

# Revealing the Minimum Energy Pathways for Formamide Hydrogenation Reactions in the Presence of Platinum–Vanadium Clusters: A Quantum Chemical DFT/Nudged Elastic Band Study

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## Nudged Elastic Band Method

In elastic band methods finite number of images of the system are connected together to give a discreet representation of a path on the PES. The images are connected with springs and the object function is defined as

$$S(\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_n) = \sum_{i=0}^{n+1} E(\mathbf{R}_i) + \sum_{i=1}^{n+1} \frac{k}{2} \|\mathbf{R}_i - \mathbf{R}_{i-1}\|^2$$

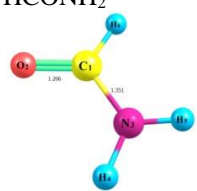
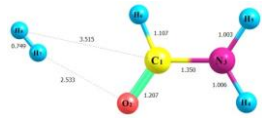
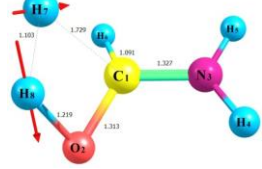
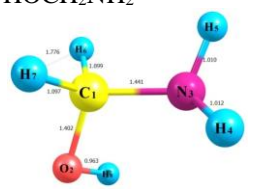
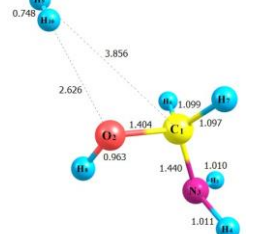
where  $\mathbf{R}_0$  and  $\mathbf{R}_{n+1}$  represent positions of reagents and products. A spring interaction between adjacent images prevents them to move far away from the path and ensures path continuity.  $E(\mathbf{R}_i)$  is the electronic energy of the  $i$ -th image and is a subject to the standard minimization routine in the frameworks of some quantum chemical or MM method. An important feature of the NEB method which distinguishes it from other elastic band methods [61-63] is the use of such a projection of the object function gradient that spring forces act along the path whereas true forces act in the directions perpendicular to the local tangent vectors. Such algorithm ensures that spring forces do not hinder to the convergence of elastic band to MEP. In general, many MEPs may exist between the chosen reagents and products. The minimization technique used in ORCA package will likely converge to the MEP closest to the initial guess. NEB method exists in several versions: NEB, NEB-CI, NEB-TS.

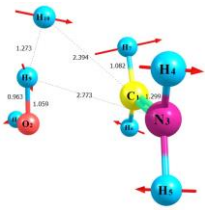
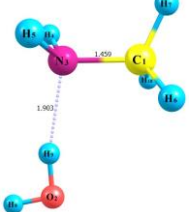
The construction of MEP curves by the NEB method in the case of complex molecular processes involving multi-electron systems is a time-consuming technical task. Often, due to a

small given number of images, some TSs may be missed, and if their number is large, there may be repeated images of TSs, between which false minima appear. In addition, if a conformational rearrangement of the system becomes necessary on the reaction pathway, false TSs with high barriers may appear, corresponding to the breaking of some bonds with the rearrangement and the subsequent formation of former bonds. Such unreliable MEPs often can be improved by increasing the number of images.


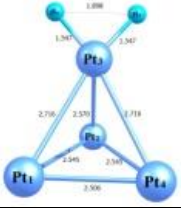
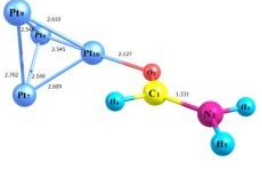

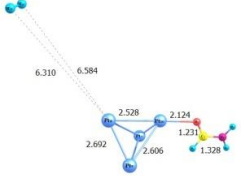
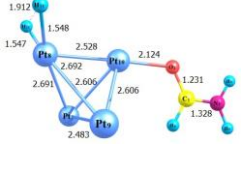
The first obtained MEP curve which connects reagents and products should only be considered as a starting point for further analysis. This MEP should then be thoroughly analysed, with mandatory re-optimisation of all significant critical points. In complex cases, obtaining optimised geometries of all images is rarely achieved. Usually, the NEB method works well when there are only a few critical points between the reagent and the product. In other cases, it is necessary to partition the initial MEP into several sections, each preferably including one or two TSs, and to apply the NEB method to each section, with subsequent refinement of all critical points. All optimised sections of the MEP should be stitched together to produce a final overall MEP.

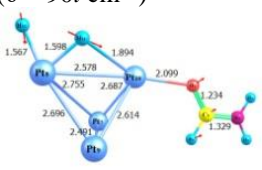
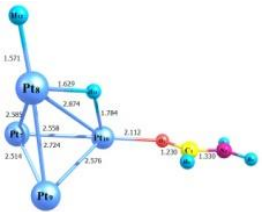
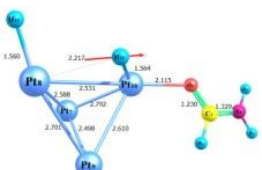
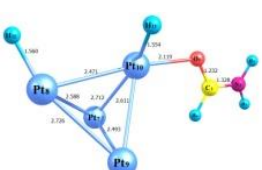
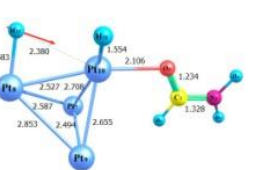
**Table S1.** Cartesian coordinates of compounds and their absolute energy characteristics  $E_{\text{el}}+ZPE$  and  $G^0$  (298.15 K, 1.00 atm.) for critical points (minima and transition states) of MEP curves of reaction (1)

