-0.008230267	4.780822909	6.850224000
Pt	1.483125139	7.159588347	7.005451000
Pt	7.058272982	2.499981626	6.832844000
Pt	4.197055486	2.476881499	6.876264000
Pt	2.748191081	0.010674632	6.845259000
Pt	5.655178230	4.867440276	6.880777000
Pt	1.393456177	2.407986997	6.880004000
Pt	5.614614040	9.724539191	6.880199000
Pt	9.842522321	2.406530990	6.879010000
Pt	-2.789632214	4.874919373	6.880752000
Pt	-4.195485055	7.297834876	6.880306000
Pt	5.550067368	0.094602771	6.990658000
Pt	2.778657800	9.707002842	7.040852000
Pt	-1.384133182	7.309137209	7.050073000
C	0.697198393	7.090833275	9.060387000
C	1.945568378	7.796461560	9.061201000
C	2.035050559	9.269187293	9.028921000
C	6.360373940	0.210866942	9.134430000
C	-0.521062389	9.257483750	9.044865000
C	-0.600896967	7.781936158	9.008450000
O	6.438471386	1.462585727	9.665992000
H	0.693279614	6.054211719	9.403615000
H	2.837063581	7.263924546	9.401909000
H	2.813007957	9.711267061	9.664410000
H	4.221506627	0.039114040	9.418224000
H	-1.387317810	7.349695273	9.640695000

H	5.604872513	1.954522126	9.493741000
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Phenol on Pt BriO

Pt	-1.403896216	5.704682579	4.542070000
Pt	7.011467436	5.675022141	4.594987000
Pt	-2.810224679	8.138558281	4.548341000
Pt	0.000043765	8.138640059	4.547593000
Pt	8.443189258	3.250695028	4.558169000
Pt	7.036929982	0.804938411	4.554193000
Pt	0.001155844	3.250706083	4.557896000
Pt	1.405521173	0.804486133	4.555507000
Pt	1.432625820	5.673902913	4.595591000
Pt	9.848892974	0.802283233	4.567694000
Pt	5.622052511	3.271806798	4.624706000
Pt	4.221402485	5.670821838	4.632745000
Pt	2.821625746	3.272487307	4.626884000
Pt	2.839478771	8.097633805	4.599243000
Pt	5.603440599	8.097822171	4.603354000
Pt	4.220310733	0.879614718	4.615750000
Pt	-4.155906306	7.365607282	6.851333000
Pt	-2.739689084	4.878245414	6.858939000
Pt	7.097483073	2.382809493	6.847067000
Pt	5.782002232	4.866817893	6.995397000
Pt	1.350591899	7.364792045	6.846171000
Pt	-0.063576519	4.878172391	6.858963000
Pt	1.351763427	2.382711035	6.847738000
Pt	-1.402819932	7.337330810	6.877762000
Pt	-1.400961101	2.411552245	6.878171000
Pt	-5.629726228	9.724294345	6.892093000
Pt	2.826399047	9.725177109	6.881385000
Pt	5.627196086	0.017619628	6.879564000
Pt	2.819633967	0.017729342	6.881828000
Pt	2.667257375	4.867349493	7.002661000
Pt	4.220140364	7.265093831	7.041554000
Pt	4.225349440	2.448186064	7.054061000
C	5.467039182	4.159119861	9.050855000
C	5.473524478	5.595836768	9.019843000
C	4.217070092	6.403795937	9.018946000
C	2.975084225	5.589301264	9.038850000

C	2.987828958	4.154169744	9.056088000
C	4.228656676	3.364262394	9.017360000
O	4.151095126	7.433681976	9.960056000
H	6.372717873	3.655269369	9.397493000
H	6.364033961	6.111706470	9.389955000
H	2.084502687	3.643586715	9.397659000
H	4.232392201	2.466710485	9.649341000
H	2.093743428	6.111688226	9.417021000
H	4.843665685	8.095051404	9.753358000

Phenol on Pt H0

Pt	-1.404405987	5.694741630	4.553140000
Pt	6.989970248	5.662983918	4.619132000
Pt	-2.805285836	8.118134606	4.551801000
Pt	-0.007955309	8.121955256	4.550524000
Pt	8.436487856	3.260809860	4.552249000
Pt	7.023294836	0.814967646	4.551468000
Pt	0.002587537	3.263145849	4.552372000
Pt	1.416428097	0.813889481	4.551337000
Pt	1.449482731	5.665501940	4.618491000
Pt	9.845216043	0.816404603	4.560077000
Pt	5.607412723	3.265717940	4.645557000
Pt	4.220539419	5.664130964	4.644339000
Pt	2.833852817	3.258331215	4.632504000
Pt	2.803858241	8.118079238	4.551255000
Pt	5.635187557	8.119205517	4.547443000
Pt	4.222194654	0.862357765	4.614323000
Pt	-4.186293497	7.348143124	6.869096000
Pt	-2.766922507	4.890677741	6.869184000
Pt	7.100980751	2.402417649	6.827657000
Pt	5.699168224	4.923659184	7.086246000
Pt	1.379143331	7.342610577	6.879941000
Pt	-0.035547442	4.890886177	6.876763000
Pt	1.337387432	2.407313081	6.824677000
Pt	-1.402342139	7.316718370	6.891414000
Pt	-1.404759712	2.443612858	6.870267000
Pt	0.000609323	0.011629380	6.868570000
Pt	8.440594177	0.009338114	6.867892000
Pt	5.639209745	-0.033852106	6.869928000

Pt	2.803448076	-0.033569446	6.867600000
Pt	2.750094275	4.921525215	7.057627000
Pt	4.224834594	7.402446480	6.815677000
Pt	4.205852117	2.368909708	7.061413000
C	4.900584248	2.791381081	9.102783000
C	5.682376623	4.030081249	9.109677000
C	5.018730263	5.300200063	9.137421000
C	3.555204265	5.354886652	9.187525000
C	2.776883801	4.150204012	9.097030000
C	3.469340579	2.853418304	9.090481000
O	3.071633611	6.502669736	9.737457000
H	5.390780169	1.891495303	9.477063000
H	6.713235870	3.970511857	9.462907000
H	5.532867544	6.179579993	9.530394000
H	1.764604421	4.164706675	9.506341000
H	2.899096412	1.995524397	9.450149000
H	2.141021295	6.650727912	9.450362000

Phenol on Pt BentC₄

Pt	-1.416155433	5.686408991	4.566844000
Pt	7.011378426	5.671717971	4.604578000
Pt	-2.812221276	8.118058072	4.561139000
Pt	-0.003226090	8.122200504	4.570660000
Pt	8.436819924	3.247667019	4.569179000
Pt	7.027073687	0.811896807	4.564576000
Pt	-0.003162544	3.248878416	4.571367000
Pt	1.405980376	0.807889496	4.570018000
Pt	1.399054138	5.688169054	4.558978000
Pt	9.841433369	0.811596819	4.571697000
Pt	5.622372448	3.270396945	4.607462000
Pt	4.231351075	5.674507302	4.602635000
Pt	2.808869015	3.243432000	4.564789000
Pt	2.814326769	8.113737259	4.571883000
Pt	5.622084544	8.119238433	4.570852000
Pt	4.222128904	0.817589881	4.570176000
Pt	-4.206422294	7.328673023	6.857460000
Pt	-2.800736070	4.868922930	6.874393000
Pt	7.041210296	2.418796183	6.866703000
Pt	5.606630270	4.875900742	7.056062000

Pt	1.393694051	7.309447162	6.879771000
Pt	-0.011811635	4.872035802	6.881599000
Pt	1.391873041	2.428836926	6.879906000
Pt	-1.409310814	7.308676271	6.882575000
Pt	-1.410031411	2.434382007	6.884105000
Pt	-0.005773300	0.006842351	6.880667000
Pt	8.432632921	0.001090814	6.881552000
Pt	5.622983315	-0.003415106	6.882952000
Pt	2.809722898	-0.002461134	6.880842000
Pt	2.768682438	4.868042856	6.848648000
Pt	4.201752218	7.322408630	6.883664000
Pt	4.202185726	2.420079333	6.876905000
C	5.644651897	4.964404135	9.353618000
C	5.078763012	6.243357866	9.680668000
C	3.821088297	6.348371341	10.249692000
C	3.092057973	5.178867728	10.541416000
C	3.629647130	3.906225432	10.267909000
C	4.894325714	3.797547013	9.710722000
O	1.876384436	5.343465380	11.113958000
H	6.738337247	4.884644746	9.319221000
H	5.680748842	7.140415947	9.523514000
H	3.382629698	7.317772793	10.488842000
H	3.053603162	3.009275973	10.509031000
H	5.347357590	2.813809217	9.575031000
H	1.455650457	4.474922718	11.263836000

Phenol Dissociation on Pt Product

Pt	4.230072218	4.061660207	4.558543000
Pt	2.784302150	6.504137044	4.592112000
Pt	5.633679803	6.484033960	4.556041000
Pt	7.040705856	4.060690519	4.565999000
Pt	1.397226726	4.053717832	4.553481000
Pt	-1.418539259	4.045442033	4.554840000
Pt	2.809769923	1.624892367	4.560658000
Pt	-4.246966869	8.920127808	4.552568000
Pt	5.617590660	1.605534592	4.588547000
Pt	-0.019751877	1.613222796	4.563022000
Pt	0.004273512	6.509562145	4.628702000
Pt	1.381544165	8.920318993	4.631024000

Pt	-1.419051159	8.919691550	4.580684000
Pt	8.410586434	1.585355228	4.614553000
Pt	4.172893549	8.936617998	4.601461000
Pt	-2.766896086	6.514657555	4.618553000
Pt	4.273514473	7.276168501	6.840895000
Pt	2.804924123	4.811937295	6.848407000
Pt	-0.027896440	4.793214099	6.853283000
Pt	1.452007557	7.191415115	7.005374000
Pt	7.050018894	2.449229125	6.889618000
Pt	4.139211034	2.442749966	6.893701000
Pt	2.721499699	0.005251801	6.843467000
Pt	5.636607848	4.902909432	6.916090000
Pt	1.360014314	2.408397991	6.874247000
Pt	5.589413177	9.728722015	6.875285000
Pt	9.816445898	2.410465299	6.880378000
Pt	-2.787504807	4.886216151	6.879020000
Pt	-4.214835881	7.301350261	6.881886000
Pt	5.498212166	0.042514923	6.915884000
Pt	2.741505959	9.719888000	7.062108020
Pt	-1.399408710	7.333845218	7.084592000
C	0.717201702	7.149422024	9.070649000
C	2.007253805	7.782585856	9.071682000
C	2.186343633	9.248480586	9.084942000
C	6.556871778	0.250883185	9.454885000
C	-0.369853405	9.392719400	8.989255000
C	-0.535499041	7.915360693	9.017635000
O	6.579003073	1.276683745	10.136389000
H	0.657317718	6.113261889	9.413940000
H	2.862332926	7.179852334	9.390407000
H	3.051142738	9.591482600	9.667460000
H	4.396113940	0.205506786	9.375773000
H	-1.348556871	7.529553195	9.649493000
H	5.591207872	3.262754314	7.760924000

Phenoxy Hydrogenation on Pt Reactant

Pt	5.622580141	1.658184624	4.548581004
Pt	-1.403240685	8.927856165	4.584879004
Pt	2.803007837	1.657508093	4.545568006
Pt	4.208459644	4.091902134	4.551963002

Pt	1.413445721	8.952414135	4.563729003
Pt	2.825085548	6.513165977	4.554601003
Pt	8.442105785	1.638744344	4.575670003
Pt	0.008334185	1.635141287	4.562078002
Pt	7.052740557	4.082807234	4.588086003
Pt	4.225011241	8.946734508	4.572074006
Pt	-0.020526413	6.513453426	4.627555003
Pt	-2.796500062	6.502920012	4.629538004
Pt	-1.400115511	4.075960911	4.599074003
Pt	5.667540761	6.524178877	4.609684006
Pt	-4.206891952	8.917069646	4.595793004
Pt	1.357193835	4.116024836	4.622643005
Pt	2.809854673	0.125661107	6.836382995
Pt	5.643989818	0.094309228	6.840485018
Pt	1.477608824	7.353903833	6.848637998
Pt	-1.330448377	7.461638047	6.992720993
Pt	5.598642164	4.892150941	6.859736009
Pt	6.991844154	2.454909523	6.909789981
Pt	-1.359964124	2.422609094	6.895719001
Pt	4.207631879	2.502446352	6.871753994
Pt	8.466049039	-0.011064774	6.925131993
Pt	0.039573764	0.014477772	6.864626982
Pt	4.248631445	7.332789848	6.880475998
Pt	2.800124177	4.916929558	6.882241016
Pt	1.401799345	2.495849796	6.883602007
Pt	8.421146722	4.812140293	6.938978020
Pt	-4.173776907	7.318000476	7.057828999
Pt	-0.051189569	4.918727236	7.101730016
C	-0.925539264	6.879555190	9.066210020
C	-2.092739269	7.718253440	9.050997022
C	-3.470409827	7.182692061	9.080561994
C	7.725964199	5.736332864	9.490863035
C	-2.390351539	4.861989809	9.014080985
C	-1.008053639	5.414454050	9.029101997
O	6.833241693	5.291308095	10.211322987
H	0.016895129	7.322157469	9.397531998
H	-1.961857407	8.761615514	9.354176033
H	-4.177820317	7.804271087	9.644616002
H	8.778685299	3.852721260	9.430589010

