

Electronic Supplementary Information

Approaching complexity of alkyl hydrogenation on Pd by density-functional modelling

Hristiyan A. Aleksandrov,^{1,2*} Sergey M. Kozlov,¹ Georgi N. Vayssilov,²
Konstantin M. Neyman^{1,3}

¹ Departament de Ciència dels Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Martí i Franquès 1, 08028 Barcelona, Spain

² Faculty of Chemistry and Pharmacy, University of Sofia, 1126 Sofia, Bulgaria

³ ICREA (Institució Catalana de Recerca i Estudis Avançats), 08010 Barcelona, Spain

* corresponding author, e-mail: haa@chem.uni-sofia.bg

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Table S1. Activation barriers (ΔE^\ddagger) for ethyl hydrogenation to ethane on Pd(111) slab and Pd₇₉ nanoparticle models. Binding energies of both reactants (ethyl+H), E_b ; binding energies of attacking H atom, $E_b(\text{H})$; binding energies of ethyl species, $E_b(\text{ethyl})$; (full) metal-adsorbates (Pd-(ethyl+H^{att})) interaction energies, E_{int} ; deformation energies of the Pd surface and the ethyl adsorbate, $E_d(\text{Pd})$ and $E_d(\text{C}_2\text{H}_5)$, respectively; energies describing the lateral interaction between ethyl species and attacking H atom, E_{coads} are also shown for the IS and TS structures. H^{fcc} and H^{tss} indicate surface and subsurface H atoms, respectively. All energies are given in kJ/mol.

Table S2. Activation barriers (ΔE^\ddagger) for ethyl hydrogenation to ethane on Pd(111) slab and Pd₇₉ nanoparticle. The energy difference between TS and IS structures in the binding energies of both reactants (ethyl+H), ΔE_b ; (full) metal-adsorbates (Pd-(ethyl+H^{att})) interaction energies, ΔE_{int} ; deformation energies of the Pd surface and the ethyl adsorbate, $\Delta E_d(\text{Pd})$ and $\Delta E_d(\text{ethyl})$, respectively; energies describing the lateral interaction between ethyl species and attacking H atom, ΔE_{coads} . H^{fcc} and H^{tss} indicate surface and subsurface H atoms, respectively. All energies are given in kJ/mol.

Table S3

Relative energies (in kJ/mol) of the IS, TS and FS structures of the reaction: $\text{C}_2\text{H}_5 + 78 \text{H}^{fcc} + 24 \text{H}^{tss} \rightarrow \text{C}_2\text{H}_6 + 77 \text{H}^{fcc} + 24 \text{H}^{tss}$ when ethyl species is located at terrace and edge sites of Pd₇₉ nanoparticle.

Structures of the obtained transition states

Table S1. Activation barriers (ΔE^\ddagger) for ethyl hydrogenation to ethane on Pd(111) slab and Pd₇₉ nanoparticle models. Binding energies of both reactants (ethyl+H), E_b; binding energies of attacking H atom, E_b(H); binding energies of ethyl species, E_b(ethyl); (full) metal-adsorbates (Pd-(ethyl)+H^{att}) interaction energies, E_{int}; deformation energies of the Pd surface and the ethyl adsorbate, E_d(Pd) and E_d(C₂H₅), respectively; energies describing the lateral interaction between ethyl species and attacking H atom, E_{coads} are also shown for the IS and TS structures. H^{fcc} and H^{ss} indicate surface and subsurface H atoms, respectively. All energies are given in kJ/mol.

N ^a	Elementary reaction	ΔE^\ddagger	E _b		E _b (H)		E _b (ethyl)		E _{int}		E _d (Pd)		E _d (ethyl)		E _{coads}	
			IS	TS	IS	TS	IS	TS	IS	TS	IS	TS	IS	TS	IS	TS
(a)	C ₂ H ₅ + H ^{fcc} → C ₂ H ₆	53	-424	-372	-261	-147	-468	-141	15	5	19	23	10	-259		
(b)	C ₂ H ₅ + H ^{fcc} → C ₂ H ₆	50	-425	-375	-262	-148	-468	-148	15	6	20	21	8	-253		
(a)	C ₂ H ₅ + 7 H ^{fcc} → C ₂ H ₆ + 6 H ^{fcc}	47	-390	-343	-250	-122	-444	-151	24	15	18	22	11	-229		
(b)	C ₂ H ₅ + 7 H ^{fcc} → C ₂ H ₆ + 6 H ^{fcc}	41	-394	-353	-253	-124	-446	-135	24	11	18	20	11	-249		
(a)	C ₂ H ₅ + 7 H ^{fcc} + 9 H ^{ss} → C ₂ H ₆ + 6 H ^{fcc} + 9 H ^{ss}	42	-369	-326	-243	-113	-434	-157	36	18	19	22	10	-209		
(a-b)	C ₂ H ₅ + 7 H ^{fcc} + 9 H ^{ss} → C ₂ H ₆ + 6 H ^{fcc} + 9 H ^{ss}	37	-372	-335	-246	-116	-439	-150	38	14	18	20	11	-219		
(c-b)	C ₂ H ₅ + 8 H ^{fcc} + 8 H ^{ss} → C ₂ H ₆ + 7 H ^{fcc} + 8 H ^{ss}	3 ^b	-340	-305	-240	-85	-425	-139	58	34	17	18	10	-218		
(d-b)	C ₂ H ₅ + 8 H ^{fcc} + 8 H ^{ss} → C ₂ H ₆ + 7 H ^{fcc} + 8 H ^{ss}	3 ^b	-356	-320	-242	-101	-422	-138	39	18	18	19	9	-218		
terrace	C ₂ H ₅ + H ^{fcc} → C ₂ H ₆	54	-439	-385	-267	-157	-488	-145	18	9	20	24	12	-274		
terrace	C ₂ H ₅ + 78 H ^{fcc} → C ₂ H ₆ + 77 H ^{fcc}	46	-398	-353	-247	-128	-451	-152	22	13	21	23	8	-237		
terrace	C ₂ H ₅ + 78 H ^{fcc} + 24 H ^{ss} → C ₂ H ₆ + 77 H ^{fcc} + 24 H ^{ss}	16	-354	-339	-231	-119	-420	-202	29	16	22	22	15	-175		
terrace	C ₂ H ₅ + 79 H ^{fcc} + 23 H ^{ss} → C ₂ H ₆ + 78 H ^{fcc} + 23 H ^{ss}	14	-321	-306	-230	-105	-406	-193	28	18	21	22	14	-175		

^a Initial position of attacking H atom or change in the position is shown for the slab models, while the location of ethyl species at the terrace site is indicated for the NP models; ^b barrier for ethyl hydrogenation from the H already located at the surface

Table S2. Activation barriers (ΔE^\ddagger) for ethyl hydrogenation to ethane on Pd(111) slab and Pd₇₉ nanoparticle. The energy difference between TS and IS structures in the binding energies of both reactants (ethyl+H), ΔE_b ; (full) metal-adsorbates (Pd-(ethyl+H^{att})) interaction energies, ΔE_{int} ; deformation energies of the Pd surface and the ethyl adsorbate, $\Delta E_d(\text{Pd})$ and $\Delta E_d(\text{ethyl})$, respectively; energies describing the lateral interaction between ethyl species and attacking H atom, ΔE_{coads} . H^{fcc} and H^{ass} indicate surface and subsurface H atoms, respectively. All energies are given in kJ/mol.