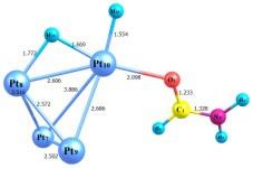
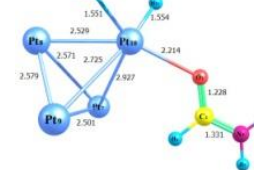
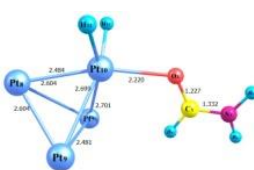
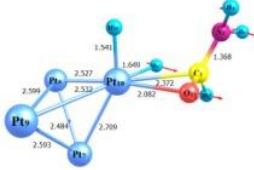
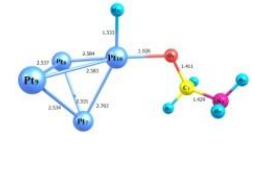
N <sup>o</sup>		x	y	z	$E_{\text{el}}+ZPE$ (Eh)	$G^0$ (Eh)
1	HCONH <sub>2</sub> 	C -1.618563000 O -1.318776000 N -0.740693000 H 0.245234000 H -1.053605000 H -2.668478000	-5.625411000 -4.533655000 -6.564245000 -6.364814000 -7.455742000 -5.967342000	0.438205000 0.022906000 0.854347000 0.826662000 1.191856000 0.518499000	-169.73162324	-169.75611381
2	reagent I {H <sub>2</sub> +HCONH <sub>2</sub> } 	C -1.161411000 O -0.463109000 N -0.772403000 H 0.164952000 H -1.399638000 H -2.210205000 H -2.172119000 H -2.823093000	-5.990544000 -5.304219000 -6.542144000 -6.386666000 -7.105577000 -6.234283000 -4.855423000 -4.878319000	0.258067000 -0.448068000 1.426759000 1.757556000 1.970458000 0.002400000 -2.263384000 -2.632536000	-170.88914588	-170.91697493
3	TS1 ( $\nu = 2267i \text{ cm}^{-1}$ ) 	C -0.164668000 O 0.611030000 N 0.391957000 H 1.353889000 H -0.169756000 H -1.198521000 H -0.753679000 H -0.070252000	0.323779000 1.228648000 -0.648260000 -0.881638000 -1.290091000 0.537180000 -0.070293000 0.800674000	0.103388000 -0.449578000 0.814346000 0.630099000 1.346087000 0.378900000 -1.469990000 -1.353252000	-170.78205729	-170.80707851
4	product I – HOCH <sub>2</sub> NH <sub>2</sub> 	C -1.549525000 O -1.182165000 N -0.604127000 H 0.241679000 H -0.995402000 H -2.538474000 H -1.620415000 H -0.930622000	-5.805373000 -4.464515000 -6.473419000 -6.725203000 -7.304017000 -5.891563000 -6.220027000 -4.135102000	0.169563000 -0.013771000 1.027351000 0.533028000 1.449302000 0.641033000 -0.843500000 0.855563000	-170.88926191	-170.91441307
5	reagent II – {H <sub>2</sub> +HOCH <sub>2</sub> NH}	C -1.292845000 O -1.158481000 N -0.386932000 H 0.556313000 H -0.685766000 H -2.310200000 H -1.124379000 H -1.094939000 H -4.381961000 H -3.642666000	-6.183261000 -4.803927000 -6.613562000 -6.729427000 -7.476485000 -6.439400000 -6.646942000 -4.397805000 -3.976469000 -4.089323000	0.268649000 0.044074000 1.302158000 0.956073000 1.734244000 0.595225000 -0.710826000 0.915463000 -0.404673000 -0.416234000	-172.04755813	-172.07627259
6	TS2 ( $\nu = 542i \text{ cm}^{-1}$ ) 	C 0.487656000 O -1.457586000 N 0.725755000 H 1.341447000	-0.496628000 0.665451000 -1.175279000 -0.767091000	-0.603142000 0.073741000 0.479116000 1.168064000	-171.9376478	-171.96468770

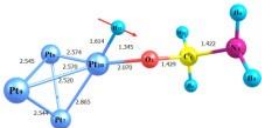
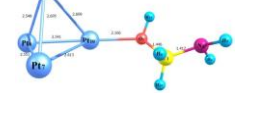
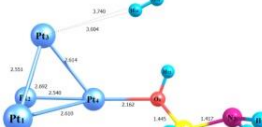
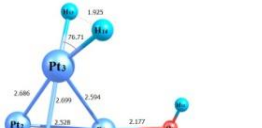
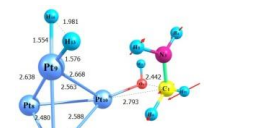
		H 0.079665000 -1.876598000 0.800791000 H -0.267384000 -0.857774000 -1.283867000 H 1.119517000 0.352524000 -0.829270000 H -2.019741000 1.223512000 -0.473762000 H -0.602662000 1.251144000 0.287408000 H 0.593333000 1.680738000 0.380921000		
7	<p>product II – H<sub>2</sub>O···NH<sub>2</sub> CH<sub>3</sub></p> 	C 1.022152000 -0.155398000 -0.685129000 O -2.008310000 1.091072000 0.109328000 N 0.301722000 -0.555932000 0.518684000 H 0.857140000 -0.374814000 1.345260000 H 0.106953000 -1.549162000 0.505241000 H 0.395886000 -0.349034000 -1.557157000 H 1.983086000 -0.664303000 -0.828438000 H -2.583876000 1.141199000 0.873807000 H -1.277085000 0.496331000 0.371105000 H 1.202332000 0.920042000 -0.652699000	-172.07848258	-172.10743269

**Table S2.** Cartesian coordinates of compounds and their energy characteristics (298.15 K, 1.00 atm) for critical points (minima and transition states) of MEP curves of reaction (2)

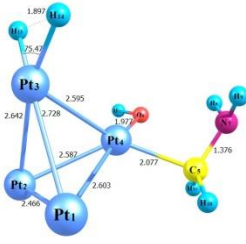
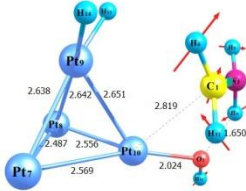
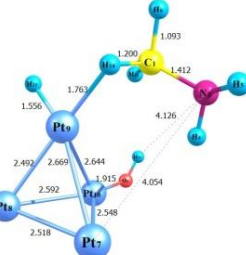
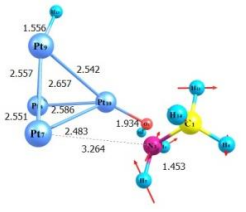
N <sup>o</sup>		x	y	z	$E_{el} + ZPE$ (Eh)	$G^0$ (Eh)
1	Pt4 triplet 	Pt 0.875935000 Pt 0.887334000 Pt -0.886662000 Pt -0.876607000	-0.967007000 0.966706000 0.899704000 -0.899404000	-0.962692000 0.952412000 -0.903515000 0.913796000	-477.34495741	-477.38354486
2	{Pt <sub>3</sub> Pt <sub>(3)</sub> (H) <sub>2</sub> } 	Pt 0.930468000 Pt 0.867866000 Pt -0.797037000 Pt -0.965520000 H -1.780087000 H -0.343962000	-1.115225000 0.996536000 0.910647000 -0.758971000 2.103704000 1.833641000	-0.718875000 0.700521000 -1.254812000 0.881213000 -1.200266000 -2.410737000	-478.55965765	-478.59864777
3	Pt <sub>3</sub> Pt <sub>(10)</sub> —OC(H)NH <sub>2</sub> } 	C -0.869782000 O 0.210563000 N -0.999980000 H -0.192693000 H -1.894866000 H -1.789895000 Pt -0.973069000 Pt 0.646100000 Pt -1.486597000 Pt 0.375782000	-5.651059000 -5.085120000 -6.761596000 -7.166045000 -7.203352000 -5.268756000 -2.946440000 -1.169435000 -1.476580000 -3.304646000	0.442196000 0.290492000 1.164214000 1.610371000 1.271709000 -0.012663000 -3.066157000 -2.219723000 -0.857632000 -0.861467000	-647.10710218	-647.15131812
4		H -2.074516000 H -2.155771000	0.000000000 0.000000000	-0.899512000 -0.158060000	-1.15826981	-1.16976531
5	reagent (a) – {H <sub>2</sub> +Pt <sub>3</sub> Pt <sub>(10)</sub> —OC(H)NH <sub>2</sub> } 	C -1.427809000 O -0.779357000 N -2.476619000 H -2.763878000 H -2.986348000 H -1.168337000 Pt 2.193696000 Pt 2.828467000 Pt 0.679704000 Pt 0.874208000 H 7.007985000 H 7.519981000	-6.412901000 -5.786922000 -7.160495000 -7.229758000 -7.663851000 -6.381422000 -5.517235000 -3.220264000 -3.577706000 -4.607218000 -0.167789000 -0.665676000	0.184245000 1.023303000 0.509522000 1.472611000 -0.193860000 -0.879871000 -1.653434000 -0.402587000 -1.985121000 0.401344000 3.206742000 3.446504000	-648.25931885	-648.30780740
6	min1(a) 	C -1.427809000 O -0.779357000 N -2.476619000 H -2.763878000 H -2.986348000 H -1.168337000 Pt 2.193696000 Pt 2.828467000 Pt 0.679704000 Pt 0.874208000 H 2.799451000	-6.412901000 -5.786922000 -7.160495000 -7.229758000 -7.663851000 -6.381422000 -5.517235000 -3.220264000 -3.577706000 -4.607218000 -1.885534000	0.184245000 1.023303000 0.509522000 1.472611000 -0.193860000 -0.879871000 -1.653434000 -0.402587000 -1.985121000 0.401344000 0.380542000	-648.32281527	-648.36707510