H	-0.281106727	4.886051029	9.663340990
H	8.434277375	1.617819101	7.780229021

Phenoxy Hydrogenation on Pt Product

Pt	5.601108014	1.638375810	4.547692002
Pt	-1.410396672	8.921507587	4.593835006
Pt	2.788513673	1.644985458	4.551215004
Pt	4.194183842	4.081621719	4.566230006
Pt	1.403631899	8.936956087	4.559373007
Pt	2.819765630	6.502101606	4.559211004
Pt	8.438289810	1.630246884	4.559393004
Pt	0.004767871	1.622570244	4.567198003
Pt	7.016280969	4.063089374	4.536378003
Pt	4.224702555	8.932283852	4.568674005
Pt	-0.021954569	6.499325793	4.629111006
Pt	-2.799950135	6.510886331	4.602071003
Pt	-1.393758469	4.069737631	4.590654005
Pt	5.659211312	6.510289842	4.614947007
Pt	-4.218694363	8.905115274	4.613176004
Pt	1.357656806	4.102808726	4.633990004
Pt	2.788087301	0.093670916	6.842028998
Pt	5.651489298	0.077710707	6.850203993
Pt	1.472173803	7.338720100	6.847573982
Pt	-1.333001403	7.415842072	6.994486011
Pt	5.585921830	4.869434674	6.877912981
Pt	7.009214797	2.426696357	6.854630031
Pt	-1.420505877	2.418225703	6.873105988
Pt	4.189537356	2.473217719	6.873909015
Pt	8.455549742	0.011439934	6.874664997
Pt	0.001287674	0.009010317	6.880656024
Pt	4.234698278	7.318148894	6.884347988
Pt	2.779855147	4.894876566	6.893494022
Pt	1.372608348	2.477937506	6.895286980
Pt	8.381080809	4.804048092	6.807155003
Pt	-4.169219576	7.265155998	7.066684991
Pt	-0.106761724	4.889767437	7.153534031
C	-0.821221542	6.919170785	9.068729009
C	-2.088827255	7.591109317	9.061298991
C	-3.382878396	6.886624868	9.047666010

C	7.934166447	5.414323725	9.394255015
C	-1.948334314	4.805008106	9.747240026
C	-0.701594569	5.449790738	9.145716990
O	6.903288511	4.770918723	9.641390984
H	0.060798956	7.509839141	9.332501993
H	-2.102829199	8.648563261	9.341138006
H	-4.181313537	7.390110734	9.613982992
H	9.379950543	4.941887229	10.849004913
H	0.214123335	5.135110670	9.667183029
H	9.252960005	3.719541182	9.586243946

Phenol Hydrogenation on Pt Reactant

Pt	-1.401607522	5.698438713	4.544058000
Pt	7.009241185	5.671110160	4.589473000
Pt	-2.811189387	8.139877357	4.544875000
Pt	-0.006860785	8.141601029	4.542229000
Pt	8.441456388	3.249449609	4.554229000
Pt	7.031331566	0.807043670	4.551321000
Pt	0.008717970	3.244444070	4.580852000
Pt	1.405756662	0.811410013	4.565650000
Pt	1.425917907	5.667234467	4.600304000
Pt	9.846196405	0.805090639	4.564083000
Pt	5.607051409	3.270454125	4.619957000
Pt	4.210670817	5.658882043	4.627679000
Pt	2.792296644	3.252139810	4.648085000
Pt	2.836096086	8.094212823	4.597888000
Pt	5.602326482	8.096256464	4.594836000
Pt	4.216092451	0.882134438	4.618873000
Pt	-4.152209954	7.353563552	6.840665000
Pt	-2.748563723	4.875434087	6.858958000
Pt	7.074506234	2.383746439	6.844447000
Pt	5.769663380	4.870132375	6.990576000
Pt	1.345099329	7.356098634	6.829925000
Pt	-0.067642775	4.878649429	6.877456000
Pt	1.328448917	2.357787118	6.963876000
Pt	-1.402061580	7.330282314	6.877781000
Pt	-1.430993878	2.417719948	6.869693000
Pt	-0.017769868	-0.042464179	6.866020902
Pt	8.433561904	-0.015318025	6.871559072

Pt	5.615397018	0.022963043	6.879107000
Pt	2.827621034	0.000685347	6.875726000
Pt	2.675658034	4.846111861	7.004601000
Pt	4.210050405	7.266875510	7.017997000
Pt	4.212889794	2.471477324	7.072365000
C	5.469017061	4.196475648	9.054855000
C	5.490557722	5.630157214	9.040316000
C	4.265167560	6.453529197	9.020501000
C	3.022734209	5.680939462	9.159080000
C	2.986816628	4.247556340	9.070943000
C	4.216180259	3.425460607	9.020524000
O	1.986528613	6.382762726	9.688884000
H	6.366017769	3.672138448	9.392810000
H	6.406177841	6.132555813	9.361833000
H	4.290727374	7.358386123	9.640056000
H	2.093274903	3.758638642	9.465884000
H	4.198391263	2.531627134	9.657912000
H	1.145184883	5.892856608	9.563582000
H	1.099105571	2.008108776	8.475421000

Phenol Hydrogenation on Pt Product

Pt	-1.406459418	5.708554984	4.546252000
Pt	7.015334018	5.680623257	4.599570000
Pt	-2.813442720	8.147516471	4.550115000
Pt	-0.001054621	8.147905599	4.553767000
Pt	8.443171306	3.253933935	4.559097000
Pt	7.038060392	0.809216340	4.556008000
Pt	0.006297207	3.251697184	4.557878000
Pt	1.406058705	0.811859166	4.563821000
Pt	1.413652482	5.685730128	4.560204000
Pt	9.849601546	0.808206516	4.567414000
Pt	5.618109004	3.272022442	4.627263000
Pt	4.229753483	5.678210191	4.612888000
Pt	2.827485909	3.267965406	4.623343000
Pt	2.839355152	8.099231691	4.605012000
Pt	5.598451167	8.101452221	4.614833000
Pt	4.222523104	0.878988657	4.620325000
Pt	-4.160282779	7.370067009	6.851149000
Pt	-2.741596572	4.885167548	6.857881000

Pt	7.094963004	2.392886605	6.843672000
Pt	5.753008830	4.858489847	7.004731000
Pt	1.359836904	7.359300864	6.847113000
Pt	-0.033642316	4.881065953	6.859039000
Pt	1.385331230	2.439304177	6.866046000
Pt	-1.402196744	7.343884204	6.872834000
Pt	-1.386464768	2.425118629	6.875255000
Pt	0.002923992	-0.002653497	6.882554000
Pt	8.456148091	-0.009007717	6.878376000
Pt	5.624223420	0.035554821	6.881134000
Pt	2.822608324	0.040733080	6.886107000
Pt	2.718956941	4.924875770	6.936918000
Pt	4.208237855	7.253390080	7.073712000
Pt	4.195856729	2.498955191	7.103959000
C	5.542391600	4.119190077	9.065996000
C	5.413873372	5.549572019	9.069346000
C	4.113733978	6.236402530	8.999950000
C	2.927233375	5.316417152	9.007846000
C	3.136981640	3.936817764	9.643920000
C	4.368746708	3.219011444	9.105526000
O	1.826642298	5.997955490	9.535222000
H	6.509590863	3.700296346	9.359495000
H	6.267118180	6.143093412	9.406084000
H	4.004130730	7.115502162	9.651385000
H	2.228838545	3.329235747	9.517926000
H	4.580849574	2.284732360	9.643383000
H	1.016554326	5.471709932	9.356445000
H	3.274840011	4.096399474	10.735413000

Cyclohexenol on Pt

Pt	7.004886426	4.136415449	4.530407000
Pt	-1.424691910	4.132667332	4.558734000
Pt	8.422063187	1.697411551	4.514238000
Pt	5.613242991	1.700506211	4.495471000
Pt	-2.837416200	6.571493135	4.536754000
Pt	-1.419658270	9.006976004	4.505435000
Pt	5.611684591	6.568681136	4.542792000
Pt	4.201052718	8.997463113	4.509677000
Pt	4.187052650	4.149536131	4.607177000

Pt	-4.238247761	9.001691749	4.514334000
Pt	-0.023847944	6.573794356	4.561282000
Pt	1.418442758	4.145879081	4.651902000
Pt	2.798684063	6.553207248	4.609779000
Pt	2.795759575	1.690301733	4.525751000
Pt	-0.014635344	1.693404893	4.532448000
Pt	1.397028172	9.002574082	4.496719000
Pt	9.799152710	2.486492622	6.848533000
Pt	8.388725285	4.931996713	6.853226000
Pt	-1.455365493	7.377955229	6.839257000
Pt	-0.075400865	4.927312025	6.871687000
Pt	4.198960363	2.466280842	6.806365000
Pt	5.603681814	4.930193869	6.879133000
Pt	4.205731793	7.395867459	6.838759000
Pt	7.000562491	2.497774121	6.832336000
Pt	-4.253057143	7.370111096	6.846875000
Pt	11.217182513	0.058558236	6.833578000
Pt	2.778815475	0.052161640	6.824032000
Pt	5.595251824	0.065022545	6.812208000
Pt	8.407245527	0.070044560	6.823263000
Pt	2.751975373	4.955865374	7.124484000
Pt	1.353881821	2.466416203	6.854503000
Pt	1.357407325	7.412236712	6.834098000
C	0.464376528	5.237419914	10.209678000
C	0.845988084	3.983938485	10.993864000
C	1.919577873	3.170104540	10.260137000
C	3.028681582	4.005948561	9.719787000
C	2.856043094	5.356705968	9.300929000
C	1.679202642	6.109500515	9.916345000
O	4.208024212	3.398397918	9.713071000
H	-0.011523787	4.938910371	9.245157000
H	-0.034720802	3.347175911	11.164590000
H	1.465712639	2.663610870	9.373396000
H	3.792520453	5.932054368	9.319161000
H	1.398452753	6.961087465	9.266150000
H	4.862991779	3.906807049	9.151584000
H	2.345037518	2.362664244	10.873729000
H	1.225213913	4.271196905	11.990048000
H	2.047378371	6.560809605	10.858193000

H	-0.294254259	5.822258851	10.751076000
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Cyclohexanone on Pt

Pt	7.032038680	4.142858532	4.531225000
Pt	-1.409672273	4.141330105	4.570247000
Pt	8.439033099	1.702828302	4.515810000
Pt	5.625470315	1.702006557	4.508825000
Pt	-2.818823664	6.582394353	4.540449000
Pt	-1.406667735	9.013160272	4.509968000
Pt	5.629878400	6.583381739	4.540389000
Pt	4.219988602	9.013577026	4.515831000
Pt	4.221488565	4.141860886	4.561041000
Pt	-4.219076920	9.012882621	4.517765000
Pt	-0.007112962	6.581410195	4.565920000
Pt	1.406839477	4.138003609	4.598857000
Pt	2.816671917	6.584637126	4.564843000
Pt	2.812735927	1.698139638	4.535634000
Pt	0.002991399	1.697247308	4.545081000
Pt	1.405686972	9.012791565	4.507006000
Pt	-1.410598020	2.505524613	6.850594000
Pt	-2.818481482	4.947208977	6.853682000
Pt	-1.411627550	7.390325570	6.846205000
Pt	-0.005495894	4.952446988	6.894941000
Pt	4.224524147	2.506248617	6.841114000
Pt	5.631333908	4.946882702	6.850997000
Pt	4.224086021	7.391773914	6.847373000
Pt	7.032173518	2.508324028	6.829083000
Pt	-4.219501358	7.386287420	6.843827000
Pt	-0.000296504	0.073082442	6.836876000
Pt	2.813903039	0.073421084	6.831538000
Pt	5.625686663	0.077003233	6.820474000
Pt	8.437414613	0.077134950	6.824799000
Pt	2.820087571	4.955939162	6.881146000
Pt	1.407675462	2.504827525	6.874113000
Pt	1.404901000	7.397318170	6.848100000
C	0.194721986	5.203438540	10.520854000
C	0.347946758	3.768893589	11.023177000
C	1.669446517	3.134546317	10.562715000
C	2.875052934	4.013957935	10.830677000