N ^a	Elementary reaction	ΔE^\ddagger	ΔE_b	ΔE_{int}	$\Delta E_d(\text{Pd})$	$\Delta E_d(\text{ethyl})$	ΔE_{coads}
(a)	$\text{C}_2\text{H}_5 + \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6$	53	52	327	-10	4	-269
(b)	$\text{C}_2\text{H}_5 + \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6$	50	50	320	-9	1	-261
(a)	$\text{C}_2\text{H}_5 + 7 \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6 + 6 \text{H}^{fcc}$	47	47	293	-9	4	-241
(b)	$\text{C}_2\text{H}_5 + 7 \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6 + 6 \text{H}^{fcc}$	41	41	311	-13	2	-260
(a)	$\text{C}_2\text{H}_5 + 7 \text{H}^{fcc} + 9 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 6 \text{H}^{fcc} + 9 \text{H}^{ass}$	42	43	277	-18	3	-219
(b)	$\text{C}_2\text{H}_5 + 7 \text{H}^{fcc} + 9 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 6 \text{H}^{fcc} + 9 \text{H}^{ass}$	37	37	289	-24	2	-230
(c-b)	$\text{C}_2\text{H}_5 + 8 \text{H}^{fcc} + 8 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 7 \text{H}^{fcc} + 8 \text{H}^{ass}$	35 ^b	35	286	-24	1	-228
(d-b)	$\text{C}_2\text{H}_5 + 8 \text{H}^{fcc} + 8 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 7 \text{H}^{fcc} + 8 \text{H}^{ass}$	36 ^b	37	284	-21	1	-227
terrace	$\text{C}_2\text{H}_5 + \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6$	53	58	343	-9	4	-281
terrace	$\text{C}_2\text{H}_5 + 78 \text{H}^{fcc} \rightarrow \text{C}_2\text{H}_6 + 77 \text{H}^{fcc}$	46	47	299	-9	2	-244
terrace	$\text{C}_2\text{H}_5 + 78 \text{H}^{fcc} + 24 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 77 \text{H}^{fcc} + 24 \text{H}^{ass}$	16	16	218	-13	0	-189
terrace	$\text{C}_2\text{H}_5 + 78 \text{H}^{fcc} + 24 \text{H}^{ass} \rightarrow \text{C}_2\text{H}_6 + 78 \text{H}^{fcc} + 23 \text{H}^{ass}$	14	15	213	-10	1	-188

^a Initial position of attacking H atom or change in the position is shown for the slab models, while the location of ethyl species at the terrace site is indicated for the NP models; ^b barrier for ethyl hydrogenation from the H already located at the surface.

Table S3

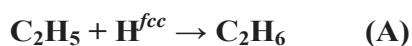
Relative energies (in kJ/mol) of the IS, TS and FS structures of the reaction: $C_2H_5 + 78 H^{fcc} + 24 H^{tss} \rightarrow C_2H_6 + 77 H^{fcc} + 24 H^{tss}$ when ethyl species is located at terrace and edge sites of Pd₇₉ nanoparticle.

site	IS	TS	FS
terrace	0	16	-98
edge	-31	-2	-80

Structures of the obtained transition states

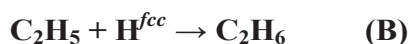
Transition states on Pd(111) slabs

All Pd(111) slabs are hexagonal cells with 8.39×8.39 Å dimensions.



C	4.04325752607290	2.31675051486829	4.49485989575851
C	5.42780313304679	2.33106673626886	3.88771477046444
H	3.38008074607404	1.60048301360661	3.99290862131367
H	3.52992963746283	3.28866734049503	4.49707148333653
H	5.34578855716078	2.58273046548158	2.81485949802561
H	6.08007644553040	3.08470599081664	4.35489061829885
H	5.92567195686870	1.35504971713452	3.96355141349212
H	3.75515606352429	1.25001894366306	5.64269559408264
Pd	0.02890215557717	0.04808766226785	6.85963996606994
Pd	2.83253910135301	0.04336365595836	6.80548885519102
Pd	5.63246665519054	0.03044601963765	6.86430499822081
Pd	9.79098790215931	2.47559189607361	6.87687222209505
Pd	11.20487811412488	4.90147668923974	6.86412555778878
Pd	4.22911616814175	2.47732563063569	6.70455308609573
Pd	5.62475998454773	4.91280147204401	6.85284671823861
Pd	7.03270454105008	2.47173733900461	6.85952879551997
Pd	8.41424492573934	4.89086726023025	6.85317416269771
Pd	1.41103000141396	0.82452645707513	9.14308821173664
Pd	4.20255873317366	0.83201750736633	9.12591365786186
Pd	7.00353867424868	0.82948965262960	9.15018040730723
Pd	2.81697529771538	3.24504488165770	9.12395622447490
Pd	4.20550041316405	5.67080519482376	9.14991865873646
Pd	5.57870452376092	3.24154845292893	9.09168784156523
Pd	6.99739664876287	5.67320361053610	9.13737615157885
Pd	8.39309323610388	3.25195651992226	9.15411650052329
Pd	9.79762795803233	5.66834201823496	9.15194218724539
Pd	2.79590021281160	1.61421374049411	11.41421482187893
Pd	5.59180042562322	1.61421374049411	11.41421482187893
Pd	8.38770063843479	1.61421374049411	11.41421482187893
Pd	4.19385031921741	4.03553435123529	11.41421482187893
Pd	5.59180042562322	6.45685496197637	11.41421482187893
Pd	6.98975053202903	4.03553435123529	11.41421482187893
Pd	8.38770063843485	6.45685496197637	11.41421482187893
Pd	9.78565074484060	4.03553435123529	11.41421482187893
Pd	11.18360085124635	6.45685496197637	11.41421482187893
Pd	0.00000000000000	0.00000000000000	13.69705778625463
Pd	2.79590021281163	0.00000000000000	13.69705778625463
Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
Pd	5.59180042562322	4.84264122148232	13.69705778625463
Pd	6.98975053202900	2.42132061074118	13.69705778625463

Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640584	0.80710687024708	15.97990075063048
Pd	4.19385031921741	0.80710687024708	15.97990075063048
Pd	6.98975053202903	0.80710687024708	15.97990075063048
Pd	2.79590021281160	3.22842748098816	15.97990075063048
Pd	4.19385031921747	5.64974809172934	15.97990075063048
Pd	5.59180042562316	3.22842748098816	15.97990075063048
Pd	6.98975053202897	5.64974809172934	15.97990075063048
Pd	8.38770063843479	3.22842748098816	15.97990075063048
Pd	9.78565074484066	5.64974809172934	15.97990075063048



C	4.24949167341306	2.10836538783027	4.48005983341306
C	5.48907493946611	2.40942253610872	3.66450814562456
H	3.74945654656293	1.17704086593935	4.19254821690746
H	3.51258645585047	2.92569915231079	4.46392382686019
H	6.21933972681199	1.59015580149388	3.69939657610726
H	5.19488897353890	2.55388441962878	2.61022178953809
H	4.95218683042831	1.30496223998856	5.67516594026382
H	5.98946496469902	3.32733130903414	3.99965136195534
Pd	0.01883255464245	0.02838597665321	6.86596626974603
Pd	2.79550420003740	0.01137849798293	6.88005609206291
Pd	5.61159797349819	0.01835328158600	6.81461223160982
Pd	9.78653051686470	2.45032532513796	6.85834662234482
Pd	11.19702500910512	4.88601389062103	6.84969861290727
Pd	4.19997602389667	2.45013612817770	6.68319345095547
Pd	5.61405482676368	4.88201749303992	6.86701429136104
Pd	7.02981650055183	2.45701729249875	6.87430014330707
Pd	8.40405535015127	4.87204538304482	6.86475505647992
Pd	1.40975498828014	0.82405816657663	9.15917635860968
Pd	4.21461709452919	0.82539161385423	9.12345219833894
Pd	7.00602697941508	0.82105395590384	9.14958167603310
Pd	2.83741152265522	3.23441514282228	9.08401734864024
Pd	4.20915130909736	5.66744319428907	9.15406547114307
Pd	5.59949485875249	3.23930451779956	9.11644860691001
Pd	7.00451339396731	5.66200872019254	9.16542630008460
Pd	8.41019729491562	3.24561007458925	9.16204787590915
Pd	9.80695692578752	5.66591959514938	9.14416783021997
Pd	2.81019138897854	1.62431981215211	11.40679501746723
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Pd	8.39793584469211	1.62064034614140	11.43090975127038
Pd	4.20228758732351	4.03561698004007	11.40165458391215
Pd	5.60222314763575	6.46296847470447	11.43006928181006
Pd	6.99901794975132	4.03914559664618	11.43068739272610
Pd	8.40010210472772	6.46084446638760	11.42801348957058
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Pd	11.19054060795263	6.46226691356076	11.42182310085551
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Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
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Pd	8.38770063843479	4.84264122148232	13.69705778625463
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Pd	2.79590021281163	3.22842748098821	15.97990075063048
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Pd	6.98975053202900	5.64974809172940	15.97990075063048
Pd	8.38770063843482	3.22842748098821	15.97990075063048
Pd	9.78565074484063	5.64974809172940	15.97990075063048



C	3.86207643650462	2.05531508467953	4.30958155814122
C	5.25545962055592	1.95630897999585	3.69989270006751
C	3.01837476730687	3.24743764090592	3.91047610230645
C	6.08157465029814	3.23514299996028	3.63904580286813
H	3.32103496352204	1.14096067658657	4.02030458552805
H	5.09561379715004	1.59369562885518	2.66451206772193
H	5.82201295384477	1.15675562517239	4.20556060466228
H	3.49286775973881	1.28905543250316	5.63938863644886
H	1.99988761929192	3.17979053262514	4.32189238127417
H	2.93142807601071	3.26319194336739	2.80663470501460
H	3.45000577090687	4.20886692309822	4.22230041452688
H	7.05509037522970	3.04448963009237	3.16774156416706
H	6.27722169562094	3.63596252926270	4.65523036401403
H	5.57963361229111	4.02562155609219	3.06416438140210
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Pd	11.19778750655227	4.87321233543789	6.86884408198199
Pd	4.22193296342074	2.44538940127045	6.61890900294109
Pd	5.61123746910087	4.87615941168672	6.84672569305841
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Pd	8.40543370258370	4.86395289180360	6.86219548598543
Pd	1.40390809209149	0.81291105345682	9.14781903429189
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Pd	4.20128451879970	5.65710342942531	9.14871512291425
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Pd	6.98896072169332	5.65510851837261	9.14221705835915
Pd	8.38723729354408	3.23793757069185	9.15542906581907
Pd	9.79130963963848	5.65601476430330	9.15365221294606
Pd	2.79590021281163	1.61421374049405	11.41421482187893
Pd	5.59180042562319	1.61421374049405	11.41421482187893
Pd	8.38770063843476	1.61421374049405	11.41421482187893
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Pd	9.78565074484060	4.03553435123529	11.41421482187893
Pd	11.18360085124638	6.45685496197622	11.41421482187893
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Pd	5.59180042562322	4.84264122148232	13.69705778625463
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Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640581	0.80710687024703	15.97990075063048
Pd	4.19385031921738	0.80710687024703	15.97990075063048
Pd	6.98975053202900	0.80710687024703	15.97990075063048
Pd	2.79590021281163	3.22842748098811	15.97990075063048
Pd	4.19385031921744	5.64974809172919	15.97990075063048
Pd	5.59180042562319	3.22842748098811	15.97990075063048
Pd	6.98975053202900	5.64974809172919	15.97990075063048
Pd	8.38770063843482	3.22842748098811	15.97990075063048
Pd	9.78565074484063	5.64974809172919	15.97990075063048