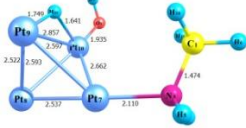
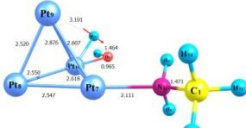
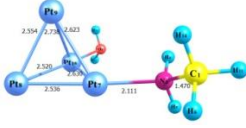
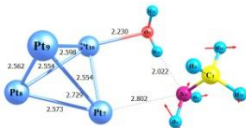
		H	3.964326000	-3.379547000	0.636236000		
7	TS1(a) ( $\nu = 90i \text{ cm}^{-1}$ ) 	C O N H H H Pt Pt Pt Pt H H H	-1.554946000 -0.831906000 -2.582932000 -2.792669000 -3.153584000 -1.382120000 2.428088000 2.715281000 0.650318000 0.832318000 1.809824000 3.862328000	-1.033668000 -0.481722000 -1.797914000 -1.941521000 -2.240789000 -0.918928000 -0.312570000 2.166400000 1.359303000 0.649821000 2.096940000 2.454650000	0.233472000 1.065175000 0.583802000 1.558583000 -0.113527000 -0.842645000 -1.549201000 -0.559818000 -2.068048000 0.434058000 0.794587000 0.463562000	-648.30190879	-648.34556610
8	min2(a) 	C O N H H H Pt Pt Pt Pt H H H	-1.515682000 -0.393341000 -2.585325000 -2.490539000 -3.489444000 -1.697391000 3.470220000 2.033209000 1.281999000 1.314577000 1.425830000 2.645887000	-0.919250000 -1.414700000 -1.472423000 -2.325691000 -1.044403000 0.010097000 0.437383000 2.286060000 0.921373000 -0.495541000 1.028458000 2.988637000	0.304571000 0.388615000 0.868881000 1.395549000 0.783976000 -0.245382000 -1.460248000 -0.364530000 -2.598714000 -0.447431000 0.474193000 0.900520000	-648.31378768	-648.35832012
9	TS2(a) ( $\nu = 665i \text{ cm}^{-1}$ ) 	C O N H H H Pt Pt Pt Pt H H H	-1.605508000 -0.591167000 -2.591425000 -2.517300000 -3.404840000 -1.749314000 2.974423000 2.707404000 0.924517000 1.012624000 1.171076000 3.669510000	-0.959547000 -0.726592000 -1.722391000 -2.137360000 -1.905706000 -0.549301000 -0.105352000 2.183255000 1.193856000 0.448564000 1.888150000 2.392422000	0.250248000 0.906731000 0.711883000 1.626823000 0.152823000 -0.755218000 -1.719259000 -0.539837000 -2.311062000 0.188653000 0.817229000 0.670984000	-648.29908909	-648.34345837
10	min3(a) 	C O N H H H Pt Pt Pt Pt H H H	-1.345890000 -0.681370000 -2.400926000 -2.683312000 -2.927742000 -1.094256000 2.256234000 2.850480000 0.577052000 0.960013000 0.539365000 3.950350000	-0.961070000 -0.321362000 -1.683994000 -1.713512000 -2.197244000 -0.961640000 -0.343306000 1.982889000 1.445923000 0.836506000 1.943183000 1.973625000	0.226680000 1.042804000 0.585076000 1.551681000 -0.098013000 -0.840324000 -1.701567000 -0.736357000 -2.141824000 0.367945000 1.374066000 0.369830000	-648.31336605	-648.35718620
11	TS3(a) ( $\nu = 486i \text{ cm}^{-1}$ ) 	C O N H H H Pt Pt Pt Pt H H H	-1.217064000 -0.538130000 -2.286876000 -2.568013000 -2.827873000 -0.965133000 2.180007000 3.002360000 0.469100000 1.114892000 0.735938000 2.900791000	-0.891615000 -0.264725000 -1.588655000 -1.609032000 -2.089464000 -0.893747000 -0.400189000 1.911781000 1.374568000 0.862839000 1.918180000 1.670061000	0.211851000 1.029512000 0.576454000 1.543665000 -0.104755000 -0.854949000 -1.770486000 -0.948109000 -2.149706000 0.379866000 1.456876000 0.629782000	-648.29644351	-648.34022424

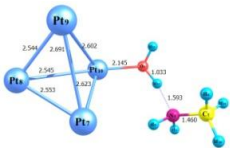
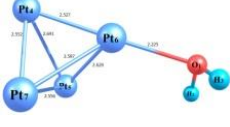
12	min4(a) 	C	-1.267130000	-0.802464000	0.290246000	-648.30275109	-648.34722432
		O	-0.881504000	0.142590000	0.981318000		
		N	-2.345229000	-1.512990000	0.602082000		
		H	-2.869293000	-1.291963000	1.433532000		
		H	-2.643181000	-2.273997000	0.019277000		
		H	-0.738288000	-1.094748000	-0.625107000		
		Pt	2.734060000	-0.208362000	-2.672941000		
		Pt	2.883321000	1.734771000	-1.082371000		
		Pt	0.640870000	1.056924000	-2.144947000		
		Pt	0.938893000	1.079876000	0.524258000		
		H	1.099484000	1.386127000	2.039651000		
		H	2.447996000	1.784235000	0.635002000		
		C	-1.215665000	-0.798692000	0.192301000		
		O	-0.543282000	-0.186791000	1.017515000		
13	TS4(a) ( $\nu = 319i\text{ cm}^{-1}$ ) 	C	-1.215665000	-0.798692000	0.192301000	-648.2958571	-648.34017570
		O	-0.543282000	-0.186791000	1.017515000		
		N	-2.285931000	-1.515828000	0.528363000		
		H	-2.568694000	-1.569859000	1.493624000		
		H	-2.808894000	-2.016014000	-0.167298000		
		H	-0.962322000	-0.786304000	-0.876241000		
		Pt	2.100497000	-0.719193000	-1.686158000		
		Pt	3.047466000	1.620530000	-1.194646000		
		Pt	0.730544000	1.287261000	-2.276057000		
		Pt	1.164571000	1.096880000	0.405530000		
		H	1.680353000	1.059972000	1.869552000		
		H	1.661356000	2.528038000	0.693515000		
		C	-1.188462000	-0.796716000	0.237618000		
		O	-0.582812000	-0.018506000	0.968224000		
14	min5(a) 	N	-2.300489000	-1.422818000	0.620066000	-648.30231564	-648.34648548
		H	-2.671202000	-1.263518000	1.542810000		
		H	-2.774035000	-2.054519000	0.000337000		
		H	-0.842214000	-1.018920000	-0.779342000		
		Pt	2.204481000	-0.575698000	-1.779578000		
		Pt	3.122358000	1.793033000	-1.205466000		
		Pt	0.856200000	1.403908000	-2.427907000		
		Pt	1.248200000	0.981435000	0.209278000		
		H	1.977346000	0.735740000	1.551101000		
		H	0.950628000	2.236579000	1.062858000		
		C	-0.887978000	-0.922758000	0.129368000		
		O	-1.217330000	0.122377000	-0.630170000		
		N	-1.522431000	-1.051904000	1.368272000		
		H	-2.067378000	-0.239849000	1.614677000		
15	TS5(a) ( $\nu = 295i\text{ cm}^{-1}$ ) 	H	-2.003057000	-1.922965000	1.519082000	-648.25186007	-648.29442531
		H	-0.800764000	-1.889238000	-0.388483000		
		Pt	2.365881000	0.439219000	-2.515605000		
		Pt	3.205206000	1.249816000	-0.320650000		
		Pt	1.570050000	2.754361000	-1.662593000		
		Pt	0.722483000	0.748078000	-0.378968000		
		H	0.394530000	-0.803569000	0.396944000		
		H	0.240788000	1.516432000	0.868127000		
		C	-0.509386000	-1.139553000	0.759719000		
		O	-0.306136000	0.225327000	1.053221000		
		N	-1.890155000	-1.499160000	0.672636000		
		H	-2.363653000	-1.278624000	1.540285000		
		H	-2.346804000	-0.974566000	-0.063605000		
		H	-0.013762000	-1.415683000	-0.183214000		
16	min6(a) 	Pt	1.911768000	0.011683000	-2.403223000	-648.26867845	-648.31255245
		Pt	3.146054000	1.800042000	-1.105443000		
		Pt	1.077544000	2.404471000	-2.443281000		
		Pt	0.811014000	1.208629000	-0.168909000		
		H	-0.047596000	-1.725018000	1.564545000		
		H	0.531111000	2.382452000	0.777268000		