C	2.720110064	5.476621055	10.470273000
C	1.381742994	6.077867285	10.922783000
O	3.923872152	3.562154112	11.282226000
H	0.109707530	5.193141182	9.406888000
H	-0.493751619	3.147331200	10.679252000
H	1.637191679	2.997151293	9.455063000
H	2.770103875	5.511580878	9.352365000
H	1.276878821	7.092663239	10.505233000
H	3.589950758	6.034903364	10.843949000
H	1.844640701	2.144293517	11.005257000
H	0.310193778	3.761365507	12.127088000
H	1.394588130	6.195359717	12.021184000
H	-0.746430646	5.641346361	10.888814000

Cyclohexenol Hydrogenation on Pt Reactant

Pt	7.013524439	4.135612925	4.525823000
Pt	-1.415808629	4.132711626	4.556381000
Pt	8.428976212	1.686799261	4.519552000
Pt	5.621020534	1.697997310	4.491534000
Pt	-2.830033770	6.569611879	4.533695000
Pt	-1.414070403	9.003142475	4.503074000
Pt	5.610159627	6.573429821	4.547864000
Pt	4.203173432	8.994526297	4.521897000
Pt	4.195648273	4.150356186	4.603824000
Pt	-4.231818826	8.999524991	4.510627000
Pt	-0.008351172	6.575597553	4.568142000
Pt	1.428108957	4.146815429	4.653500000
Pt	2.805706770	6.554998935	4.623182000
Pt	2.802233142	1.688520281	4.525655000
Pt	-0.008396154	1.693473488	4.529256000
Pt	1.405025668	8.996870152	4.510791000
Pt	9.818298372	2.492493797	6.846366966
Pt	8.408134421	4.928564320	6.851622974
Pt	-1.444042301	7.370199572	6.842803000
Pt	-0.056067984	4.922997556	6.877654000
Pt	4.214092185	2.464175926	6.803000000
Pt	5.627075655	4.924993190	6.875673000
Pt	4.256185617	7.367724045	6.876548000
Pt	7.012902821	2.500112200	6.829420000

Pt	7.022753954	7.365872945	6.845029049
Pt	11.254734512	0.067926336	6.825546949
Pt	2.792869865	0.047258557	6.826086000
Pt	5.584982482	0.070391522	6.806375000
Pt	8.417637100	0.110623293	6.860670000
Pt	2.776781679	4.906945155	7.135208000
Pt	1.367302170	2.466422930	6.857250000
Pt	1.335503188	7.379169632	6.874189000
C	0.556710089	5.092192329	10.288262000
C	0.990260449	3.855393550	11.072199000
C	2.082354194	3.072847397	10.331622000
C	3.151121542	3.936884793	9.754894000
C	2.923933742	5.276186018	9.323262000
C	1.743541751	5.994741118	9.973479000
O	4.342752832	3.359540735	9.716679000
H	0.070475735	4.781067705	9.336360000
H	0.134034967	3.189313475	11.256618000
H	1.638013809	2.535183251	9.461081000
H	3.842929699	5.879887744	9.313864000
H	1.426476305	6.843027678	9.340416000
H	4.971251778	3.871940869	9.125863000
H	2.550483865	2.293551757	10.950847000
H	1.370234601	4.161068102	12.062555000
H	2.123406837	6.442976767	10.912452000
H	-0.202333627	5.658448052	10.849035000
H	2.824339613	8.220632018	7.707361000

Cyclohexenol Hydrogenation on Pt Product

Pt	7.014069614	4.124005197	4.524773000
Pt	-1.412617594	4.122646659	4.563678000
Pt	8.426535460	1.676275755	4.507049000
Pt	5.613127760	1.689502625	4.500844000
Pt	-2.830999056	6.562471954	4.537161000
Pt	-1.412361224	8.995640860	4.503023000
Pt	5.613179889	6.565237069	4.539523000
Pt	4.202888100	8.976464086	4.515245000
Pt	4.184676824	4.137437078	4.603072000
Pt	-4.232126802	8.993453562	4.513489000
Pt	-0.012008242	6.561559322	4.565913000

Pt	1.418740374	4.132408567	4.636453000
Pt	2.805297620	6.527932264	4.621466000
Pt	2.804342728	1.683502191	4.532240000
Pt	-0.006111747	1.679776196	4.534876000
Pt	1.401389884	8.976274789	4.504213000
Pt	9.805752995	2.459824649	6.837784000
Pt	8.409082603	4.910444621	6.847224000
Pt	-1.437416377	7.354304009	6.835492000
Pt	-0.042124541	4.908192308	6.888604000
Pt	4.215292517	2.460116962	6.829962000
Pt	5.616212999	4.920350518	6.843616000
Pt	4.193191082	7.330754307	6.867864000
Pt	7.013528957	2.473760700	6.819628000
Pt	7.004843673	7.348559499	6.843097000
Pt	11.220678608	0.023323649	6.828307000
Pt	2.791822415	0.026262320	6.818187000
Pt	5.609029555	0.035648274	6.810745000
Pt	8.416430727	0.031371792	6.820620000
Pt	2.766256788	4.864309507	7.219704000
Pt	1.367560136	2.451791740	6.856065000
Pt	1.387424897	7.353626670	6.860751000
C	0.249936234	5.402364431	10.215311000
C	0.743867868	4.063905083	10.750519000
C	1.838621931	3.477634742	9.852217000
C	2.879983635	4.496800175	9.372446000
C	2.773413896	5.838950013	10.099975000
C	1.369197329	6.452777567	10.153602000
O	4.134912736	3.901355141	9.550373000
H	-0.143950744	5.230744159	9.178787000
H	-0.085391572	3.343923563	10.827448000
H	1.342986612	2.988667165	8.970759000
H	3.505773258	6.558021672	9.699783000
H	1.212197047	7.106091120	9.268078000
H	4.835063429	4.509111746	9.208449000
H	2.384009775	2.662714183	10.352773000
H	1.137672524	4.190294767	11.775296000
H	1.321267369	7.121254463	11.027982000
H	-0.610892968	5.774162513	10.790697000
H	3.103100330	5.601045664	11.130599000

Cyclohexanol on Pt

Pt	-0.075619590	8.162111283	4.531096000
Pt	6.955748716	0.846784333	4.566620000
Pt	2.738019141	8.154890570	4.513094000
Pt	1.320483041	5.716661921	4.531237000
Pt	4.136493691	0.850117339	4.540430000
Pt	2.737587325	3.289042490	4.510443000
Pt	-2.893501875	8.167011945	4.536034000
Pt	5.546980759	8.160324862	4.513088000
Pt	-1.476037225	5.723690686	4.571967000
Pt	1.329446145	0.853530321	4.514476000
Pt	5.540570176	3.286819252	4.563794000
Pt	8.365779457	3.288257320	4.595111000
Pt	6.952408428	5.732288939	4.562545000
Pt	-0.070343405	3.294923751	4.549937000
Pt	9.778424512	0.851470277	4.541302000
Pt	4.139496362	5.724648273	4.504696000
Pt	8.361553925	0.025618381	6.849576000
Pt	5.547265002	0.035374928	6.857912000
Pt	4.136176928	2.472096741	6.849602000
Pt	6.940470667	2.463790027	6.882875000
Pt	-0.085607645	4.903247362	6.911190000
Pt	-1.483050172	7.366037957	6.843676000
Pt	6.946640713	7.358905014	6.842417000
Pt	1.331589902	7.349457620	6.834306000
Pt	2.733957840	0.039953935	6.843920000
Pt	11.177092768	0.031602759	6.834624000
Pt	1.338425730	2.465559468	6.826687000
Pt	2.736772784	4.908147715	6.821948000
Pt	4.136912828	7.343309511	6.825212000
Pt	8.341439037	4.916894527	6.875346000
Pt	9.766389178	2.453554518	6.867268000
Pt	5.531344484	4.913133936	6.848747000
C	7.389630777	3.083700187	10.803461000
C	8.731654002	2.426784601	11.136340000
C	-1.375043344	3.026779135	10.314353000
C	-1.309906909	4.540154799	10.446276000
C	-2.650524190	5.207961552	10.165982000
C	7.456048555	4.602547201	10.980924000

O	-0.247241336	5.021705598	9.572377000
H	7.121248250	2.853392002	9.751809000
H	8.686016094	1.341719391	10.958583000
H	-1.535197744	2.786899567	9.233106000
H	-2.875130376	5.064110218	9.072224000
H	6.505770800	5.072089845	10.680817000
H	-0.250693197	5.999482830	9.589929000
H	-0.405085512	2.584599385	10.586804000
H	8.943863825	2.556660804	12.213388000
H	7.597494738	4.842511187	12.050516000
H	6.586796126	2.659703753	11.427310000
H	-1.003441673	4.789672172	11.484329000
H	-2.584188373	6.298548593	10.316614000

Phenol hydrogenation on Pt Product 1

Pt	-1.409226651	5.698667995	4.547074000
Pt	7.010746382	5.665599238	4.599088000
Pt	-2.800285197	8.131701968	4.548855000
Pt	0.021082556	8.128374315	4.577376000
Pt	8.437302951	3.244219645	4.559883000
Pt	7.038593929	0.802042453	4.559850000
Pt	-0.002926110	3.240553930	4.554317000
Pt	1.405215737	0.783469103	4.555087000
Pt	1.417264602	5.673544504	4.572303000
Pt	9.844316844	0.795303143	4.565250000
Pt	5.616444360	3.261725195	4.635755000
Pt	4.220555469	5.658180764	4.628399000
Pt	2.818361123	3.226524812	4.570997000
Pt	2.838515202	8.084416854	4.611852000
Pt	5.602501164	8.087769022	4.598673000
Pt	4.232535529	0.863554685	4.626835000
Pt	-4.149029012	7.351093104	6.838979000
Pt	-2.743602880	4.861288519	6.863343000
Pt	7.083823638	2.382118656	6.858422000
Pt	5.756638258	4.865178202	7.015832000
Pt	1.385770118	7.306016508	6.894184000
Pt	-0.045789855	4.857927798	6.853189000
Pt	1.354886969	2.371723169	6.840721000
Pt	-1.393191125	7.322320392	6.881762000

Pt	-1.405193522	2.399893476	6.874701000
Pt	-5.627869181	9.713620844	6.874086000
Pt	2.819133274	9.710804420	6.876851000
Pt	5.626879268	0.021484883	6.891143000
Pt	2.830530607	0.009278875	6.885556000
Pt	2.692246149	4.799099317	6.885204000
Pt	4.214824976	7.240953308	7.042648000
Pt	4.187406212	2.488214466	7.100148000
C	5.377103682	4.236951005	9.086226000
C	5.509230459	5.667399344	9.062687000
C	4.343967580	6.583640842	9.063985000
C	3.101711083	5.875255428	9.586312000
C	2.899502647	4.501640095	8.946658000
C	4.069824050	3.568454220	9.004372000
O	1.959568372	6.742968229	9.456830000
H	6.224982610	3.644434385	9.438344000
H	6.472955635	6.088304345	9.363293000
H	4.547111011	7.517515617	9.606869000
H	1.982714050	4.019953635	9.316847000
H	3.958336704	2.675184441	9.636485000
H	1.148982732	6.217104685	9.612319000
H	3.259982880	5.717932220	10.679420000

Phenol hydrogenation on Pt Product 2

Pt	-1.403882942	5.701089570	4.557451000
Pt	6.992148131	5.675644123	4.628060000
Pt	-2.809471857	8.124752206	4.556896000
Pt	-0.004253913	8.127730263	4.553543000
Pt	8.439714957	3.270043364	4.558073000
Pt	7.025535024	0.825463766	4.552862000
Pt	-0.000313730	3.271320706	4.559298000
Pt	1.414282627	0.824303419	4.552986000
Pt	1.446033770	5.672852164	4.626840000
Pt	9.846869121	0.824187817	4.563392000
Pt	5.617234898	3.284524446	4.629413000
Pt	4.217839643	5.668780814	4.660515000
Pt	2.821363160	3.276442495	4.616952000
Pt	2.808927451	8.125123367	4.548715000
Pt	5.631458333	8.125148312	4.550648000