C	3.88257444581220	2.13717749693172	4.32052890900984
C	5.24137965640260	1.82844063012514	3.74116208479409
H	3.11438422359000	1.45813235483104	3.93069966309811
H	3.53181951241432	3.16092566100877	4.16952065492475
H	5.17052284246645	1.89710741028055	2.63939824677022
H	6.01382678646188	2.53522336092976	4.07259397935519
H	5.57809764593979	0.81248519299738	3.98524889687879
H	3.24369507794316	1.37430921817980	5.63154681296998
H	8.37827041378641	1.66620507746989	5.99826794514612
H	4.25775179577076	4.18308947203817	6.00834092256345
H	5.61946105238743	6.45303850586675	5.98659411620065
H	8.42484575323717	6.42392259349989	6.03334672883316
H	9.77198297896356	4.03210155303990	6.00679903316790
H	11.17572425641173	6.49205877845571	5.99670432567590
Pd	0.01667013403533	0.01959329404724	6.77894548364437
Pd	2.82147561756181	0.01951131229820	6.79472976751893
Pd	5.60801962784190	0.03492678641405	6.82841997587849
Pd	1.41644949382527	2.42704848355941	6.81201056731361
Pd	11.19295781103616	4.86421914289734	6.80065645787606
Pd	4.22725691391477	2.42153576445438	6.54642406351620
Pd	5.64471704081038	4.85404825460976	6.82078632409792
Pd	6.99944777602089	2.44465787059822	6.83594481073325
Pd	8.38597231308639	4.83048918558060	6.82216610657408
Pd	1.40367616955705	0.80943936788822	9.12577272465382
Pd	4.19543280944936	0.82408220078756	9.10640322479050
Pd	6.99847482582856	0.81065594150583	9.13332394344997
Pd	2.80861329465381	3.22569193572329	9.09588948800793
Pd	4.20088688325870	5.65576793959743	9.12684805258657
Pd	5.56155436925553	3.21387659992246	9.05901231688761
Pd	6.99542762419023	5.65424130129590	9.13838533513994
Pd	8.38981510615448	3.22949160698258	9.14186081725110
Pd	9.79107551361302	5.65385324224426	9.14256315900966
Pd	2.79968788803518	1.61704975581752	11.41186935789910
Pd	5.58957889171095	1.61908176534220	11.40911711377505
Pd	8.38925601044769	1.61197527449941	11.43064730544507
Pd	4.19434814639555	4.03210266321926	11.40626736744709

Pd	5.59207205631225	6.45809462519832	11.42579321060855
Pd	6.98042286052437	4.02995919156175	11.40576636457038
Pd	8.38672318486489	6.46190000268403	11.42810335890759
Pd	9.78565479437877	4.03417970996980	11.41761118289209
Pd	11.18570244523489	6.45825556141933	11.42047944908311
Pd	0.00000000000000	0.00000000000000	13.69705778625463
Pd	2.79590021281163	0.00000000000000	13.69705778625463
Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
Pd	5.59180042562322	4.84264122148232	13.69705778625463
Pd	6.98975053202900	2.42132061074118	13.69705778625463
Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640581	0.80710687024703	15.97990075063048
Pd	4.19385031921738	0.80710687024703	15.97990075063048
Pd	6.98975053202900	0.80710687024703	15.97990075063048
Pd	2.79590021281163	3.22842748098811	15.97990075063048
Pd	4.19385031921741	5.64974809172914	15.97990075063048
Pd	5.59180042562319	3.22842748098811	15.97990075063048
Pd	6.98975053202897	5.64974809172914	15.97990075063048
Pd	8.38770063843482	3.22842748098811	15.97990075063048
Pd	9.78565074484060	5.64974809172914	15.97990075063048



C	4.49722941131729	1.96356943370794	4.38938635867658
C	5.40696572211201	2.85416394974477	3.57681871279417
H	4.59300756580411	0.90153779001979	4.14737267752106
H	3.43611735114224	2.24437725014804	4.33776927162901
H	5.13851455054728	2.74355514501833	2.51134650036147
H	5.30096611159454	3.91306161946569	3.84109077408972
H	6.46464280407647	2.58009914948157	3.68394192787466
H	5.42574344916115	1.64570527828546	5.68712855517867
H	8.36409622930440	1.65252122787238	5.98135636063629
H	4.20025389607298	4.15173870874515	6.01238963225097
H	5.61976043801000	6.45214287679222	6.00194298544100
H	8.35410342772265	6.42393457174212	6.03488438344568
H	9.74820389894564	4.01200695339640	5.98747546674844
H	11.16919300543621	6.47754232027612	5.97612322328677
Pd	8.38780921701967	0.00821889753111	6.77422285908156
Pd	2.79062465189813	0.01423395607360	6.83760243638105
Pd	5.58321221785305	0.01335379510365	6.80109018376371
Pd	1.39132981431498	2.41245287273006	6.79798630261797
Pd	11.16117764885087	4.85503796437002	6.78251648210559
Pd	4.18168966713230	2.40733240541831	6.59481180440909
Pd	5.61100083411978	4.84451475067859	6.82942868048993
Pd	6.97155889914793	2.43197584081366	6.81200076782980
Pd	8.35821125108502	4.82088097584469	6.81022133293345
Pd	1.39597731190296	0.80647205732026	9.12804231771015
Pd	4.19973187365341	0.81482467550374	9.11259242831198
Pd	6.99291876547170	0.80318637771133	9.12601657397842
Pd	2.82808167221940	3.20869800183874	9.04953324253614
Pd	4.19159686597377	5.64978274915230	9.12395840867023
Pd	5.58694507888740	3.21770973975963	9.10394998777566
Pd	6.99361773687698	5.64577134226059	9.14443157426521

Pd	8.39062831310780	3.22184131937632	9.12739366661596
Pd	9.78753431688932	5.64516530218238	9.12827437544327
Pd	2.79919881525971	1.61598125674483	11.40626545843342
Pd	5.59067698102881	1.61370112156909	11.41558369130549
Pd	8.38989180533866	1.60975709738403	11.42650185530513
Pd	4.19354413699282	4.02859211105195	11.40541526114041
Pd	5.59177991196710	6.45439934056861	11.42732070213079
Pd	6.99283302327465	4.03109252419637	11.41554059845297
Pd	8.39131100776011	6.45775701203187	11.42804840311261
Pd	9.79572255876518	4.02763722454183	11.40016371400530
Pd	11.18579295588929	6.45362828077305	11.41549268216811
Pd	0.00000000000000	0.00000000000000	13.69705778625463
Pd	2.79590021281163	0.00000000000000	13.69705778625463
Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
Pd	5.59180042562322	4.84264122148232	13.69705778625463
Pd	6.98975053202900	2.42132061074118	13.69705778625463
Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640581	0.80710687024703	15.97990075063048
Pd	4.19385031921738	0.80710687024703	15.97990075063048
Pd	6.98975053202900	0.80710687024703	15.97990075063048
Pd	2.79590021281157	3.22842748098800	15.97990075063048
Pd	4.19385031921738	5.64974809172909	15.97990075063048
Pd	5.59180042562313	3.22842748098800	15.97990075063048
Pd	6.98975053202894	5.64974809172909	15.97990075063048
Pd	8.38770063843476	3.22842748098800	15.97990075063048
Pd	9.78565074484057	5.64974809172909	15.97990075063048