17	TS6(a) $(\nu = 1156i \text{ cm}^{-1})$ 	C -0.956244000 -0.874839000 0.318977000 O -0.242011000 0.186620000 0.950771000 N -1.986697000 -1.376880000 1.160412000 H -1.605002000 -1.737506000 2.025370000 H -2.657279000 -0.654515000 1.390057000 H -1.397989000 -0.520989000 -0.618491000 Pt 3.658944000 0.323405000 -1.496418000 Pt 2.914660000 2.718322000 -1.255654000 Pt 1.551156000 1.115099000 -2.684974000 Pt 1.247566000 1.101434000 -0.133342000 H -0.259287000 -1.686287000 0.087455000 H -0.267820000 1.406137000 0.255838000	-648.23647914	-648.28027141
18	product (a) – $\{\text{Pt}_3\text{Pt}_{(10)}\text{—O(H)—CH}_2\text{N H}_2\}$ 	C -0.644233000 -0.841369000 0.561895000 O -0.163660000 0.468694000 0.950644000 N -1.948033000 -1.032015000 1.081710000 H -1.990867000 -1.518800000 1.962839000 H -2.605419000 -1.413633000 0.422130000 H -0.654005000 -0.896392000 -0.527910000 Pt 2.445968000 -0.030809000 -2.250088000 Pt 3.566928000 2.101629000 -1.409834000 Pt 1.272534000 2.386995000 -2.481705000 Pt 1.530953000 1.238418000 -0.156896000 H 0.115081000 -1.522671000 0.949635000 H -0.925248000 1.059952000 0.897579000	-648.26249591	-648.30715334
19	reagent (c) – $\{\text{H}_2+\text{Pt}_3\text{Pt}_{(4)}\text{—O(H)—CH}_2\text{NH}_2\}$ 	C 0.147902000 -1.551725000 -0.216401000 O 0.805770000 -0.313351000 0.131137000 N 0.169511000 -2.422263000 0.900864000 H 0.941983000 -3.068720000 0.925118000 H -0.703585000 -2.888796000 1.081372000 H -0.881327000 -1.332645000 -0.506669000 Pt -1.508336000 2.000452000 -2.584376000 Pt 0.553861000 3.494525000 -2.607946000 Pt -0.812168000 3.490666000 -0.453755000 Pt 0.598334000 1.406860000 -1.161674000 H 0.700306000 -1.903919000 -1.090058000 H 0.527975000 -0.089688000 1.029299000 H -0.265791000 1.768631000 1.945821000 H -0.274437000 1.409975000 2.607265000	-649.4204705	-649.46832874
20	min1(c) 	C 0.118576000 -1.852088000 -0.337539000 O 0.820952000 -0.657643000 0.142466000 N 0.289569000 -2.986159000 0.468567000 H 1.249551000 -3.272892000 0.587088000 H -0.201016000 -2.965137000 1.349478000 H -0.940408000 -1.606253000 -0.429274000 Pt -1.581988000 2.072301000 -1.988341000 Pt 0.459164000 3.491176000 -2.031703000 Pt -0.657819000 3.018202000 0.364716000 Pt 0.624745000 1.202525000 -0.971592000 H 0.543208000 -2.008125000 -1.327795000 H 0.479462000 -0.427000000 1.015018000 H 0.190319000 3.541111000 1.550260000 H -1.394315000 2.449982000 1.608651000	-649.48095798	-649.52581812
21	TS1(c) $(\nu = 228i \text{ cm}^{-1})$ 	C -0.113726000 -1.640293000 -0.420389000 O 2.061859000 -0.655924000 -0.955994000 N -0.309894000 -1.515721000 0.848732000 H 0.265155000 -2.011082000 1.513103000 H -0.826965000 -0.683543000 1.173687000 H -0.751885000 -1.078127000 -1.093606000 Pt -1.442807000 1.857665000 -1.997472000 Pt 0.284962000 3.396310000 -1.104511000 Pt -0.908493000 1.791308000 0.615270000 Pt 0.805854000 0.887250000 -1.161761000	-649.44953169	-649.49369932

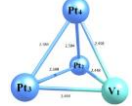

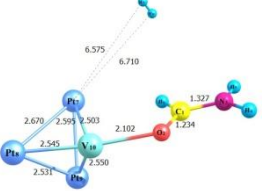
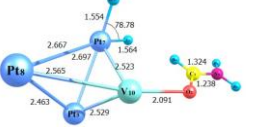
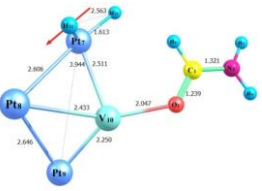