Pt	4.220587163	0.863447508	4.590603000
Pt	-4.192285858	7.360860049	6.872142000
Pt	-2.768956377	4.902114975	6.878332000
Pt	7.090201936	2.413540195	6.835347000
Pt	5.701345700	4.913942682	7.120192000
Pt	1.387699219	7.359159810	6.860614000
Pt	-0.031991044	4.900784040	6.894084000
Pt	1.351561481	2.413823255	6.834176000
Pt	-1.401790137	7.333692467	6.886259000
Pt	-1.403942431	2.453392431	6.875509000
Pt	0.002357148	0.018266700	6.870357000
Pt	8.440695175	0.018343048	6.867464000
Pt	5.625497899	0.010040282	6.866448000
Pt	2.815684328	0.005982365	6.866662000
Pt	2.760510270	4.899006248	7.106383000
Pt	4.221942047	7.383358442	6.824782000
Pt	4.214907783	2.418588582	6.979949000
C	5.451762277	3.846315475	9.088310000
C	5.483306888	5.260988389	9.260099000
C	4.242605251	5.986700118	9.713693000
C	2.963454549	5.300582066	9.319358000
C	2.945129414	3.888771956	9.070468000
C	4.189065908	3.092945163	8.998876000
O	1.874668335	5.955459026	9.819186000
H	6.356186594	3.263854341	9.283642000
H	6.424113514	5.702857296	9.598294000
H	4.230480237	7.038701010	9.375409000
H	2.029329050	3.342773161	9.318393000
H	4.164017932	2.148546765	9.557891000
H	1.053266655	5.586543555	9.417507000
H	4.253491020	6.026562823	10.823922000

Phenol hydrogenation on Pt Product 3

Pt	-1.401010606	5.695052602	4.548936000
Pt	7.021414510	5.667530978	4.578605000
Pt	-2.816568397	8.131672638	4.555148000
Pt	-0.005492699	8.133320622	4.545345000
Pt	8.447938717	3.241223332	4.558334000
Pt	7.042846985	0.787748960	4.558022000

Pt	0.006507420	3.241913284	4.560321000
Pt	1.402817540	0.794397303	4.559724000
Pt	1.429233251	5.662718812	4.596878000
Pt	9.853306392	0.793557497	4.569975000
Pt	5.625914661	3.234154236	4.580926000
Pt	4.222088552	5.660158141	4.641767000
Pt	2.827115046	3.255793052	4.619563000
Pt	2.840297011	8.086597039	4.603883000
Pt	5.596735565	8.078930712	4.621229000
Pt	4.215093355	0.865757953	4.625416000
Pt	-4.175846147	7.304948462	6.864792000
Pt	-2.758621666	4.860895219	6.861864000
Pt	7.091483838	2.380416512	6.845809000
Pt	5.761364297	4.816405939	6.932752000
Pt	1.354958738	7.351371632	6.826943000
Pt	-0.054684054	4.854790591	6.873611000
Pt	1.368596047	2.378659988	6.851011000
Pt	-1.408599976	7.319175479	6.873068000
Pt	9.855853438	2.397445162	6.877386000
Pt	5.634192505	9.701782086	6.887586000
Pt	2.830817339	9.712531815	6.878609000
Pt	5.621205709	0.015321991	6.881496000
Pt	2.822545546	0.009502344	6.884185000
Pt	2.710464216	4.856853936	7.000634000
Pt	4.254678375	7.231487421	7.099291000
Pt	4.258024123	2.495684276	7.091839000
C	5.516327587	4.482697893	8.993640000
C	5.320897670	5.845975388	9.646315000
C	4.084795662	6.576311906	9.129898000
C	2.908707458	5.680495334	9.152553000
C	3.025252917	4.246001947	9.069371000
C	4.332723496	3.566311421	8.998154000
O	1.769940474	6.260637056	9.622663000
H	6.423956192	3.976968752	9.347105000
H	6.224238569	6.458455757	9.517336000
H	3.866706562	7.505212530	9.674165000
H	2.181065485	3.659672389	9.442754000
H	4.414281673	2.662326300	9.621897000
H	0.985416177	5.712577083	9.383537000

H	5.193216141	5.695210485	10.741468000
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Phenol hydrogenation on Pt Product 4

Pt	-1.403002015	5.709145381	4.549177000
Pt	7.028212899	5.689254135	4.562481000
Pt	-2.807755449	8.147399113	4.553126000
Pt	0.001271079	8.149749829	4.548584000
Pt	8.434291609	3.255195848	4.560717000
Pt	7.035455252	0.813726104	4.564793000
Pt	-0.002425228	3.256131485	4.559568000
Pt	1.402717306	0.806177693	4.555827000
Pt	1.426650756	5.678637799	4.598936000
Pt	9.845111720	0.810329910	4.567690000
Pt	5.612402242	3.270158041	4.627760000
Pt	4.211089488	5.675217204	4.616546000
Pt	2.822870207	3.263602775	4.613915000
Pt	2.843830945	8.101867991	4.614578000
Pt	5.599607901	8.097741744	4.606522000
Pt	4.219314519	0.876699224	4.621171000
Pt	-4.162945589	7.358978887	6.849381000
Pt	-2.775548003	4.891449944	6.861173000
Pt	7.053090269	2.440954902	6.866085000
Pt	5.734800533	4.921988154	6.942308000
Pt	1.361699950	7.370365755	6.839296000
Pt	-0.062524540	4.886480473	6.866859000
Pt	1.348238021	2.394258852	6.839689000
Pt	-1.399633499	7.347319874	6.876998000
Pt	-1.421324652	2.429141539	6.875251000
Pt	-0.011919446	-0.012471086	6.878391000
Pt	8.444857418	0.000006263	6.879904000
Pt	5.620212340	0.046445425	6.888388000
Pt	2.816700888	0.029763099	6.883559000
Pt	2.705155444	4.845564874	6.997070000
Pt	4.245990407	7.238787419	7.083647000
Pt	4.229290165	2.494701601	7.109889000
C	5.258926479	3.918812073	9.649705000
C	5.491095780	5.278717147	8.998468000
C	4.335698215	6.238913871	9.025699000
C	3.027736474	5.580743635	9.163791000

C	2.859965417	4.152453592	9.052759000
C	4.018995175	3.223272013	9.106416000
O	2.051307000	6.367048184	9.691295000
H	6.152699090	3.290333643	9.538379000
H	6.413898825	5.758496938	9.348722000
H	4.444579998	7.129550680	9.661348000
H	1.890817910	3.752418840	9.370977000
H	3.767001952	2.298374914	9.642981000
H	1.179851617	5.922339153	9.613987000
H	5.109012995	4.070486305	10.741969000

Phenol hydrogenation on Pt Product 5

Pt	-1.403523694	5.665887804	4.556683000
Pt	7.008237814	5.652102271	4.606672000
Pt	-2.818336523	8.093594152	4.550918000
Pt	-0.001922312	8.099644712	4.542722000
Pt	8.440970185	3.228533481	4.565497000
Pt	7.030407988	0.794283986	4.555969000
Pt	0.001702810	3.229193455	4.568443000
Pt	1.409002280	0.789535587	4.556566000
Pt	1.430718338	5.649655057	4.605856000
Pt	9.847632418	0.789529887	4.564046000
Pt	5.627874247	3.271190340	4.633146000
Pt	4.218829059	5.653288534	4.647647000
Pt	2.813539976	3.258366342	4.616709000
Pt	2.833504840	8.082510652	4.591059000
Pt	5.604113131	8.080581030	4.595414000
Pt	4.219791115	0.799018711	4.540306000
Pt	-4.160406809	7.300204180	6.841260000
Pt	-2.771296790	4.817965258	6.868763000
Pt	7.068746173	2.347793719	6.873064000
Pt	5.685472377	4.771803275	7.092164000
Pt	1.351691552	7.302298699	6.820856000
Pt	-0.027257009	4.819265627	6.884154000
Pt	1.375625036	2.346512554	6.873738000
Pt	-1.402558769	7.259069155	6.881780000
Pt	-1.402804322	2.376581690	6.884165000
Pt	-5.625599275	9.697920435	6.872012000
Pt	2.816214489	9.701116936	6.869015000

Pt	5.626782864	-0.051366095	6.871792000
Pt	2.813826421	-0.056103626	6.873856000
Pt	2.765938590	4.748360368	7.065135000
Pt	4.203286205	7.258485571	6.996285000
Pt	4.219241833	2.300557374	6.839428000
C	5.481171520	4.419617796	9.222362000
C	5.496284997	5.839201151	9.078642000
C	4.264251405	6.651388376	9.055698000
C	3.014442481	5.909045775	9.240902000
C	2.960051145	4.476451171	9.198131000
C	4.207243489	3.729045677	9.627329000
O	1.960655477	6.659717148	9.632106000
H	6.404874932	3.942691039	9.559189000
H	6.425424606	6.383594195	9.267804000
H	4.304370097	7.602188020	9.599884000
H	2.028597856	4.037068719	9.575108000
H	4.184848204	2.686911872	9.251782000
H	1.134347652	6.129645981	9.587073000
H	4.199084848	3.646272494	10.735832000

Phenol hydrogenation on Pt Product 6

Pt	-1.406459418	5.708554984	4.546252000
Pt	7.015334018	5.680623257	4.599570000
Pt	-2.813442720	8.147516471	4.550115000
Pt	-0.001054621	8.147905599	4.553767000
Pt	8.443171306	3.253933935	4.559097000
Pt	7.038060392	0.809216340	4.556008000
Pt	0.006297207	3.251697184	4.557878000
Pt	1.406058705	0.811859166	4.563821000
Pt	1.413652482	5.685730128	4.560204000
Pt	9.849601546	0.808206516	4.567414000
Pt	5.618109004	3.272022442	4.627263000
Pt	4.229753483	5.678210191	4.612888000
Pt	2.827485909	3.267965406	4.623343000
Pt	2.839355152	8.099231691	4.605012000
Pt	5.598451167	8.101452221	4.614833000
Pt	4.222523104	0.878988657	4.620325000
Pt	-4.160282779	7.370067009	6.851149000
Pt	-2.741596572	4.885167548	6.857881000

Pt	7.094963004	2.392886605	6.843672000
Pt	5.753008830	4.858489847	7.004731000
Pt	1.359836904	7.359300864	6.847113000
Pt	-0.033642316	4.881065953	6.859039000
Pt	1.385331230	2.439304177	6.866046000
Pt	-1.402196744	7.343884204	6.872834000
Pt	-1.386464768	2.425118629	6.875255000
Pt	0.002923992	-0.002653497	6.882554000
Pt	8.456148091	-0.009007717	6.878376000
Pt	5.624223420	0.035554821	6.881134000
Pt	2.822608324	0.040733080	6.886107000
Pt	2.718956941	4.924875770	6.936918000
Pt	4.208237855	7.253390080	7.073712000
Pt	4.195856729	2.498955191	7.103959000
C	5.542391600	4.119190077	9.065996000
C	5.413873372	5.549572019	9.069346000
C	4.113733978	6.236402530	8.999950000
C	2.927233375	5.316417152	9.007846000
C	3.136981640	3.936817764	9.643920000
C	4.368746708	3.219011444	9.105526000
O	1.826642298	5.997955490	9.535222000
H	6.509590863	3.700296346	9.359495000
H	6.267118180	6.143093412	9.406084000
H	4.004130730	7.115502162	9.651385000
H	2.228838545	3.329235747	9.517926000
H	4.580849574	2.284732360	9.643383000
H	1.016554326	5.471709932	9.356445000
H	3.274840011	4.096399474	10.735413000