C	3.89404525953829	2.21271553565291	3.89739551827586
C	5.25773600860493	1.90560589890333	3.32656902681786
H	3.13000696961799	1.53385814172145	3.50095390950129
H	3.54651208225640	3.23704289227451	3.74247660859131
H	5.19452796998332	1.97415452726087	2.22418634874249
H	6.02800804333636	2.61299083912786	3.66119078304934
H	5.59528216284591	0.88960806439455	3.57067805923696
H	3.18977028736897	1.44032805177043	5.23054187543585
H	8.38719388186366	1.69046724506998	5.58698533503597
H	4.26939662291459	4.20554795255643	5.61873753233669
H	5.63183957195166	6.48376289786334	5.56431115047007
H	8.45157229053652	6.44579692056062	5.63834475618993
H	9.78716082730254	4.07824799192477	5.60100587200682
H	11.19405000459130	6.52561257211718	5.58445492368201
H	9.77855947424306	2.45513205943933	8.18070743761408
H	4.18809085990410	2.44123434241308	8.10573070070954
H	7.03993917302942	2.42416746936875	8.17235313181426
H	11.17622650800051	4.87783371687503	8.24266562542207
H	8.38637357845302	0.01450567989718	8.22006587295677
H	5.57921873108397	4.90314276588594	8.21476895368051
H	2.79666527120433	0.02352081641872	8.22923067170198
H	8.41403998583235	4.87291977476375	8.23147742058377
H	9.79409334179515	7.25160337545752	8.20352889691325
Pd	8.42246104550921	0.04921632273207	6.35654143207123

Pd	2.83613383393948	0.04740443850030	6.36642893374418
Pd	5.62125764045940	0.08575911863374	6.40484291096692
Pd	1.44288875920260	2.44493486951606	6.35983557831134
Pd	11.20486384064241	4.90634658748187	6.38467118667286
Pd	4.22904168872648	2.45172118162000	6.13435788700400
Pd	5.67064651024397	4.88202469192674	6.41561799009306
Pd	7.00355215597100	2.48482160489724	6.42286086660357
Pd	8.39585833824269	4.85150113101379	6.42315473594023
Pd	1.40015586525826	0.83478521722014	9.05794959143163
Pd	4.20139329837354	0.83943062404908	9.02808767719768
Pd	6.99144680451248	0.82683764854676	9.06899731925626
Pd	2.80564136578801	3.24480030643482	9.03182565787789
Pd	4.19309897461357	5.67594045646658	9.09671143336197
Pd	5.58684080689636	3.24415895523224	8.96138085191060
Pd	6.99563520161265	5.67369593685292	9.06485558258038
Pd	8.39672184187876	3.25242163866940	9.08337532240029
Pd	9.79305598720003	5.67275643127158	9.11963675166991
Pd	2.80217418455093	1.62613456883608	11.39273012158281
Pd	5.59143735976517	1.63219134002778	11.38670327719474
Pd	8.39047127186468	1.62406390614415	11.40690920583787
Pd	4.20196729586587	4.03775501336956	11.38876225109022
Pd	5.59692396064552	6.47026603832547	11.40812619520153
Pd	6.98010988676963	4.04114177229800	11.39035281424737
Pd	8.38629414951495	6.47689138271476	11.40661712974865
Pd	9.79498318298606	4.03832340606623	11.41282886697445
Pd	11.18804481942561	6.47227165283089	11.42428437307422
Pd	0.00000000000000	0.00000000000000	13.69705778625463
Pd	2.79590021281163	0.00000000000000	13.69705778625463
Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
Pd	5.59180042562322	4.84264122148232	13.69705778625463
Pd	6.98975053202900	2.42132061074118	13.69705778625463
Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640581	0.80710687024703	15.97990075063048
Pd	4.19385031921738	0.80710687024703	15.97990075063048
Pd	6.98975053202900	0.80710687024703	15.97990075063048
Pd	2.79590021281160	3.22842748098806	15.97990075063048
Pd	4.19385031921747	5.64974809172914	15.97990075063048
Pd	5.59180042562316	3.22842748098806	15.97990075063048
Pd	6.98975053202903	5.64974809172914	15.97990075063048
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C	4.17635321900266	2.04521020869354	3.95733450960564
C	5.07026152465501	2.86156181249911	3.05405825949856
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H	3.14645133402378	2.42536616815182	4.00947173815250
H	4.64430645486046	2.83837272626438	2.03530483843412
H	5.13360090077404	3.91213295554705	3.36229367553970
H	6.08911393673298	2.45818148415567	2.99690251383379
H	5.24880879980880	1.57575524401680	5.19380121612219
H	8.35972309177656	1.68792561973618	5.56924858672475

H	4.18620978794672	4.18663568676118	5.62809534218769
H	5.60564626879498	6.49057379163573	5.58968844518616
H	8.33479813004421	6.43794989913039	5.63334822546526
H	9.73126846943800	4.06148399689261	5.59604457842617
H	11.16579949596039	6.51272918298972	5.54409463377138
H	9.75708136781600	2.44244654103111	8.19771301972171
H	4.19447449122829	2.43497357510661	8.11927337825207
H	7.00822667790003	2.42739363039165	8.12983181592853
H	11.17786597533467	4.89131898873777	8.23488165176452
H	8.38143109276448	0.00899923537222	8.20991887992775
H	5.58408337788495	4.87736173357305	8.22039879402363
H	6.99002516721794	7.26108943072620	8.21359941786390
H	8.40501238278032	4.86757856696124	8.22645027262741
H	5.59920864586961	0.00889801953438	8.19279749527508
Pd	8.37506191807346	0.04765094752131	6.34570416410108
Pd	2.77653835140816	0.06503036296471	6.41957658664267
Pd	5.56497397322826	0.06708075306097	6.32677150522894
Pd	9.77405747443345	2.44896715819366	6.39472347648602
Pd	11.14362060761989	4.90063093545411	6.37978368110528
Pd	4.16531251532675	2.44275963446916	6.18700503904077
Pd	5.60802845685218	4.88647598963986	6.41782333066909
Pd	6.94555242843303	2.47140487099725	6.35441975289273
Pd	8.33680872876116	4.84823429756670	6.41939353487343
Pd	1.39640156384778	0.82568975740981	9.05297182758102
Pd	4.19799830879200	0.82932573954712	9.02952344490461
Pd	6.98848207506687	0.82597693585711	9.05945679477669
Pd	2.80466905187804	3.24170821725795	8.99122491470348
Pd	4.19079173384119	5.67161784048414	9.09336770946080
Pd	5.59174709803815	3.23726324023915	9.00604136029967
Pd	6.99129110519064	5.66142459726517	9.08506051137785
Pd	8.37825012116381	3.24503721667381	9.07378898918846
Pd	9.78801488931524	5.67646278050223	9.09362421130269
Pd	2.79814597862675	1.62512521447664	11.38691755553734
Pd	5.58886657364861	1.62390866433676	11.38929837118774
Pd	8.38742920289143	1.61977579755871	11.40321942974406
Pd	4.19292340021766	4.03431310597557	11.38856083217125
Pd	5.59335521013025	6.46710279136388	11.40981607023316
Pd	6.98065539229834	4.03574357037941	11.40217399474376
Pd	8.38555186294815	6.47201916518986	11.40696544465800
Pd	9.79423052185162	4.03528581462056	11.39408962545026
Pd	11.18411929015097	6.46892113894984	11.41896827644021
Pd	0.00000000000000	0.00000000000000	13.69705778625463
Pd	2.79590021281163	0.00000000000000	13.69705778625463
Pd	5.59180042562319	0.00000000000000	13.69705778625463
Pd	1.39795010640581	2.42132061074118	13.69705778625463
Pd	2.79590021281160	4.84264122148232	13.69705778625463
Pd	4.19385031921744	2.42132061074118	13.69705778625463
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Pd	6.98975053202900	2.42132061074118	13.69705778625463
Pd	8.38770063843479	4.84264122148232	13.69705778625463
Pd	1.39795010640584	0.80710687024708	15.97990075063048
Pd	4.19385031921741	0.80710687024708	15.97990075063048
Pd	6.98975053202903	0.80710687024708	15.97990075063048
Pd	2.79590021281163	3.22842748098821	15.97990075063048
Pd	4.19385031921744	5.64974809172940	15.97990075063048
Pd	5.59180042562319	3.22842748098821	15.97990075063048
Pd	6.98975053202900	5.64974809172940	15.97990075063048