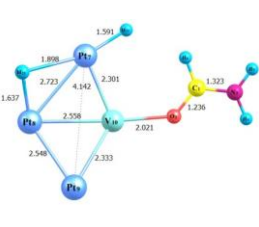
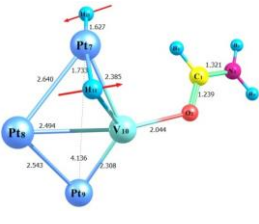
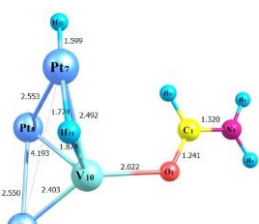
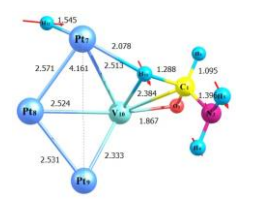
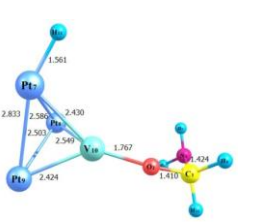
		H	0.536246000	-2.411154000	-0.804928000		
		H	2.455154000	-0.614805000	-0.078422000		
		H	-1.798349000	0.788707000	1.443452000		
		H	-0.257111000	1.889409000	2.022838000		
22	min2(c) 	C	-0.337418000	-1.568191000	-0.765853000	-649.47743304	-649.52176321
		O	2.009905000	-0.556783000	0.160550000		
		N	-0.291403000	-2.154511000	0.478390000		
		H	0.630380000	-2.203441000	0.893481000		
		H	-1.025393000	-1.919124000	1.127990000		
		H	-1.335102000	-1.501248000	-1.189749000		
		Pt	-1.761947000	1.405125000	-1.516214000		
		Pt	0.408888000	2.530082000	-1.835536000		
		Pt	-0.696735000	2.464631000	0.657334000		
		Pt	0.359670000	0.359008000	-0.429790000		
		H	0.408655000	-1.957620000	-1.456818000		
		H	2.769532000	0.029724000	0.128024000		
		H	0.246225000	3.007839000	1.766663000		
		H	-1.385257000	2.064512000	1.981528000		
23	TS2(c) ( $\nu = 174i\text{ cm}^{-1}$ ) 	C	-0.553613000	-1.352975000	0.218434000	-649.45803541	-649.50217880
		O	2.055438000	-0.800957000	-0.628981000		
		N	0.394069000	-1.656173000	1.040409000		
		H	1.347322000	-1.649690000	0.604081000		
		H	0.288741000	-1.427295000	2.017895000		
		H	-1.526345000	-1.052292000	0.580728000		
		Pt	-0.809430000	2.222656000	-2.401045000		
		Pt	0.665230000	3.252533000	-0.683142000		
		Pt	-1.321258000	1.716580000	0.137166000		
		Pt	0.816004000	0.732177000	-1.083467000		
		H	-0.415974000	-1.578806000	-0.830781000		
		H	2.946018000	-0.693932000	-0.968013000		
		H	-1.307805000	1.480065000	1.680164000		
		H	-2.578397000	0.808108000	0.316553000		
24	min3(c) 	C	-1.049004000	-1.061253000	0.741252000	-649.46612059	-649.51103927
		O	3.205175000	0.542602000	0.364223000		
		N	-0.511037000	-1.995852000	-0.170821000		
		H	0.284633000	-1.625591000	-0.674397000		
		H	-1.188769000	-2.352028000	-0.828965000		
		H	-1.863319000	-1.488336000	1.332605000		
		Pt	0.248643000	1.142876000	-2.620789000		
		Pt	0.151224000	3.279363000	-1.291758000		
		Pt	-0.808473000	1.270336000	-0.172921000		
		Pt	1.795575000	1.395427000	-0.611361000		
		H	-0.299421000	-0.681784000	1.429717000		
		H	2.944944000	-0.091879000	1.036596000		
		H	-1.203080000	1.852060000	1.215347000		
		H	-1.707091000	-0.185942000	0.251272000		
25	TS3(c) ( $\nu = 121i\text{ cm}^{-1}$ ) 	C	-1.328318000	-1.924860000	0.679389000	-649.45647562	-649.50163974
		O	2.279502000	-0.070529000	0.589461000		
		N	-0.359002000	-1.405855000	-0.271186000		
		H	0.593747000	-1.509887000	0.062882000		
		H	-0.419476000	-1.886796000	-1.159197000		
		H	-1.231198000	-3.000243000	0.879971000		
		Pt	-0.320290000	1.289611000	-2.111413000		
		Pt	1.366606000	3.157646000	-1.694299000		
		Pt	-0.721466000	3.110915000	-0.218584000		
		Pt	0.986560000	1.240435000	-0.001096000		
		H	-1.222644000	-1.394961000	1.627056000		
		H	3.179320000	0.097776000	0.297847000		
		H	-0.463520000	4.035354000	1.005577000		
		H	-2.339821000	-1.738607000	0.313591000		

26	min4(c) 	C O N H H H Pt Pt Pt Pt H H H H H	-0.858813000 3.329599000 -1.082650000 -0.633625000 -2.074955000 -1.227958000 -0.362209000 0.593344000 -0.789518000 1.806604000 0.206375000 3.330324000 0.750884000 -1.369998000	-1.582496000 1.079035000 -1.387775000 -2.139908000 -1.454211000 -2.556355000 0.446030000 2.632968000 2.682877000 1.496968000 -1.498846000 1.587441000 2.382263000 -0.790697000	0.971550000 1.020226000 -0.472212000 -0.987358000 -0.678062000 1.307256000 -1.226899000 -2.087802000 0.020434000 -0.097513000 1.176612000 1.835783000 0.793442000 1.514923000	-649.4975411	-649.54253109
27	TS4(c) ( $\nu = 1036i \text{ cm}^{-1}$ ) 	C O N H H H Pt Pt Pt Pt H H H H H	-1.811403000 2.450248000 -0.581716000 -0.727700000 0.161651000 -1.633246000 0.164219000 1.176771000 -0.744493000 1.874461000 -2.140511000 3.084045000 1.324546000 -2.596872000	-2.045590000 1.999141000 -1.270210000 -0.583799000 -1.879396000 -2.785489000 -0.141650000 1.353670000 2.261865000 1.739319000 -2.555777000 2.726311000 2.554820000 -1.373213000	0.201777000 1.405053000 0.424889000 1.158262000 0.753356000 -0.577060000 -1.195756000 -2.992396000 -1.638826000 -0.570100000 1.111946000 1.403337000 0.653897000 -0.138384000	-649.45812812	-649.50357401
28	min5(c) 	C O N H H H Pt Pt Pt Pt H H H H H	-1.829550000 2.247143000 -0.561618000 -0.680050000 0.144732000 -1.689293000 0.216345000 1.126206000 -0.863158000 1.667676000 -2.189798000 3.191829000 1.794111000 -2.574574000	-2.146686000 2.510853000 -1.452539000 -0.791833000 -2.116817000 -2.843717000 -0.274576000 1.257447000 2.077606000 1.839129000 -2.694450000 2.695597000 3.351958000 -1.411973000	0.079783000 1.405351000 0.348259000 1.109066000 0.648908000 -0.744956000 -1.220959000 -3.025193000 -1.649580000 -0.633737000 0.956491000 1.419657000 1.526626000 -0.219714000	-649.48344907	-649.52951927
29	TS5(c) ( $\nu = 170i \text{ cm}^{-1}$ ) 	C O N H H H Pt Pt Pt Pt H H H H H	-1.432849000 1.070842000 -0.044271000 0.450350000 -0.026846000 -1.905648000 1.016278000 1.998231000 -0.360507000 1.685014000 -2.025461000 0.284321000 0.746876000 -1.456331000	-1.027618000 1.428591000 -1.286017000 -1.793324000 -1.893614000 -0.432906000 -0.366826000 1.461238000 1.905628000 1.896804000 -1.935605000 1.956281000 0.535493000 -0.448125000	0.901815000 1.164745000 0.522485000 1.247698000 -0.294812000 0.119429000 -1.903763000 -3.424566000 -2.528406000 -0.927211000 1.058085000 1.336577000 0.900864000 1.827062000	-649.44645253	-649.49210026
30	product (c) – {Pt <sub>3</sub> Pt <sub>(4)</sub> –(OH) <sub>2</sub> ...NH <sub>2</sub> CH <sub>3</sub> }	C O N H H H	-1.308491000 1.835294000 -0.080804000 0.208366000 -0.225017000 -1.612052000	-1.297417000 0.332666000 -1.368424000 -2.328874000 -0.951140000 -0.253125000	1.078275000 0.762977000 0.291177000 0.149183000 -0.630126000 1.165431000	-649.46273962	-649.50892580