Pd (111) Slab

Pd	8.388904523	0.000000723	0.000000000
Pd	9.787051560	2.421662342	0.000000000
Pd	1.398147537	2.421662485	0.000000000
Pd	0.000000398	4.843326559	0.000000000
Pd	1.398147435	7.264988178	0.000000000
Pd	4.194443112	7.264988320	0.000000000
Pd	2.796313168	0.000000437	0.000000000
Pd	4.194460705	2.421662922	0.000000000
Pd	6.990757249	2.421662565	0.000000000
Pd	5.592608743	4.843326273	0.000000000
Pd	6.990756280	7.264988758	0.000000000
Pd	-1.398146876	7.264988401	0.000000000
Pd	0.000000000	0.000000000	0.000001000
Pd	2.796295575	4.843325836	0.000001000
Pd	0.000009295	9.686667840	0.000001000
Pd	-2.796295780	4.843325550	0.000001000
Pd	8.388904288	3.228884230	2.283166000
Pd	6.990756250	0.807220879	2.283166000
Pd	9.787052794	0.807220522	2.283166000
Pd	0.000000163	8.072210065	2.283166000
Pd	-1.398147875	5.650546714	2.283166000
Pd	1.398147803	5.650546857	2.283166000
Pd	2.796313433	3.228884810	2.283166000
Pd	1.398164895	0.807220593	2.283166000
Pd	4.194461939	0.807221102	2.283166000
Pd	5.592609008	8.072210645	2.283166000
Pd	4.194460470	5.650546428	2.283166000
Pd	6.990757014	5.650546071	2.283166000
Pd	-0.000000235	3.228883506	2.283166000
Pd	2.796295340	8.072209342	2.283166000
Pd	5.592609476	3.228883587	2.283166000
Pd	-2.796295515	8.072209922	2.283166000
Pd	-0.000028607	1.614478409	4.550964000
Pd	1.398250691	4.036037109	4.550993000
Pd	-1.398181321	4.036004828	4.551035000
Pd	2.796395131	6.457700228	4.550964000
Pd	4.194627744	8.879332069	4.551033000
Pd	1.398072953	8.879359127	4.551080000

Pd	5.592561679	1.614572843	4.551013000
Pd	6.990731551	4.036070012	4.551008000
Pd	4.194417821	4.036082601	4.550949000
Pd	-2.796388118	6.457697571	4.551058000
Pd	-1.398038203	8.879432584	4.551122000
Pd	-4.194664423	8.879351925	4.551067000
Pd	8.388950272	1.614575921	4.551023000
Pd	0.000036932	6.457837795	4.551105000
Pd	2.796343901	1.614601625	4.551046000
Pd	5.592572495	6.457871447	4.551020000
Pd	8.388939503	0.000001312	6.837179000
Pd	-1.398162228	2.421673940	6.837342000
Pd	1.398183734	2.421713178	6.837354000
Pd	0.000066706	4.843259408	6.837376000
Pd	1.398259358	7.264942034	6.837391000
Pd	4.194445423	7.264922323	6.837433000
Pd	2.796264278	0.000051758	6.837216000
Pd	4.194437557	2.421784828	6.837446000
Pd	6.990748679	2.421743723	6.837350000
Pd	5.592557128	4.843294874	6.837403000
Pd	-4.194496972	7.264940002	6.837374000
Pd	-1.398202223	7.264954537	6.837387000
Pd	-0.000023713	0.000022928	6.837437000
Pd	2.796358991	4.843277675	6.837418000
Pd	5.592642917	0.000075594	6.837494000
Pd	-2.796365966	4.843245983	6.837356000

Phenol on Pd Bri30

Pd	9.788061513	0.844477674	4.576738000
Pd	8.385275315	3.247842665	4.590903000
Pd	6.998469365	0.830606385	4.561974000
Pd	7.002008423	5.658314083	4.576604000
Pd	5.596141161	8.091176513	4.540062000
Pd	4.235450403	5.642945073	4.585572000
Pd	1.416846573	5.655500078	4.534874000
Pd	0.017140914	8.078666717	4.531761000
Pd	-1.400751236	5.657489560	4.559012000
Pd	4.200409911	0.816709292	4.539017000
Pd	2.797275608	3.238167346	4.539853000

Pd	1.399162391	0.820786306	4.543746000
Pd	2.813526490	8.079858569	4.537645000
Pd	5.611626896	3.237764723	4.584409000
Pd	-0.017030685	3.233743901	4.575720000
Pd	-2.789838842	8.086217206	4.537843000
Pd	4.213261278	7.281462338	6.834445000
Pd	8.403414514	-0.030721235	6.814631000
Pd	-1.430529981	2.469821347	6.978313000
Pd	6.947476311	2.363425785	6.928733000
Pd	5.632825670	4.854330033	6.983020000
Pd	-4.194556422	7.343793030	6.814174000
Pd	1.396671292	2.445681553	6.829841000
Pd	0.058832964	4.884821550	6.804295000
Pd	1.421631308	7.278029438	6.830816000
Pd	-1.366147172	7.330403512	6.820052000
Pd	2.794143382	0.032670256	6.830655000
Pd	4.158103055	2.428603625	6.814445000
Pd	0.000221737	0.033558059	6.832382000
Pd	-2.758488776	4.956639198	6.914169000
Pd	2.823021902	4.861527191	6.833521000
Pd	5.582101635	-0.016462441	6.819496000
C	6.485985453	2.967368161	9.018455000
C	7.727050455	2.260757800	9.026215000
C	9.002245241	2.952377921	9.001549000
C	-2.227313173	4.402108337	9.064059000
C	7.716969320	5.119040685	9.012247000
C	6.447878032	4.415846134	8.978935000
O	-1.076346476	4.997319100	9.509003000
H	5.578812972	2.439439362	9.318194000
H	7.731639450	1.208438201	9.319786000
H	-1.324342608	2.477133271	9.490834000
H	-3.468506333	6.162432693	9.338653000
H	5.589891785	4.915680362	9.445379000
H	-1.084696610	5.951418218	9.263411000

Phenol on Pd Bri0

Pd	9.784734047	0.795990335	4.539780000
Pd	8.381359353	3.234940019	4.589483000
Pd	6.985916422	0.841998050	4.590914000

Pd	6.985641036	5.629070938	4.584071000
Pd	5.604370092	8.048141441	4.575702000
Pd	4.194938073	5.641089660	4.552588000
Pd	1.390745601	5.656121868	4.529011000
Pd	-0.006811469	8.077569973	4.535867000
Pd	-1.413179088	5.637779891	4.558626000
Pd	4.184192211	0.793505412	4.537673000
Pd	2.787727261	3.220131124	4.536750000
Pd	1.391685366	0.791645720	4.543937000
Pd	2.792070626	8.078883923	4.537302000
Pd	5.588155239	3.232592622	4.583343000
Pd	-0.003617387	3.220690416	4.537818000
Pd	-2.819949578	8.046741884	4.571489000
Pd	4.138551148	7.276410599	6.816152000
Pd	8.378976103	-0.005923803	6.837554000
Pd	-1.367113294	2.363594272	6.815826000
Pd	6.979437864	2.434228816	6.991109000
Pd	5.467874185	4.807163685	6.899503000
Pd	-4.205934327	7.180507925	6.965321000
Pd	1.385497488	2.381717958	6.827036000
Pd	0.035754959	4.823733275	6.813915000
Pd	1.387290465	7.267277354	6.828670000
Pd	-1.364466992	7.273685671	6.810239000
Pd	2.776815797	-0.040537998	6.830740000
Pd	4.138756838	2.358554997	6.811548000
Pd	-0.006244133	-0.039091155	6.838768000
Pd	-2.702994817	4.811651557	6.928039000
Pd	2.732896473	4.824165372	6.809180000
Pd	-0.010005942	9.679184940	6.832993000
C	6.957116691	3.398105384	8.977844000
C	8.187738499	4.165096840	9.014502000
C	-3.000446529	5.595790062	9.003124000
C	6.937567229	6.351034644	8.994560000
C	5.694196457	5.576733335	8.960960000
C	5.714362730	4.145060381	8.985271000
O	-4.202786540	7.514422043	9.750463000
H	6.957553249	2.413429551	9.461570000
H	-2.084209022	3.654838014	9.330797000
H	-2.114006917	6.136976480	9.341837000

H	4.783994567	6.090473416	9.283258000
H	4.801515349	3.622896367	9.284310000
H	-4.952803336	8.092362841	9.489663000

Phenol on Pd H0

Pd	9.782742586	0.814389023	4.540648000
Pd	8.384689414	3.250359855	4.577831000
Pd	6.987730023	0.806469300	4.533989000
Pd	7.002261864	5.639547057	4.567919000
Pd	5.590683214	8.070453072	4.536613000
Pd	4.186745473	5.652059662	4.535171000
Pd	1.371924611	5.636756957	4.580388000
Pd	-0.019501752	8.059593758	4.573931000
Pd	-1.402853865	5.646687700	4.592252000
Pd	4.189674802	0.804637538	4.539749000
Pd	2.790650671	3.227096618	4.540808000
Pd	1.392774086	0.803051437	4.537999000
Pd	2.783294054	8.067510454	4.539268000
Pd	5.586764038	3.227268991	4.538923000
Pd	-0.005518357	3.245037838	4.575465000
Pd	-2.779611171	8.057478054	4.579673000
Pd	4.181968509	7.266033673	6.828995000
Pd	8.384228737	-0.004205975	6.825646000
Pd	-1.407798143	2.368762048	6.815965000
Pd	6.959995133	2.392869019	6.820018000
Pd	5.547637303	4.835171455	6.818453000
Pd	-4.254339622	7.283601493	6.805837000
Pd	1.407550388	2.393818700	6.824462000
Pd	0.029021159	4.809161993	6.978228000
Pd	1.432940275	7.284517143	6.818669000
Pd	-1.382996300	7.291051968	6.972355000
Pd	2.780881540	0.016226074	6.821466000
Pd	4.184177851	2.415640497	6.827961000
Pd	11.174815217	-0.009096452	6.833822000
Pd	-2.861642274	4.826638104	6.955344000
Pd	2.814348386	4.834188222	6.824076000
Pd	5.595292727	0.019665199	6.819812000
C	-0.760889293	4.375674979	9.051159000
C	0.003569342	5.579108131	9.073161000

C	-0.657599240	6.866106532	9.079534000
C	-2.084724814	6.930366549	9.101602000
C	-2.869471270	5.707739861	9.023802000
C	-2.205820020	4.441681568	9.030709000
O	-2.647301901	8.070622430	9.612155000
H	-0.294897123	3.437133113	9.358949000
H	1.050605652	5.546514204	9.383165000
H	-0.100793439	7.744816436	9.411011000
H	7.273307041	5.767419067	9.347237000
H	8.418693393	3.554108465	9.333908000
H	-3.543591901	8.193430621	9.217434000

Phenol on Pd BentC₄

Pd	9.785868350	0.804513005	4.542600000
Pd	8.388074156	3.243044399	4.569544000
Pd	6.992097961	0.805524790	4.543376000
Pd	7.004147102	5.644592384	4.580667000
Pd	5.597991646	8.065017647	4.552303000
Pd	4.196035436	5.648280349	4.548506000
Pd	1.391067845	5.646734012	4.552088000
Pd	-0.004461654	8.066611971	4.549884000
Pd	-1.412389793	5.644950989	4.579741000
Pd	4.194457964	0.805214218	4.547785000
Pd	2.795242857	3.227626518	4.548764000
Pd	1.396803174	0.805314022	4.548538000
Pd	2.796117826	8.068945878	4.546105000
Pd	5.590619225	3.228500371	4.545696000
Pd	0.000165065	3.229793815	4.547581000
Pd	-2.796114548	8.068365366	4.559833000
Pd	4.185468319	7.264225522	6.836453000
Pd	2.795786750	9.678840396	6.835814000
Pd	-1.392286857	2.394856382	6.816568000
Pd	6.980359470	2.398521084	6.819496000
Pd	5.572598272	4.840569120	6.831092000
Pd	-4.210187282	7.276303589	6.857083000
Pd	1.398871755	2.416836866	6.835778000
Pd	0.009626592	4.841685617	6.842413000
Pd	1.407061654	7.265518058	6.834321000
Pd	-1.382238726	7.278870124	6.853341000

Pd	2.794482167	0.003793051	6.834817000
Pd	4.189247567	2.417505502	6.834638000
Pd	-0.001925630	-0.002389289	6.835451000
Pd	-2.802509380	4.829755278	6.976104000
Pd	2.793898138	4.838435354	6.835816000
Pd	5.592842860	-0.000482094	6.832709000
C	-2.781198062	4.661409569	9.290231000
C	-1.498369557	5.235737681	9.498565000
C	-1.365903527	6.554307538	9.935493000
C	-2.518204036	7.307246509	10.223535000
C	-3.799336171	6.760814594	10.024254000
C	7.255982513	5.446976114	9.575496000
O	-2.330289515	8.560481970	10.719926000
H	8.303313924	3.574031363	9.198081000
H	-0.606235347	4.611969464	9.381799000
H	-0.384392026	6.993887299	10.115781000
H	6.498030257	7.347866256	10.272031000
H	6.263058879	4.995427959	9.503205000
H	-3.193124121	8.997156595	10.847582000