Pd	8.38770063843482	3.22842748098821	15.97990075063048
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C	4.65003294142942	2.04981176433938	3.87111158877348
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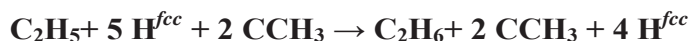
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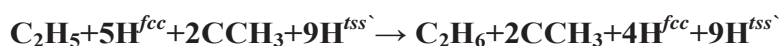
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Pd	8.38770063843482	3.22810463824014	15.98035731922317
Pd	9.78593033486186	5.64990951310338	15.98035731922317



C	4.42175444228375	1.88198635336307	3.90275472147116
C	5.26494290454141	2.74223224040844	2.99042477447232
C	5.61006502706014	6.52682424455213	5.13618859512570
C	9.65130126509032	4.08946903592811	5.12992423326296
C	5.64146228022533	6.56329638641482	3.65071124279855
C	9.57165355642907	4.14530508057130	3.64664610564381
H	4.57451730328569	0.81247188268392	3.73811164723971
H	3.34668273177747	2.09365054327436	3.83439373905581
H	4.99390682336078	2.53784714059542	1.93982494179931
H	5.11349017630362	3.81180586757569	3.17380270962275
H	6.33701103553487	2.53162397945365	3.10281767343051
H	5.47331520191632	1.71789115252087	5.25414943070950
H	8.29481109664474	1.71431667561148	5.49535134343090
H	4.15514068322109	4.15377835745098	5.50445999216166
H	8.34370504255979	6.50474254557223	5.60526948912610
H	11.08851690366528	6.56104437112195	5.49749616284607
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H	4.15292379972079	2.45226356203625	8.04100864685456
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H	11.15485452615612	4.90418552010230	8.27552029619270
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H	5.56876762722422	4.87622074847091	8.26454335652218
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H	8.37586709939280	4.86514847951227	8.33101096679889
H	9.77245677359461	7.24746346090285	8.21992317997980
H	1.58604253687152	0.33102752015982	3.29124553368045
H	4.69817076374273	6.18239749869460	3.22988851875276
H	6.46877362848073	5.94969866646913	3.26192650369290
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Pd	8.36372799652212	0.06271223870536	6.26877909926343
Pd	2.73809775832716	0.07297398210955	6.37711962492873
Pd	5.55260118653352	0.09214866452014	6.37642719280133
Pd	9.73189408273638	2.49366344141021	6.31187137776620
Pd	11.09215207438936	4.89168958652125	6.27535004127335
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Pd	8.32690112400964	4.88250847164395	6.38508040222468
Pd	1.37112002366912	0.82828811130877	9.05776815289283
Pd	4.17537205080409	0.84531200570788	9.00274513041845
Pd	6.96339227408769	0.82810166073022	9.06218055925241
Pd	2.78579952880409	3.24160860980066	8.97348894650098
Pd	4.16784437270596	5.67127069141422	9.08417597212812
Pd	5.56054060099033	3.23907969896817	8.96982217923414
Pd	6.96715429221531	5.65989993273575	9.09804601871875
Pd	8.35189096169289	3.24016370552706	9.10060927526824
Pd	9.76812130641331	5.67545558839236	9.12996561896775
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Pd	5.57415272372686	1.62841370806321	11.37892032529800
Pd	8.37488814156854	1.61976486283338	11.40788291854524
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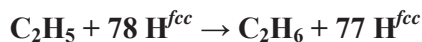
Transition states on terraces of Pd₇₉ nanoparticles



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H	14.18202825975301	5.94156598176562	13.99617659209533
H	13.06002897487531	6.47814579888917	15.28588106527070
H	12.55767240040131	4.09289853862853	13.36019159569754
H	11.39059158856920	4.69049437692430	14.55786553566138
H	12.93123998344354	3.98768524127219	15.09818275827443
H	12.62697324907595	6.37183779589199	12.88214875992997
Pd	13.66414133067191	13.81906374454024	7.12800757386401
Pd	13.70130432273533	15.13505879925074	9.50604715254434
Pd	13.93375743942453	13.80538671812260	11.83113609430067
Pd	13.87424899055154	11.14004862366694	7.01430584170762
Pd	14.05379318197364	12.45221035931197	9.43507175725345
Pd	14.23517464656679	11.06777469396075	11.74663601716844
Pd	13.94674528378076	8.44526465071718	7.04537783668812
Pd	14.02749721543281	12.36976074830294	14.10055278417549
Pd	14.18289317051514	9.76456603261978	9.38983651439553
Pd	14.25551653712128	8.33206228950798	11.73147061719534
Pd	14.20237392125159	9.67503673686697	14.07924437496779
Pd	14.13437633406275	7.05101434688935	9.362605443363028
Pd	11.36809211560364	16.36198658008649	8.85080644368013
Pd	11.33801922711393	15.05436795763054	6.46704519450215
Pd	11.53883815225654	13.65186401400045	8.79967382644715
Pd	11.61778708271301	15.13561722411812	11.24660765465163
Pd	11.55254713669730	12.37154010499863	6.22771413745152
Pd	11.77674901645316	13.73534631209062	13.53939686558082