		Pt -0.774374000 1.213442000 -2.394378000 Pt 1.135168000 2.692555000 -3.222325000 Pt -0.146738000 3.539144000 -1.194273000 Pt 1.433834000 1.480442000 -1.004020000 H -1.125280000 -1.682806000 2.082659000 H 1.700706000 0.873557000 1.545714000 H 1.099483000 -0.391875000 0.729696000 H -2.140093000 -1.858144000 0.640013000		
31	{Pt <sub>3</sub> Pt—OH <sub>2</sub> } 	O -10.365185000 0.781005000 2.355422000 H -9.889195000 1.237084000 3.058152000 H -10.848344000 0.061659000 2.774728000 Pt -6.899294000 -0.987474000 -0.369535000 Pt -6.280598000 0.380818000 1.864057000 Pt -8.743848000 -0.093390000 1.108048000 Pt -7.211006000 -1.997840000 1.952839000	-553.72339995	-553.76496670

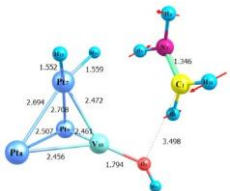
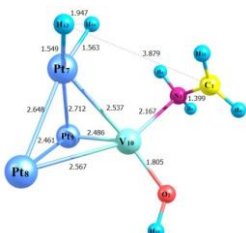
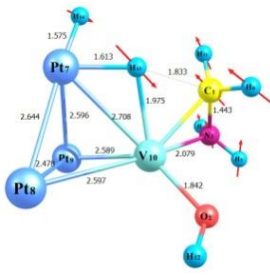
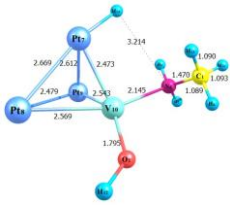
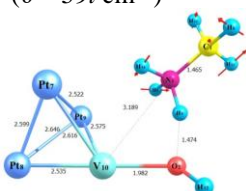
**Table S3.** Cartesian coordinates of compounds and their energy characteristics (298.15 K, 1.00 atm) for critical points (minima and transition states) of MEP curves of reaction (**3a**)

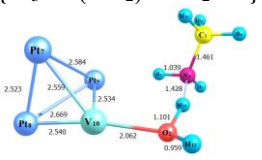
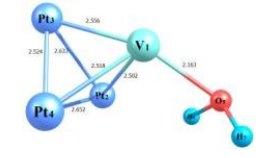
N <sup>o</sup>			x	y	z	$E_{\text{el}} + ZPE$ (Eh)	$G^0$ (Eh)
1	Pt <sub>3</sub> V 	V	-0.173582000	-0.006451000	1.783481000	-1301.81665941	-1301.85443045
		Pt	0.035693000	1.526975000	-0.141413000		
		Pt	-1.333343000	-0.798590000	-0.250454000		
		Pt	1.240465000	-0.751747000	-0.163197000		
2	Pt <sub>3</sub> V+ OC(H)NH <sub>2</sub> 	C	-0.773516000	-5.575095000	0.346531000	-1471.59145088	-1471.63536193
		O	0.296902000	-4.965754000	0.407920000		
		N	-1.001505000	-6.700000000	1.012180000		
		H	-0.284301000	-7.089309000	1.603039000		
		H	-1.886798000	-7.168514000	0.940050000		
		H	-1.598781000	-5.203740000	-0.275164000		
		Pt	-0.813848000	-3.248171000	-2.816827000		
		Pt	0.270922000	-1.039322000	-2.118650000		
		Pt	-1.661199000	-1.866943000	-0.668236000		
		V	0.477685000	-3.176183000	-0.669503000		
3	reagent (a) — {H <sub>2</sub> + Pt <sub>3</sub> V—OC(H)NH <sub>2</sub> } 	C	0.166571000	-0.007808000	1.588742000	-1472.74892612	-1472.79563209
		O	0.773173000	1.018536000	1.907589000		
		N	-0.094795000	-0.984922000	2.446967000		
		H	0.204582000	-0.908419000	3.406011000		
		H	-0.591926000	-1.805838000	2.151177000		
		H	-0.183514000	-0.152887000	0.556854000		
		Pt	0.662135000	1.536421000	-1.807475000		
		Pt	1.486850000	4.059968000	-1.520642000		
		Pt	-0.863414000	3.403756000	-0.849212000		
		V	1.130338000	2.496933000	0.455958000		
		H	-0.988930000	-4.328592000	-4.278895000		
		H	-1.701069000	-4.327148000	-4.057075000		
4	min1(a) 	C	-0.728137000	-5.699862000	0.775210000	-1472.81905059	-1472.86258454
		O	-0.149201000	-4.652525000	1.091522000		
		N	-0.954274000	-6.677826000	1.638346000		
		H	-0.652760000	-6.587832000	2.595780000		
		H	-1.424241000	-7.516572000	1.347037000		
		H	-1.079791000	-5.856067000	-0.253800000		
		Pt	-0.562230000	-4.080453000	-2.577375000		
		Pt	0.727697000	-1.751811000	-2.417999000		
		Pt	-1.562538000	-1.812313000	-1.515062000		
		V	0.215767000	-3.183548000	-0.351726000		
		H	0.364432000	-5.233979000	-3.052826000		
		H	-1.509006000	-5.315586000	-2.420453000		
5	TS1(a) ( $\nu = 439i \text{ cm}^{-1}$ ) 	C	-0.194829000	-0.947620000	1.064674000	-1472.79523155	-1472.83895026
		O	0.118810000	0.238180000	1.240708000		
		N	-0.339923000	-1.795574000	2.067737000		
		H	-0.205579000	-1.485961000	3.017687000		
		H	-0.593430000	-2.752131000	1.893567000		
		H	-0.365030000	-1.332044000	0.050165000		
		Pt	-0.189818000	0.458718000	-2.247474000		
		Pt	1.146507000	2.695656000	-2.235356000		
		Pt	-0.212516000	3.892029000	-0.306312000		
		V	0.360795000	1.721819000	-0.148300000		
		H	1.334571000	0.301541000	-2.351522000		
		H	-0.859558000	-0.994611000	-2.045574000		
6	min2(a) 	C	-0.375232000	-1.113064000	1.151265000	-1472.81822519	-1472.86194347
		O	-0.270548000	0.118175000	1.126014000		
		N	-0.550986000	-1.786176000	2.276625000		