Phenol Dissociation on Pd Product

Pd	4.173404520	8.883248366	4.554652000
Pd	1.382705665	8.867024205	4.569507000
Pd	2.780985190	6.462695428	4.557456000
Pd	-1.411433746	8.869508824	4.553150000
Pd	-4.209657632	8.871860926	4.533467000
Pd	-2.767940646	6.464260039	4.594277000
Pd	6.998589064	4.011463624	4.600242000
Pd	4.196792706	4.041396022	4.538551000
Pd	5.592510536	1.612168261	4.567670000
Pd	1.389096729	4.034229981	4.536079000
Pd	-1.406998119	4.027185686	4.541729000
Pd	-0.018075421	1.610310410	4.540605000
Pd	5.600608438	6.451860109	4.535920000
Pd	-0.001195847	6.466476559	4.593005000
Pd	8.359677929	1.597838735	4.606498000
Pd	2.787020630	1.614243247	4.531149000
Pd	-4.189001697	7.262736097	6.835419000
Pd	4.227983865	7.240182608	6.803532000

Pd	2.781647320	9.625980186	6.911909000
Pd	1.418023597	7.170698701	6.931156000
Pd	-1.379044780	7.297956200	7.025593000
Pd	2.729226483	0.008084892	6.803636000
Pd	9.769307562	2.408088836	6.833059000
Pd	6.981653425	2.395320280	7.031465000
Pd	5.595399266	4.879419600	6.853396000
Pd	4.119473691	2.435099604	6.820941000
Pd	1.361192893	2.407625163	6.824136000
Pd	-0.026562550	4.791870186	6.818581000
Pd	5.578205060	9.674138234	6.823048000
Pd	5.507023241	0.011327966	6.832734000
Pd	-2.779426463	4.854508064	6.850949000
Pd	2.782118824	4.809048984	6.814030000
C	0.728298738	7.156256213	9.037023000
C	2.018047090	7.773177852	9.023408000
C	2.177194066	9.208062459	8.950005000
C	6.564206751	0.368263492	9.006691000
C	-0.344409541	9.397326929	8.960531000
C	-0.479431242	7.954872524	9.007394000
O	6.677669491	1.639396687	9.168405000
H	0.648308582	6.114991228	9.358553000
H	2.883195366	7.175332625	9.322882000
H	3.070661676	9.648101729	9.409747000
H	4.399367415	0.319885808	9.284580000
H	-1.381459991	7.533150926	9.470943000
H	5.465120745	3.312986626	7.618094000

Phenoxy Hydrogenation on Pd Reactant

Pd	1.423465166	0.801879946	4.545245000
Pd	4.223323441	0.811888689	4.572709000
Pd	2.817270503	3.215085520	4.552235000
Pd	7.005291315	0.813468349	4.568578000
Pd	9.807968836	0.815406169	4.527080000
Pd	8.360703610	3.217327224	4.600682000
Pd	-1.402159146	5.674458988	4.600972000
Pd	1.400039510	5.633367391	4.521043000
Pd	0.004148213	8.072274699	4.568685000
Pd	4.206814598	5.644896405	4.536675000

Pd	7.000829337	5.652157847	4.541715000
Pd	5.613140842	8.072636825	4.539194000
Pd	-0.007205146	3.232692235	4.536285000
Pd	5.598161225	3.212453498	4.601375000
Pd	-2.767231337	8.082560555	4.593922000
Pd	2.810966836	8.067981119	4.535433000
Pd	9.793981561	2.428351487	6.838019083
Pd	1.367795840	2.447797803	6.801760000
Pd	2.815668175	0.044668291	6.876924000
Pd	4.182276407	2.494647097	6.931560000
Pd	6.976093593	2.396508370	7.066521000
Pd	2.919489485	9.696857924	6.812929084
Pd	7.015838552	7.266638654	6.827391923
Pd	-1.377109753	7.261785767	7.003700000
Pd	0.003434375	4.831218382	6.835126000
Pd	1.452765103	7.171010755	6.799285000
Pd	4.252730109	7.253654359	6.823286000
Pd	5.628268564	4.877500893	6.823696000
Pd	5.630761479	9.693870653	6.816055092
Pd	0.095033618	9.663156794	6.884704000
Pd	8.389577077	4.829027391	6.853438057
Pd	2.810247810	4.854395814	6.807950000
C	4.753053702	2.507462362	9.058899000
C	3.479686110	1.858077033	9.012733000
C	3.353115932	0.420767094	8.930290000
C	-1.019269892	9.285674527	8.990344000
C	5.862657450	0.293602471	9.058641000
C	5.971359107	1.729319225	9.084774000
O	-1.096321326	7.995081564	9.076572000
H	4.802027115	3.551944772	9.375431000
H	2.592209954	2.436441238	9.282383000
H	-3.137479523	9.643663848	9.354837000
H	6.705679330	-0.296802778	9.420584973
H	6.862440108	2.176008767	9.544575000
H	1.647535117	8.732788269	7.499599000

Phenoxy Hydrogenation on Pd Product

Pd	-4.209267724	8.870482267	4.563118000
Pd	-2.800592658	6.475449095	4.540277000

Pd	-1.413894555	8.869690579	4.566785000
Pd	-1.405669947	4.045096147	4.565332000
Pd	-0.006968252	1.615518590	4.538827000
Pd	1.356236290	4.064936032	4.601387000
Pd	4.185867799	4.064139528	4.593567000
Pd	5.566316982	1.617569694	4.535746000
Pd	6.963617330	4.034992804	4.522893000
Pd	1.383528380	8.878163188	4.540848000
Pd	2.783048985	6.463968026	4.546025000
Pd	4.186318607	8.877194220	4.544539000
Pd	2.775016101	1.632136793	4.537202000
Pd	-0.028473870	6.455855638	4.602552000
Pd	5.593657401	6.453740560	4.594288000
Pd	8.375314856	1.615546687	4.533308000
Pd	1.354448073	2.445260792	6.844446000
Pd	2.766219833	0.057445251	6.808588000
Pd	-4.182228505	7.285151610	6.910702000
Pd	-1.378717227	7.319065539	6.941346000
Pd	-0.111862623	4.845372125	7.079740000
Pd	9.761878929	2.401460066	6.806856000
Pd	4.170885817	7.274205888	6.833651000
Pd	5.555650549	4.822892804	6.946710000
Pd	4.145518223	2.429992056	6.832745000
Pd	6.963604999	2.399119491	6.802668000
Pd	8.373042825	0.000395457	6.821928000
Pd	1.406219152	7.281412801	6.826297000
Pd	11.162906831	0.011697619	6.829875000
Pd	8.324512678	4.838850648	6.765422000
Pd	2.741400710	4.858865141	6.854702000
Pd	5.582879687	0.034843183	6.817505000
C	-0.954654116	6.655868404	9.048500000
C	-2.194369264	7.372054781	9.007784000
C	-3.469523829	6.695540324	8.862447000
C	7.710600742	5.210893983	8.900694000
C	-2.220810218	4.526541781	9.454721000
C	-0.911245614	5.208094173	9.064162000
O	6.578875535	4.579116458	8.928914000
H	-0.051636097	7.202293464	9.333389000
H	-2.205403020	8.415827726	9.332272000

H	6.832051107	7.169627338	9.318623000
H	8.944849938	3.455180327	9.194997000
H	-0.027221278	4.783157236	9.559924000
H	-2.305816830	4.570348011	10.564869000

Phenol Hydrogenation on Pd Reactant

Pd	5.602032119	8.087525952	4.542129000
Pd	4.196717488	5.647857698	4.578780000
Pd	6.966676641	5.636471642	4.581959000
Pd	2.809923367	3.238319906	4.607289000
Pd	1.412992301	0.837700411	4.586355000
Pd	4.200532701	0.824061969	4.558483000
Pd	0.000416068	8.069204434	4.529105000
Pd	-1.403931713	5.649868812	4.528696000
Pd	1.422190777	5.646054510	4.562249000
Pd	8.406233886	3.228641974	4.543058000
Pd	6.998869176	0.809500878	4.535749000
Pd	9.801742356	0.815601590	4.553704000
Pd	-2.798913463	8.074595504	4.534722000
Pd	5.588793872	3.230162766	4.579101000
Pd	2.802846752	8.077770720	4.536613000
Pd	0.031812846	3.224669379	4.583603000
Pd	-2.767143469	9.637176704	6.814578000
Pd	7.003580021	7.269044241	6.829406010
Pd	4.220925672	7.320397457	6.810060000
Pd	5.593603091	4.845822534	6.969680000
Pd	4.271770773	2.354097888	6.926216000
Pd	1.478582299	2.475295575	7.038015000
Pd	2.810409907	9.694796505	6.826852022
Pd	1.394029193	7.306689173	6.813387000
Pd	-1.394312621	7.261407526	6.825397000
Pd	-0.026004123	4.887003408	6.797069000
Pd	9.796125932	2.451297555	6.867170904
Pd	7.053337923	2.415409471	6.808958000
Pd	5.622569774	9.680462174	6.860493042
Pd	2.793227038	4.938006972	6.949248000
Pd	0.036767282	9.655480540	6.812073000
Pd	8.397861228	4.851052063	6.831887021
C	4.821368401	2.969354879	9.011136000

C	4.850539796	4.416517177	8.989307000
C	3.581015905	5.114001298	9.049533000
C	2.348191111	4.394174155	9.135360000
C	2.305490849	2.943331173	9.050916000
C	3.584540761	2.255136605	9.030943000
O	1.283591463	5.081203474	9.645894000
H	5.736263131	2.440893035	9.286142000
H	5.719490556	4.917584016	9.433645000
H	3.567288787	6.160299205	9.362982000
H	-0.034831244	1.595980474	7.660557000
H	3.590830385	1.202420580	9.326043000
H	0.446630187	4.649942044	9.357008000
H	1.490061888	2.454082808	9.594866000

Phenol Hydrogenation on Pd Product

Pd	5.587677666	8.065515311	4.540036000
Pd	4.183762451	5.639338916	4.582501000
Pd	6.962781278	5.633376677	4.571948000
Pd	2.810211262	3.236622556	4.613163000
Pd	1.397625104	0.805273647	4.535823000
Pd	4.189375453	0.826939049	4.578984000
Pd	-0.005753752	8.064797993	4.536705000
Pd	-1.406535246	5.647441362	4.537028000
Pd	1.418754550	5.632224792	4.584074000
Pd	8.381035868	3.226527728	4.540597000
Pd	6.985873021	0.801998878	4.539444000
Pd	9.785469122	0.805191523	4.543951000
Pd	-2.801234122	8.068312004	4.539831000
Pd	5.574665598	3.222093878	4.585794000
Pd	2.789491920	8.068577474	4.540665000
Pd	-0.001241398	3.226223748	4.534230000
Pd	-2.810130521	9.654356947	6.822998000
Pd	6.988806006	7.258986783	6.827371000
Pd	4.195820926	7.300370762	6.814127000
Pd	5.575074262	4.836303662	6.937552000
Pd	4.208812188	2.356958421	7.000296000
Pd	1.363717585	2.401372060	6.802186000
Pd	2.795938181	9.684602681	6.827080000
Pd	1.371637267	7.280819220	6.824941000

Pd	-1.412589429	7.250101166	6.833592000
Pd	-0.032129550	4.838469858	6.816381000
Pd	9.782083179	2.418208853	6.828274000
Pd	7.026887613	2.402314192	6.812309000
Pd	5.588498952	9.678739777	6.825060000
Pd	2.765025239	4.876586025	7.022356000
Pd	0.004717601	9.648788866	6.823228000
Pd	8.382390716	4.840244349	6.829390000
C	5.022107059	3.084450427	9.041374000
C	5.028902513	4.537328459	8.991713000
C	3.754639802	5.232466703	9.064323000
C	2.533623229	4.522137999	9.210639000
C	2.539014750	3.046628428	9.521384000
C	3.816887684	2.346483274	9.135888000
O	1.472035648	5.241308369	9.701851000
H	5.975924607	2.576258880	9.208702000
H	5.902086604	5.054659642	9.405714000
H	3.748457145	6.302519998	9.288439000
H	1.649930224	2.542608884	9.072420000
H	3.882237583	1.296286646	9.434603000
H	0.636260955	4.771506163	9.486485000
H	2.399202156	2.949409915	10.620563000

Cyclohexanone on Pd

Pd	-4.196635611	8.883667727	4.548025000
Pd	-2.796697383	6.459247909	4.543228000
Pd	-1.401947449	8.880629573	4.550113000
Pd	-1.399123447	4.023063017	4.566070000
Pd	-0.015450505	1.622804896	4.577663000
Pd	1.399148301	4.035749814	4.548178000
Pd	4.191572545	4.035076439	4.549404000
Pd	5.590094911	1.613416276	4.546575000
Pd	6.986024548	4.036329244	4.543284000
Pd	1.394514945	8.879824476	4.544717000
Pd	2.794360612	6.457654339	4.551017000
Pd	4.194712485	8.877526844	4.546497000
Pd	2.790552184	1.613770078	4.548989000
Pd	-0.003765417	6.457441934	4.545049000
Pd	5.592190283	6.459251436	4.548513000