Pd	11.75183522295010	10.96589054648570	8.69056684981623
Pd	11.79166086558079	12.28373361842097	11.13925816054908
Pd	11.69552080308309	9.67283874910488	6.19696845425687
Pd	11.81322356030941	8.26472804736256	8.71693992796830
Pd	11.88150048108199	10.81738904982744	13.42055304312200
Pd	11.88445870599928	12.20617756805266	15.75875651299370
Pd	11.93903712342875	9.48065264451452	11.10421256900657
Pd	11.78546545755298	6.96931463692750	6.32500814360615
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Pd	12.11333600264028	6.63573813841558	11.11991241730156
Pd	12.20049296144591	7.85346957167069	13.59281793713707
Pd	9.24135655730108	16.29304868096898	10.49383328592862
Pd	9.18171695231017	13.64680269357298	5.68025632601508
Pd	9.14767669841691	15.04188882429799	8.05035344664297
Pd	9.41226199175992	13.57394989288299	10.46464994080650
Pd	9.39356665100972	10.90922481011750	5.52674205681865
Pd	9.48359930946323	14.98249671522554	12.89941902416929
Pd	9.37542070179117	12.23313885631067	8.01076873008733
Pd	9.59332878498247	13.49217904641368	15.19478878722229
Pd	9.56015204377824	10.76739153825379	10.41299845893991
Pd	9.48084202847686	8.15917369552784	5.56899083696595
Pd	9.57657511385579	12.12112091772647	12.85030787361714
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Pd	9.58539821749534	6.64208162295219	7.86272589646768
Pd	9.87401077532787	8.00424065514243	15.13491328945341
Pd	9.82721609562359	5.31762699796385	10.27721397965046
Pd	9.91927170215614	6.56234849476874	12.74541885443333
Pd	7.51973788603226	9.29810176943760	14.53402761453224
Pd	7.45074706560478	6.50937488535921	9.52230996071396
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Pd	7.18083513464055	9.43497224360593	4.99015185101281
Pd	7.29594496684829	14.68792426220473	14.47282977329526
Pd	7.20732894054083	10.74358194881505	7.36331631593010
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Pd	7.01956718596839	14.89557227114616	9.70051549712503
Pd	7.03402396784234	12.14763173318714	5.03824665041183
Pd	6.99043435294270	13.58742008677778	7.33537544489002
Pd	7.12653682298671	16.06965793082481	12.14114110794201
Pd	5.38052234757884	6.53228893792290	11.26835732832839
Pd	5.41586980844088	7.85740164324197	13.63606657095211
Pd	5.05567897438951	9.22086646842665	11.33300562015132
Pd	5.19039550791867	10.54742250810880	13.74349978116640
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Pd	4.89553570935177	11.92152391579380	11.37820893015710
Pd	5.03154663807430	9.29694300264361	6.65171157679076
Pd	4.86886066819898	10.60713094778777	9.01970509435317

Pd	5.12055881824062	13.23588063466720	13.73672064752458
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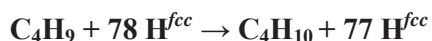


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H	5.35099406748195	16.24110228013093	12.14523578404134
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Pd	13.82876659717211	13.88709282499037	7.02567099009028
Pd	13.87275687533354	15.23735489256105	9.47528095064023
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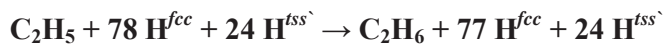


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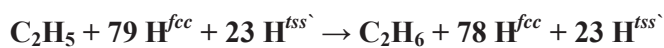


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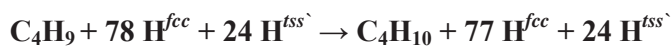


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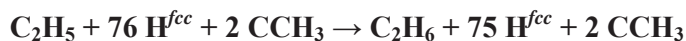
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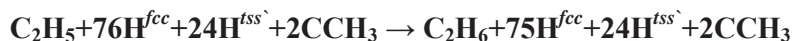


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Pd	7.52046313199658	6.35204197849972	9.66963264191851
Pd	7.79666860672603	4.93303667656986	12.11807934783558
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Pd	7.41188064874539	10.59868284531620	12.22543994576971
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Pd	7.20208690955848	12.03292925893203	9.80700344763895
Pd	7.11897206457700	9.30648512949870	4.92825881859673
Pd	7.30155158266498	14.75488256375257	14.70651140032204
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Pd	7.03199754523872	14.89050887333059	9.82244936961776
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Pd	11.86002318977954	15.45507182753857	11.38194127716943
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Pd	9.71022815672296	13.58374971487237	15.50617853626981
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Pd	9.64511538506500	12.19277573894379	12.99917030266278

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Pd	9.70537578567648	7.90893533547055	10.32507858600424
Pd	9.82764206717000	9.23958048575945	12.92365768657392
Pd	9.56917172529379	6.27327435343307	7.70375398905728
Pd	10.00306300628588	7.81795000953258	15.37425891640856
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Pd	10.07858208074854	6.20702037904885	12.94665726502198
Pd	7.46086410555033	9.12339051420498	14.91310477457895
Pd	7.29811908640927	6.09650335544771	9.45508348747673
Pd	7.70078345458563	4.90984472520331	12.04264337047920
Pd	7.72418456950728	6.33149463808104	14.48330979118030
Pd	7.44485730757831	7.76711936691099	12.13791805582630
Pd	7.19997860947404	9.21187612269895	9.64174253984583
Pd	7.29499150187417	12.00491979920042	14.99722332567288
Pd	7.32337247370044	10.64646171932828	12.20538830722484
Pd	7.12587421142296	7.59038089516919	7.02253850442943
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Pd	4.49045929637384	10.55723455728700	9.02083584120925
Pd	4.96798947771556	13.33699459561525	13.98783131486816
Pd	4.75116688287688	14.81489829314908	11.55436103539203
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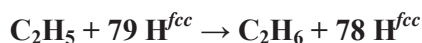
Transition states on edges of Pd₇₉ nanoparticles



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H	15.67455065772268	5.817711030291295	12.39812580868424
H	18.11619655560022	6.53838703316481	11.99285089262929
H	17.52784917920238	7.93719598771016	11.07362718833773
H	17.24569288030786	6.29532601364872	10.46149165611156
H	15.00891972376914	6.88973928301974	10.91506859013367
Pd	13.65138677380926	13.67941359959145	7.12085964416520
Pd	13.69742038997657	15.02462566257934	9.48361039293454