		H -0.597451000 H -0.633642000 H -0.326547000 Pt 0.205404000 Pt 0.560183000 Pt 1.047847000 V 0.092940000 H 1.066846000 H -0.218817000	-1.297345000 -2.787227000 -1.696013000 0.244437000 2.944530000 3.507740000 1.423560000 1.665520000 -1.224136000	3.156831000 2.265209000 0.225312000 -2.345935000 -2.375666000 0.061446000 -0.372810000 -3.262407000 -1.905883000		
7	TS2(a) ( $\nu = 448i \text{ cm}^{-1}$ ) 	C -0.187729000 O 0.352392000 N -0.380579000 H -0.091289000 H -0.823505000 H -0.525915000 Pt 0.201655000 Pt 0.462431000 Pt -0.088656000 V 0.559372000 H 1.688364000 H -1.166540000	-0.957338000 0.152875000 -1.752007000 -1.461976000 -2.646268000 -1.324275000 0.077830000 2.692944000 3.666792000 1.455091000 0.865514000 -0.769182000	1.110506000 1.215455000 2.147521000 3.068759000 2.029867000 0.131369000 -2.258636000 -2.508176000 -0.223990000 -0.345400000 -1.858262000 -2.509011000	-1472.78444015	-1472.82803979
8	min3(a) 	C -0.107790000 O 0.638582000 N -0.352254000 H 0.064547000 H -0.962455000 H -0.587618000 Pt 0.261715000 Pt -1.002328000 Pt 0.519811000 V 0.874448000 H 1.839622000 H -1.186281000	-0.937818000 0.038701000 -1.811567000 -1.694915000 -2.592539000 -1.109435000 0.223980000 2.274197000 3.731289000 1.434909000 0.618278000 -0.175081000	0.999194000 1.168017000 1.957595000 2.868237000 1.792421000 0.025805000 -2.364898000 -1.517964000 -0.082447000 -0.274848000 -1.657692000 -2.913419000	-1472.79875139	-1472.84265187
9	TS3(a) ( $\nu = 87i \text{ cm}^{-1}$ ) 	C -0.386455000 O -1.202138000 N 0.689085000 H 1.198975000 H 1.300763000 H -0.896677000 Pt -0.418726000 Pt 0.415978000 Pt 0.939641000 V -0.604352000 H 0.045433000 H -1.081527000	-1.025480000 -0.056022000 -1.331507000 -0.521008000 -2.054823000 -1.927211000 0.089245000 2.501208000 2.889027000 1.225995000 -0.609625000 0.820202000	0.798076000 1.237287000 1.628724000 1.953345000 1.281509000 0.445800000 -2.217685000 -1.907622000 0.540187000 0.012515000 -0.361815000 -3.410323000	-1472.77612155	-1472.81848934
10	min4(a) 	C 0.757826000 O 0.798920000 N -0.246684000 H -0.124620000 H -1.177580000 H 0.601267000 Pt -0.804844000 Pt -1.163198000 Pt 1.193238000 V 0.363576000 H 1.737048000 H -1.934950000	-1.587356000 -0.654043000 -1.358404000 -0.471063000 -1.394256000 -2.576251000 1.867730000 2.866736000 3.134200000 0.880748000 -1.580289000 0.872247000	0.925916000 -0.130742000 1.908383000 2.378434000 1.514376000 0.484749000 -2.778120000 -0.419696000 -1.220022000 -0.890363000 1.414808000 -3.187722000	-1472.80666895	-1472.85053789
11	TS4(a) ( $\nu = 966i \text{ cm}^{-1}$ )	C 0.638051000 O -0.350546000 N 0.107233000 H -0.393536000 H -0.485563000	-0.716828000 0.342765000 -2.000391000 -2.050593000 -2.329218000	0.758970000 0.757126000 1.009898000 1.886203000 0.260294000	-1472.75790116	-1472.80067033

		H 1.146649000 Pt -1.912542000 Pt 0.367493000 Pt 1.022431000 V -0.379961000 H 1.349935000 H -1.109645000	-0.712475000 0.706249000 1.506018000 3.587798000 1.989057000 -0.447129000 0.124748000	-0.208652000 -1.696342000 -2.559012000 -1.261975000 -0.294503000 1.541288000 -0.193296000			
12	product (a) — {Pt <sub>3</sub> V—O(H)CH <sub>2</sub> NH <sub>2</sub> }		C 0.757062000 O 0.857460000 N -0.386257000 H -0.241236000 H -1.218074000 H 0.737751000 Pt -1.205840000 Pt 0.175925000 Pt 2.264828000 V 0.615295000 H 1.661626000 H 0.451626000	-5.581131000 -4.156484000 -6.103094000 -6.987680000 -6.112319000 -5.628466000 -3.340117000 -1.259243000 -1.186810000 -2.732323000 -6.058850000 -4.033733000	0.471293000 0.762346000 1.114960000 1.572754000 0.543677000 -0.620441000 -2.039337000 -2.671330000 -1.184809000 -0.731480000 0.850599000 1.630970000	-1472.75617256	-1472.80105145
13	reagent (b) — {H <sub>2</sub> +Pt <sub>3</sub> V—O(H)CH <sub>2</sub> NH <sub>2</sub> }		C 0.118258000 O 0.914734000 N -1.119871000 H -1.517491000 H -1.782831000 H 0.054307000 Pt -1.746057000 Pt -0.539235000 Pt -1.784622000 V 0.345009000 H 0.664196000 H 0.774799000 H -5.335128000 H -5.770952000	-5.862411000 -4.702310000 -5.794174000 -6.699158000 -5.200315000 -5.794839000 -3.370235000 -0.988063000 -1.734330000 -2.930659000 -6.762732000 -4.596991000 -6.415418000 -6.515820000	-0.154210000 0.210910000 0.528430000 0.728844000 0.033790000 -1.245020000 -2.202652000 -2.258981000 -0.186688000 -0.889714000 0.137879000 1.162141000 -3.991317000 -3.394399000	-1473.90317508	-1473.95154112
14	min1(b)		C 0.041693000 O 0.808919000 N -1.188184000 H -1.499078000 H -1.911381000 H -0.043664000 Pt -1.679850000 Pt -0.289454000 Pt -1.510673000 V 0.413417000 H 0.630451000 H 0.627877000 H -1.398651000 H -2.469487000	-5.844864000 -4.690657000 -5.885502000 -6.818079000 -5.357241000 -5.684025000 -3.143100000 -0.867904000 -1.380064000 -2.875649000 -6.740772000 -4.639149000 -4.017874000 -4.451447000	-0.215328000 0.247672000 0.476283000 0.697680000 -0.000865000 -1.293985000 -2.194105000 -2.233673000 -0.156634000 -0.810745000 -0.008619000 1.196202000 -3.445851000 -1.859983000	-1473.97272664	-1474.01630519
15	TS1(b) ( $\nu = 131i \text{ cm}^{-1}$ )		C 0.495848000 O 1.956600000 N -0.835458000 H -1.322729000 H -1.260373000 H 1.030456000 Pt -1.265864000 Pt 0.707172000 Pt -0.587947000 V 0.844224000	-2.171136000 0.913590000 -2.098753000 -2.869527000 -1.190376000 -1.299708000 1.428887000 3.030314000 3.804746000 1.809856000	0.469946000 1.233854000 0.300783000 -0.122377000 0.161890000 0.817818000 -1.081710000 -1.977262000 0.027302000 0.147986000	-1473.95335143	-1473.99902046


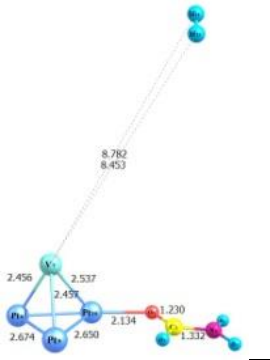
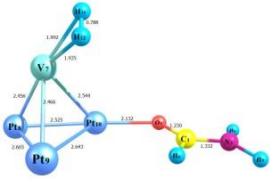
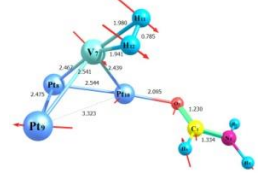