Pd	8.394054424	1.618380571	4.559976000
Pd	1.408558990	2.422497649	6.837801000
Pd	-2.797251933	9.686293314	6.840593000
Pd	6.988261486	7.266507647	6.835597000
Pd	-1.401184602	7.268172906	6.837677000
Pd	0.005277387	4.856280573	6.822950000
Pd	-1.391243016	2.415710367	6.925823000
Pd	4.192652825	7.260263452	6.837615000
Pd	5.585472807	4.846552469	6.832914000
Pd	4.188852841	2.421729816	6.836097000
Pd	6.969677221	2.421970886	6.819501000
Pd	2.786044883	9.666954987	6.815274000
Pd	1.394193618	7.263389966	6.835209000
Pd	5.599350229	9.672302739	6.833609000
Pd	-2.806784424	4.863484684	6.814453000
Pd	2.795615324	4.843651606	6.839811000
Pd	-0.007473224	9.683731736	6.835119000
C	-1.688182152	5.736680612	11.487491000
C	8.146619244	5.189826175	11.021942000
C	8.158990976	3.645976685	10.937712000
C	9.303358584	3.193761518	10.070732000
C	-0.523164184	3.734564961	10.412664000
C	-0.548509806	5.269283015	10.580542000
O	9.090697981	2.443184573	9.102013000
H	-1.498557891	5.412447472	12.527027000
H	7.337479040	5.505460236	11.698788000
H	8.302447383	3.232674480	11.952226000
H	0.200123020	3.418063143	9.645548000
H	0.425057124	5.605166378	10.966985000
H	-0.230294499	3.272052143	11.374582000
H	-0.661032078	5.726082712	9.578500000
H	-1.717523320	6.838322190	11.504027000
H	7.902637156	5.599258796	10.024687000
H	7.219371431	3.247523918	10.530523000

Cyclohexanone Hydrogenation on Pd Reactant

Pd	-0.005823784	1.612618866	4.547530000
Pd	1.391375107	4.037174249	4.545432000
Pd	-1.404462657	4.036137235	4.546292000

Pd	2.801846790	6.465144779	4.575695000
Pd	4.188993142	8.869772651	4.570082000
Pd	1.392216823	8.883366013	4.546899000
Pd	5.587645065	1.615475018	4.548858000
Pd	6.985729503	4.038900211	4.545190000
Pd	4.191422319	4.035462240	4.547572000
Pd	-2.804236679	6.459299465	4.546998000
Pd	-1.402363992	8.879564098	4.549324000
Pd	-4.199877427	8.881018738	4.547981000
Pd	8.385763127	1.615151623	4.545385000
Pd	-0.006059677	6.456502158	4.543423000
Pd	2.790708374	1.617230606	4.550174000
Pd	5.577207450	6.464592408	4.569198000
Pd	8.370945240	0.026438333	6.829689000
Pd	-1.407889911	2.425983099	6.836617000
Pd	1.384728644	2.417776279	6.837831000
Pd	-0.025058566	4.836423161	6.828012000
Pd	1.339649874	7.291347429	6.846834000
Pd	4.209826739	7.294001542	6.968473000
Pd	2.788477434	0.004204548	6.833917000
Pd	4.186708717	2.416902085	6.838619000
Pd	6.981864241	2.424531423	6.835965000
Pd	5.598023567	4.829183024	6.826721000
Pd	-4.192676870	7.269034511	6.829243000
Pd	-1.416930837	7.267923627	6.835856000
Pd	-0.004510854	0.014058972	6.833573000
Pd	2.782391194	4.794978744	6.850458000
Pd	5.576961661	0.009126862	6.838547000
Pd	-2.804544243	4.845370792	6.835707000
C	1.401651424	5.379221315	11.525549000
C	2.646744177	4.597829225	11.103794000
C	3.903516223	5.494850218	11.114648000
C	3.685115793	6.724285547	10.265692000
C	2.418859455	7.500675234	10.535661000
C	1.173909572	6.590850828	10.619663000
O	4.501268140	7.038848858	9.388600000
H	1.512676985	5.710901216	12.574086000
H	2.814946060	3.733099453	11.764535000
H	4.098473563	5.824216226	12.151662000

H	2.303497895	8.284011132	9.771388000
H	0.313780080	7.185278843	10.964321000
H	2.560937509	8.000571626	11.513160000
H	0.921074856	6.244278267	9.599628000
H	0.517404973	4.723201566	11.496381000
H	2.502684376	4.193112344	10.085209000
H	4.794658491	4.967263904	10.748661000
H	2.706448892	6.417292776	7.544191000

Cyclohexanone Hydrogenation on Pd Product

Pd	-0.009341242	1.610714452	4.545799000
Pd	1.391376583	4.038034804	4.546058000
Pd	-1.406267365	4.035583388	4.545416000
Pd	2.794054785	6.459948629	4.557841000
Pd	4.188720636	8.851610658	4.603439000
Pd	1.394236292	8.885519836	4.542918000
Pd	5.587712196	1.619325292	4.545566000
Pd	6.978150719	4.043705372	4.558266000
Pd	4.189683031	4.042051704	4.559164000
Pd	-2.799913441	6.459319534	4.543349000
Pd	-1.403173986	8.883483148	4.547258000
Pd	-4.199941185	8.884054306	4.546336000
Pd	8.384037356	1.613188500	4.546596000
Pd	-0.004104709	6.459686263	4.544965000
Pd	2.789804760	1.619261501	4.547624000
Pd	5.582726128	6.460151038	4.565025000
Pd	8.373763760	0.028678152	6.837150000
Pd	-1.411383529	2.433805975	6.835492000
Pd	1.383392408	2.426579852	6.833675000
Pd	-0.027153999	4.850051764	6.834156000
Pd	1.357859504	7.292831433	6.812357000
Pd	4.186930370	7.282925868	6.929188000
Pd	2.787743320	0.013493025	6.835460000
Pd	4.187195252	2.421596788	6.831818000
Pd	6.979577595	2.433630836	6.834027000
Pd	5.596589822	4.851715704	6.861302000
Pd	-4.179842922	7.283201562	6.817894000
Pd	-1.413391193	7.278348469	6.830207000
Pd	-0.001744517	0.029984408	6.840178000

Pd	2.750297860	4.829209458	6.834572000
Pd	5.577540770	0.017953908	6.832460000
Pd	-2.800102993	4.851141263	6.835821000
C	1.680792592	5.428463995	11.857694000
C	2.785068439	4.462831876	11.415580000
C	3.919704434	5.186209031	10.678265000
C	3.378363387	5.999312820	9.489580000
C	2.264236496	6.954084429	9.931115000
C	1.138139907	6.228261961	10.669466000
O	4.436403251	6.622779587	8.828978000
H	2.084625838	6.126471669	12.613195000
H	3.197778471	3.925056629	12.284294000
H	4.434754546	5.888677966	11.356682000
H	1.869934804	7.482285857	9.029789000
H	0.378977898	6.954472783	11.000459000
H	2.716240087	7.733067587	10.570477000
H	0.626469242	5.545200398	9.966182000
H	0.864409133	4.874050393	12.347998000
H	2.352665657	3.695164316	10.749415000
H	4.675005979	4.474629688	10.309602000
H	2.880164414	5.216474915	8.793732000

Cyclohexanol on Pd

Pd	5.590678333	8.070192618	4.550959000
Pd	4.192249567	5.647435032	4.554673000
Pd	6.987417105	5.647957180	4.552799000
Pd	2.795068953	3.227625308	4.554126000
Pd	1.396614747	0.805839657	4.551495000
Pd	4.192570264	0.806830625	4.552605000
Pd	-0.001636065	8.070328035	4.551199000
Pd	-1.399840892	5.648808323	4.551190000
Pd	1.397784063	5.648024841	4.553219000
Pd	8.386916355	3.227211030	4.550921000
Pd	6.988814318	0.805627353	4.550974000
Pd	9.785301152	0.805408590	4.550972000
Pd	-2.798028474	8.070582348	4.551287000
Pd	5.589792252	3.227464012	4.553989000
Pd	2.794472562	8.070160198	4.551176000
Pd	-0.001392906	3.227185329	4.551450000

Pd	-2.800248968	9.683072298	6.838613000
Pd	6.986878654	7.261308512	6.837396000
Pd	4.190743048	7.261601621	6.837571000
Pd	5.588151126	4.838671454	6.846937000
Pd	4.189826989	2.417433090	6.846123000
Pd	1.393682776	2.417687291	6.839884000
Pd	2.792753247	9.683140214	6.837209000
Pd	1.394542358	7.261206001	6.838214000
Pd	-1.401988613	7.261234317	6.837474000
Pd	-0.004035810	4.839325642	6.838397000
Pd	9.783330167	2.417942701	6.837328000
Pd	6.987627682	2.417591996	6.837693000
Pd	5.588859466	9.683044205	6.837297000
Pd	2.791631432	4.838335303	6.848298000
Pd	-0.003610777	9.683083691	6.837374000
Pd	8.385217415	4.839418335	6.837465000
C	5.056885285	2.826034087	11.418616000
C	5.022376165	4.277524501	10.928524000
C	3.809897971	5.034190664	11.482537000
C	2.506083762	4.309982250	11.167340000
C	2.543418223	2.870063471	11.681810000
C	3.741840119	2.102467085	11.111021000
O	1.441635142	5.072519154	11.760706000
H	5.227120564	2.816426238	12.510784000
H	5.949788597	4.801889923	11.207335000
H	3.890005279	5.119524587	12.580740000
H	1.598959998	2.354967867	11.432891000
H	3.760168162	1.076378214	11.510985000
H	0.618290673	4.560282728	11.674875000
H	2.610954708	2.904860091	12.784291000
H	4.985985980	4.284400850	9.820246000
H	3.765723151	6.060075603	11.085136000
H	5.904364785	2.287583641	10.964863000
H	3.628172330	2.004080705	10.013570000
H	2.371707206	4.287789229	10.060031000

Phenoxy Hydrogenation on Pd Product (1)

Pd	-4.182420535	8.854988963	4.559545000
Pd	-2.777289500	6.448211349	4.570505000

Pd	-1.392682527	8.856406888	4.565690000
Pd	-1.366569784	4.016333616	4.530923000
Pd	0.023449404	1.593945517	4.531178000
Pd	1.390143712	4.052001409	4.589621000
Pd	4.225765712	4.057288739	4.605469000
Pd	5.590346462	1.607149975	4.535401000
Pd	6.998384110	4.027052633	4.556885000
Pd	1.402098868	8.868290217	4.537904000
Pd	2.807151078	6.453504076	4.543213000
Pd	4.205482339	8.864224778	4.543787000
Pd	2.806393450	1.619371954	4.538204000
Pd	-0.007780487	6.449747628	4.594779000
Pd	5.622058217	6.446426215	4.597440000
Pd	8.393741664	1.599144854	4.532684000
Pd	1.412902267	2.413730426	6.834379000
Pd	2.813341530	0.033948424	6.811481000
Pd	-4.142025987	7.255870414	6.929037000
Pd	-1.357325077	7.290465829	6.949266000
Pd	-0.028939400	4.822941359	6.983984000
Pd	9.824635641	2.340949881	6.792491000
Pd	4.223666734	7.243317118	6.833125000
Pd	5.652137214	4.824916609	6.971325000
Pd	4.202388330	2.415615972	6.832446000
Pd	7.002307373	2.364087969	6.811762000
Pd	2.819429793	9.651831348	6.824604000
Pd	1.445694679	7.257866420	6.821956000
Pd	-5.567419537	9.665656321	6.825151000
Pd	8.433489318	4.724891726	6.795157000
Pd	2.796595128	4.836836677	6.844898000
Pd	5.623594653	0.004209574	6.819343000
C	-1.161178673	6.693343381	9.046493000
C	-2.342642633	7.504141770	9.035648000
C	-3.668376571	6.935239269	8.984580000
C	7.375938029	5.454461160	9.332086000
C	-2.578881306	4.652402466	8.891594000
C	-1.263279323	5.251511906	8.951888000
O	6.155110875	4.877790535	8.944050000
H	-0.221783585	7.125847375	9.396503000
H	-2.241120752	8.562610796	9.294366000