Pd	13.88864589673565	13.70656728197564	11.81831373873829
Pd	13.78621996184182	10.99516330085842	7.02909238787734
Pd	14.00177861431186	12.32150076703954	9.43931906531096
Pd	14.15466177959395	10.94788168626959	11.76002198841998
Pd	13.81397748919906	8.29986959251402	7.03104182755843
Pd	13.97921649908571	12.30112341818680	14.11460925154786
Pd	14.10100356842514	9.61474778267563	9.38928380574642
Pd	14.28635016137555	8.14777840190865	11.77966170167918
Pd	14.13104971872474	9.59208359913706	14.09535926685011
Pd	14.04976826430694	6.89170550085752	9.35355524729168
Pd	11.39498745604113	16.31284502838110	8.81813215264721
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Pd	11.51106358960372	13.58962137985242	8.78729163654881
Pd	11.61099479054887	15.09855118355703	11.22587117255522
Pd	11.50084443882667	12.28199190433027	6.23232507444995
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Pd	11.96420290207744	9.50930387124703	15.72763037448729
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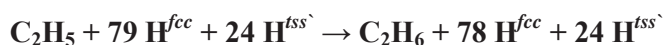


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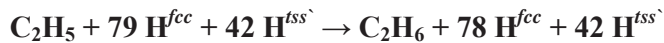


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H	8.73130028105097	10.94485840124910	6.75559367666742
H	10.95097250274555	12.38054630202186	7.64824614125599

H	11.08166281460677	9.62127239951928	7.58638752452139
Pd	13.97757460547949	14.04278857980344	6.93566525335769
Pd	13.98772532469497	15.43921043781870	9.42190894805842
Pd	14.29158821489346	14.02957596974552	11.94439084471520
Pd	14.23504129124037	11.16811870401636	6.73601982641287
Pd	14.45292431416722	12.56956100752271	9.37088524235681
Pd	14.64539083022187	11.05032349511215	11.85458319863517
Pd	14.32634105340616	8.28281975262921	6.78048064576055
Pd	14.43768767807163	12.45234713933524	14.39885228203758
Pd	14.59665723510074	9.70537486966532	9.27530334099148
Pd	14.83618284602498	8.01204891877228	11.82479771733614
Pd	14.59084905589918	9.54653459520978	14.35588616166265
Pd	14.53357532385700	6.77455097748411	9.27757366048280
Pd	11.50024164131656	16.79837448179133	8.74089413595944
Pd	11.48180702831871	15.37566512071671	6.18446117825549
Pd	11.52255594985182	13.86349371010198	8.67647898850709
Pd	11.83357311087699	15.59047169385916	11.37605810301362
Pd	11.77162067977282	12.49238255771690	5.80916145006716
Pd	12.02140920413076	14.07080835240860	13.82012279064540
Pd	11.69344317178393	11.02926524640497	8.61039878010984
Pd	11.70541621905701	12.44586392617650	11.10067589986290
Pd	11.91222082566644	9.61963549425257	5.79826577989594
Pd	11.81024629702519	8.17433117068033	8.59908684655678
Pd	11.85338082102728	10.93924694311422	13.49913862028331
Pd	12.10310614743189	12.28102364342614	16.18936149084436
Pd	12.02259034714696	9.46524885959561	11.09033765570998
Pd	11.99550021966992	6.66477105054041	6.03358782654524
Pd	12.20889760583013	5.14055934247346	8.55227744667995
Pd	12.28502445855639	9.33598076908058	16.13771916763727
Pd	12.18296877046891	6.36136847948883	11.16563079131007
Pd	12.33503981510463	7.74289911784554	13.69104028609493
Pd	9.20455578705370	16.68755935751238	10.46271308844314
Pd	9.15255976527070	13.87697130403287	5.39717159545869
Pd	9.03233039283278	15.52300165184787	7.79843973646148
Pd	9.20232316014499	13.81367470713794	10.40232432018416
Pd	9.49962826059557	10.95168264715793	5.08683184896152
Pd	9.60031218924342	15.37978198539456	13.09509765783741
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Pd	9.61045472436078	13.58597248575080	15.43825510111960
Pd	9.34836763857133	10.90478994817384	10.34161282639520
Pd	9.50538456721063	8.00013640738263	5.36120144978131
Pd	9.37652717694983	12.29835507160637	12.85670527476420
Pd	9.32520025220248	9.50422779660837	7.81496327831384
Pd	9.65452889603496	10.65820458810529	15.74437796312702
Pd	9.52524419768377	8.01668680196281	10.30132724447284
Pd	9.57902409428344	9.37421556538755	12.81939328506406
Pd	9.56475903614131	6.21225466802633	7.69472452235876
Pd	9.92474958288913	7.74470023834322	15.48211788772555
Pd	9.85041925628643	4.82745556128319	10.26651936193239
Pd	10.00018733335334	6.15466005500994	12.96561741608959
Pd	7.32949086575301	9.10003861877184	15.02160861946852
Pd	7.27714936583908	6.01547677866822	9.43540197793501
Pd	7.59018862005760	4.83724893986397	12.08597459452107
Pd	7.60508341171338	6.23198565787862	14.58446488202120
Pd	7.32722307715142	7.84715997336124	12.06092887426981
Pd	7.01801529825333	9.31798043467922	9.57968308895191
Pd	7.20241567401252	11.92465483658653	15.03632019599588

Pd	7.06050467576741	10.72430558470705	12.13645506135944
Pd	7.11121233763037	7.49837118484577	7.02164985319654
Pd	6.89522886449076	12.22124524896199	9.64829269675986
Pd	7.08401694216948	9.39329609764921	4.83795842644686
Pd	7.18818729251029	14.78170945140698	14.58380489698025
Pd	6.90549698634353	10.81687465962217	7.15349085447271
Pd	6.95914543395165	13.57813180906646	12.16281719482343
Pd	6.69837127157405	15.35733414566135	9.53938395211685
Pd	6.91782573543180	12.24142914863833	4.79219396860284
Pd	6.66527824792342	13.97164176479194	7.04503700737286
Pd	6.99920882979701	16.33566778585488	12.19905367956551
Pd	5.07160707761183	6.14236361632043	11.35779506590222
Pd	5.09103637788363	7.56157105753005	13.93331204116073
Pd	4.52971186710205	9.02728351104948	11.44727503182851
Pd	4.86425880802090	10.41867037051826	13.97050448362564
Pd	4.80691828275406	7.62407622670968	8.90549072707255
Pd	4.33222561879919	11.93912703840913	11.45547692007719
Pd	4.79609677868110	9.15156795036282	6.51774522088739
Pd	4.29739800740996	10.56285881795904	8.95738809472869
Pd	4.86624414298089	13.25372598019623	13.92988539860580
Pd	4.61438210556876	14.81072382153115	11.46527106305272
Pd	4.55564267900250	12.07210596462362	6.51636232296501
Pd	4.45000865547833	13.51883575636309	8.94981337249623