H	6.720021789	7.563312860	9.405058000
H	8.551585263	3.593521932	9.173869000
H	-0.415430174	4.646907713	9.311243000
H	7.361943099	5.399149232	10.453579000

Phenoxy Hydrogenation on Pd Product (2)

Pd	-4.199522955	8.888924700	4.523091000
Pd	-2.790133105	6.459425573	4.576414000
Pd	-1.406965305	8.860326391	4.583650000
Pd	-1.400491750	4.038565047	4.551980000
Pd	0.000372645	1.621051396	4.533469000
Pd	1.367728454	4.063623043	4.587811000
Pd	4.204717897	4.057588855	4.596086000
Pd	5.578076680	1.614750089	4.536260000
Pd	6.986185069	4.047587274	4.560874000
Pd	1.387159234	8.878486012	4.541878000
Pd	2.780948660	6.460146156	4.541036000
Pd	4.190125128	8.877719308	4.540221000
Pd	2.791652043	1.632803088	4.538411000
Pd	-0.027365333	6.459761680	4.606291000
Pd	5.584797658	6.443355035	4.557791000
Pd	8.378769994	1.613957162	4.531798000
Pd	1.387114712	2.437301071	6.832368000
Pd	2.779208472	0.046796234	6.817977000
Pd	-4.229481820	7.326556468	6.764335000
Pd	-1.396653566	7.331434887	7.016645000
Pd	-0.061784947	4.840445204	7.001526000
Pd	9.786196617	2.376905538	6.798125000
Pd	4.179420820	7.267790948	6.817546000
Pd	5.608389238	4.834778893	6.987265000
Pd	4.172073429	2.429847022	6.837837000
Pd	6.968829702	2.387488941	6.802041000
Pd	8.379379429	-0.005041223	6.824042000
Pd	1.420852159	7.274863913	6.823180000
Pd	11.170202356	0.018795837	6.818375000
Pd	8.383822947	4.813611048	6.853827000
Pd	2.774013873	4.851820796	6.843497000
Pd	5.591294998	0.026060929	6.831583000
C	-0.804128210	6.520308921	9.086541000

C	-1.940028800	7.365231383	9.137780000
C	-3.297869634	6.782832106	9.422403000
C	7.710426762	5.318874639	9.054580000
C	-2.269653422	4.498278872	8.947818000
C	-0.935686704	5.076182967	9.015396000
O	6.525816468	4.817799452	9.074159000
H	0.181860275	6.932457047	9.314976000
H	-1.787846927	8.400492088	9.458041000
H	-4.120942956	7.385211291	8.967013000
H	8.800600926	3.431831713	9.165685000
H	-0.139737674	4.470409132	9.465165000
H	-3.495051049	6.856995878	10.513999000

Phenoxy Hydrogenation on Pd Product (3)

Pd	-4.197737671	8.854334904	4.565204000
Pd	-2.796169108	6.451142908	4.588830000
Pd	-1.402239715	8.841037354	4.588820000
Pd	-1.408756128	4.029932724	4.550899000
Pd	0.003102632	1.602349874	4.535981000
Pd	1.392115114	4.029431978	4.543514000
Pd	4.206697975	4.030282451	4.576965000
Pd	5.587110655	1.595181393	4.540669000
Pd	6.986884499	4.032570722	4.573036000
Pd	1.394010512	8.867934774	4.542757000
Pd	2.791977563	6.446718776	4.536859000
Pd	4.193319229	8.866727655	4.540000000
Pd	2.797428471	1.599754156	4.538894000
Pd	-0.016982397	6.450933453	4.571137000
Pd	5.597423707	6.435539993	4.577084000
Pd	8.386209070	1.604518019	4.535056000
Pd	1.397602389	2.396032260	6.829890000
Pd	2.787306902	-0.002704873	6.830531000
Pd	-4.229584237	7.288485077	6.915787000
Pd	-1.380506852	7.251227820	7.008987000
Pd	0.029261437	4.799528166	6.828793000
Pd	-1.393818125	2.378996148	6.810815000
Pd	4.162778421	7.258097467	6.813329000
Pd	5.558274714	4.801651992	6.928189000
Pd	4.182947263	2.382151057	6.831537000

Pd	6.987117261	2.372461922	6.810111000
Pd	8.379775824	-0.019754645	6.827172000
Pd	1.406245666	7.247922725	6.822399000
Pd	-0.016710762	-0.001897888	6.826085000
Pd	-2.782348956	4.804348157	6.868980000
Pd	2.782566978	4.819247210	6.827350000
Pd	5.592315644	-0.019327259	6.836422000
C	-1.629993473	7.237898319	9.163212000
C	-2.922472058	7.900009745	9.577089000
C	-4.149282197	7.194618290	9.043106000
C	7.050748586	5.735026519	9.011888000
C	-2.831166126	5.049436334	8.990030000
C	-1.617252432	5.819776488	9.066881000
O	5.954170547	5.047695676	9.035830000
H	-0.708049015	7.716390936	9.510113000
H	-2.929908259	8.969107839	9.293750000
H	6.074030276	7.608538746	9.368177000
H	8.360576333	4.012342753	9.339305000
H	-0.674539546	5.280309103	9.218485000
H	-2.964413683	7.894860720	10.690776000

Phenoxy Hydrogenation on Pd Product (4)

Pd	-4.203199918	8.874876015	4.551992000
Pd	-2.802136585	6.460422934	4.547967000
Pd	-1.410075840	8.887578787	4.542461000
Pd	-1.396502138	4.042185257	4.554513000
Pd	-0.001344420	1.616419353	4.536062000
Pd	1.361636200	4.068808949	4.599140000
Pd	4.198263367	4.073033281	4.600627000
Pd	5.571663314	1.624953812	4.532221000
Pd	6.977256647	4.048686793	4.551432000
Pd	1.383181620	8.877894582	4.541760000
Pd	2.782351766	6.466026407	4.548437000
Pd	4.187263400	8.877976650	4.541575000
Pd	2.780805521	1.645656361	4.535254000
Pd	-0.031981288	6.457208611	4.616811000
Pd	5.598526276	6.459805697	4.599995000
Pd	8.378166851	1.616000487	4.531255000
Pd	1.369157887	2.447910937	6.843943000

Pd	2.768847000	0.071559637	6.799870000
Pd	-4.168606271	7.296792011	6.898895000
Pd	-1.435552937	7.372477201	6.914617000
Pd	-0.090801129	4.865303702	7.099989000
Pd	9.781570171	2.382470298	6.799472000
Pd	4.167152930	7.278072338	6.830226000
Pd	5.576559093	4.845105464	6.980978000
Pd	4.160231589	2.445390354	6.833020000
Pd	6.957768634	2.387870609	6.792257000
Pd	8.371228962	-0.004916245	6.821183000
Pd	1.373130721	7.280247958	6.837423000
Pd	11.166544372	0.010848024	6.822834000
Pd	8.395412125	4.801076093	6.813022000
Pd	2.737965896	4.869921869	6.854870000
Pd	5.577901025	0.028105888	6.820751000
C	-0.929483416	6.463065340	9.567854000
C	-2.000862570	7.357162204	8.973969000
C	-3.357363052	6.837332483	8.873376000
C	7.626172516	5.375208003	8.911868000
C	-2.371185231	4.511914622	8.932691000
C	-1.027024496	5.029871274	9.086559000
O	6.428270061	4.875560120	9.007733000
H	0.073231991	6.885643343	9.401213000
H	-1.944260206	8.404206346	9.296467000
H	-4.187241603	7.434280666	9.284813000
H	8.628098908	3.453505456	9.145525000
H	-0.315747041	4.332831972	9.549971000
H	-1.070135698	6.455496443	10.674309000

Phenoxy Hydrogenation on Pd Product (5)

Pd	-4.181388723	8.858684113	4.552352000
Pd	-2.774592356	6.445950939	4.585619000
Pd	-1.389353065	8.850827685	4.576764000
Pd	-1.395782067	4.030244457	4.559153000
Pd	0.015883561	1.607423091	4.535768000
Pd	1.411593426	4.033265403	4.538026000
Pd	4.220977542	4.038901386	4.582457000
Pd	5.600167045	1.601753723	4.537169000
Pd	6.996211403	4.036781393	4.572499000

Pd	1.409181601	8.869745871	4.543246000
Pd	2.801649823	6.451495622	4.542838000
Pd	4.208500839	8.868310974	4.538080000
Pd	2.811222032	1.602627305	4.539636000
Pd	-0.011890130	6.461623517	4.594150000
Pd	5.613917089	6.443049368	4.577821000
Pd	8.399449273	1.605628723	4.537348000
Pd	1.425963139	2.406740519	6.828638000
Pd	2.821007898	0.025608964	6.820148000
Pd	-4.155852875	7.270527541	6.875659000
Pd	-1.343701286	7.254988929	7.031096000
Pd	0.049332763	4.803082723	6.824281000
Pd	-1.358587660	2.372959104	6.818361000
Pd	4.207080611	7.260051110	6.817267000
Pd	5.598524341	4.814790390	6.938566000
Pd	4.213798521	2.399069002	6.831124000
Pd	7.013426100	2.368772169	6.808493000
Pd	2.824116934	9.661011713	6.828095000
Pd	1.436378282	7.250053946	6.835518000
Pd	-5.572689194	9.678807007	6.816199000
Pd	-2.740937916	4.764546183	6.896937000
Pd	2.810128393	4.829916980	6.836001000
Pd	5.628486683	-0.008537183	6.824820000
C	-1.310848135	6.882186264	9.184072000
C	-2.497825229	7.648195628	9.068754000
C	-3.805152011	7.031819257	8.965247000
C	7.269646121	5.562146173	8.994631000
C	-2.689061312	4.774363097	9.029072000
C	-1.425443497	5.422733316	9.544318000
O	6.102403490	4.997062665	9.024178000
H	-0.407978513	7.395618294	9.527180000
H	-2.457536034	8.727896531	9.247999000
H	6.516636986	7.580404050	9.357603000
H	8.342330008	3.731687199	9.330310000
H	-0.531528303	4.856783852	9.208941000
H	-1.406005918	5.344268192	10.655863000

Phenoxy Hydrogenation on Pd Product (6)

Pd	-4.209267724	8.870482267	4.563118000
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Pd	-2.800592658	6.475449095	4.540277000
Pd	-1.413894555	8.869690579	4.566785000
Pd	-1.405669947	4.045096147	4.565332000
Pd	-0.006968252	1.615518590	4.538827000
Pd	1.356236290	4.064936032	4.601387000
Pd	4.185867799	4.064139528	4.593567000
Pd	5.566316982	1.617569694	4.535746000
Pd	6.963617330	4.034992804	4.522893000
Pd	1.383528380	8.878163188	4.540848000
Pd	2.783048985	6.463968026	4.546025000
Pd	4.186318607	8.877194220	4.544539000
Pd	2.775016101	1.632136793	4.537202000
Pd	-0.028473870	6.455855638	4.602552000
Pd	5.593657401	6.453740560	4.594288000
Pd	8.375314856	1.615546687	4.533308000
Pd	1.354448073	2.445260792	6.844446000
Pd	2.766219833	0.057445251	6.808588000
Pd	-4.182228505	7.285151610	6.910702000
Pd	-1.378717227	7.319065539	6.941346000
Pd	-0.111862623	4.845372125	7.079740000
Pd	9.761878929	2.401460066	6.806856000
Pd	4.170885817	7.274205888	6.833651000
Pd	5.555650549	4.822892804	6.946710000
Pd	4.145518223	2.429992056	6.832745000
Pd	6.963604999	2.399119491	6.802668000
Pd	8.373042825	0.000395457	6.821928000
Pd	1.406219152	7.281412801	6.826297000
Pd	11.162906831	0.011697619	6.829875000
Pd	8.324512678	4.838850648	6.765422000
Pd	2.741400710	4.858865141	6.854702000
Pd	5.582879687	0.034843183	6.817505000
C	-0.954654116	6.655868404	9.048500000
C	-2.194369264	7.372054781	9.007784000
C	-3.469523829	6.695540324	8.862447000
C	7.710600742	5.210893983	8.900694000
C	-2.220810218	4.526541781	9.454721000
C	-0.911245614	5.208094173	9.064162000
O	6.578875535	4.579116458	8.928914000
H	-0.051636097	7.202293464	9.333389000

H	-2.205403020	8.415827726	9.332272000
H	6.832051107	7.169627338	9.318623000
H	8.944849938	3.455180327	9.194997000
H	-0.027221278	4.783157236	9.559924000
H	-2.305816830	4.570348011	10.564869000