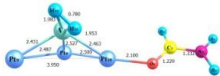
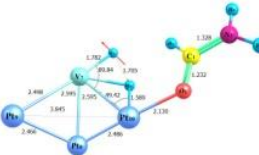
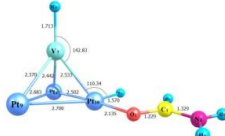
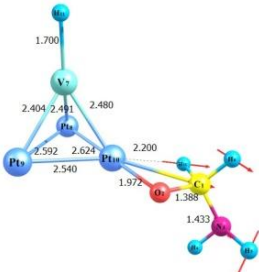
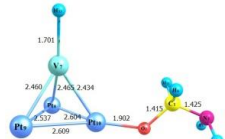
		H 0.984123000 H 2.795300000 H -1.234967000 H -2.306388000	-3.129854000 1.055258000 0.062277000 0.654424000	0.383624000 1.672209000 -1.817452000 -0.216612000		
16	min2(b) 	C 0.386989000 O 2.080549000 N -0.442379000 H -1.373658000 H -0.476435000 H 1.309151000 Pt -1.181711000 Pt 0.532730000 Pt -1.246862000 V 0.451343000 H 0.197242000 H 2.717807000 H -0.721759000 H -2.233007000	-1.967610000 0.668538000 -1.049471000 -0.982961000 -1.156172000 -2.246802000 1.042486000 2.986959000 2.623778000 0.828842000 -2.151014000 1.371378000 0.145772000 -0.113722000	0.286811000 1.093511000 0.939876000 0.537040000 1.947486000 0.771409000 -1.595425000 -1.053732000 0.606288000 0.334111000 -0.759473000 1.235123000 -2.771377000 -1.571648000	-1473.98552959	-1474.03057163
17	TS2(b) ( $\nu = 72i \text{ cm}^{-1}$ ) 	C 0.112396000 O 1.897821000 N -0.243213000 H -1.189773000 H 0.431254000 H 1.077933000 Pt -0.957263000 Pt 0.541651000 Pt -1.606615000 V 0.367536000 H -0.669192000 H 2.564326000 H -0.325117000 H -2.001742000	-1.394595000 0.490562000 -1.056255000 -1.269255000 -1.313755000 -1.886753000 1.180878000 3.009196000 2.347967000 0.674311000 -1.927517000 1.175748000 -0.152712000 0.122181000	-0.100643000 1.288102000 1.256007000 1.531433000 1.964822000 -0.184232000 -2.027582000 -0.844213000 0.198744000 0.278765000 -0.632782000 1.194049000 -1.375756000 -2.546713000	-1473.98731086	-1474.02955274
18	min3(b) 	C 0.232421000 O 2.096332000 N -0.485898000 H -1.411856000 H -0.606350000 H 1.252960000 Pt -1.126611000 Pt 0.336472000 Pt -1.600020000 V 0.378150000 H -0.255201000 H 2.873618000 H 0.266941000 H -1.950960000	-1.947893000 0.828005000 -0.830148000 -0.733129000 -0.993489000 -1.977591000 1.530495000 3.502428000 2.626803000 1.083099000 -2.907925000 1.379164000 -1.772893000 0.213076000	0.035817000 0.675117000 0.665363000 0.253504000 1.659856000 0.415770000 -1.686779000 -0.639993000 0.635770000 0.223338000 0.222202000 0.577806000 -1.039672000 -1.998099000	-1474.02456517	-1474.06878570
19	TS3(b) ( $\nu = 59i \text{ cm}^{-1}$ ) 	C -0.127010000 O 1.596493000 N -0.201919000 H -0.988579000 H 0.691344000 H 0.699066000 Pt -0.743718000 Pt -0.743278000 Pt -1.969099000 V 0.595870000 H 0.050964000 H 2.545234000	-2.254441000 0.742911000 -0.796484000 -0.460300000 -0.299672000 -2.517336000 2.020714000 4.244456000 2.062489000 2.283437000 -2.691418000 0.614685000	-0.054709000 1.014353000 0.067973000 0.635764000 0.497802000 -0.713651000 -1.959924000 -0.616340000 0.244370000 0.271500000 0.926993000 0.977290000	-1473.94555451	-1473.98936557

		H	-1.053945000	-2.653206000	-0.465417000		
		H	-0.351422000	-0.295836000	-0.826003000		
20	product ( <b>b</b> )— $\{\text{Pt}_3\text{V}-(\text{OH}_2)\cdots\text{NH}_2\text{CH}\}$ 	C	0.506289000	-7.535839000	-2.776492000	-1473.95114782	-1473.99654133
		O	0.532536000	-4.163642000	-3.458143000		
		N	1.246858000	-6.329472000	-2.415256000		
		H	0.944565000	-5.985686000	-1.482594000		
		H	2.243755000	-6.506488000	-2.367013000		
		H	0.777788000	-7.853463000	-3.784687000		
		Pt	-2.461784000	-4.175685000	-0.435476000		
		Pt	-1.087564000	-2.202262000	0.327271000		
		Pt	-0.033079000	-4.654410000	0.307088000		
		V	-0.475197000	-3.379796000	-1.838283000		
		H	0.687559000	-8.364802000	-2.087571000		
		H	-0.560403000	-7.309533000	-2.761674000		
		H	0.321492000	-4.140149000	-4.392860000		
		H	0.903084000	-5.152854000	-3.147003000		
21	$\{\text{Pt}_3\text{V}-\text{OH}_2\}$ 	V	-0.824543000	-0.688159000	1.677959000	-1378.20623079	-1378.24667250
		Pt	-0.192057000	1.438470000	0.521778000		
		Pt	-0.788746000	-0.711086000	-0.877643000		
		Pt	1.366108000	-0.705818000	0.436125000		
		O	-0.605080000	0.233822000	3.622532000		
		H	-0.347084000	1.048921000	3.136622000		
		H	0.143346000	0.003299000	4.182683000		



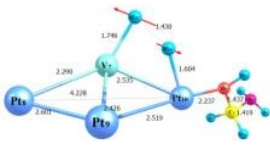
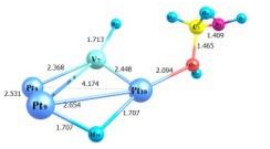
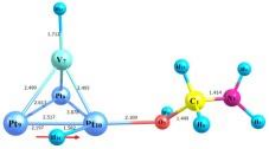
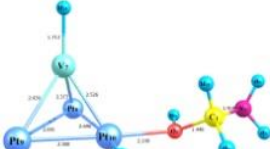
**Table S4.** Cartesian coordinates of compounds and their energy characteristics (298.15 K, 1.00 atm) for critical points (minima and transition states) of MEP curves of reaction (**3b**)

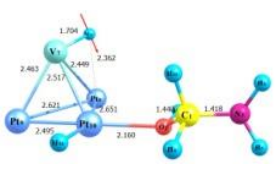
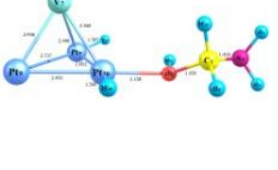
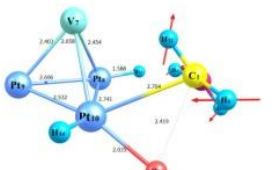

N <sup>o</sup>			x	y	z	E <sub>el</sub> + ZPE (Eh)	G <sup>0</sup> (Eh)
1	Pt3V-formamide 	C	-0.493843000	-5.911359000	0.387911000	-1471.57759947	-1471.62056793
		O	-0.505759000	-4.682703000	0.437211000		
		N	-1.123485000	-6.667749000	1.285984000		
		H	-1.612102000	-6.232632000	2.051611000		
		H	-1.087558000	-7.669179000	1.229847000		
		H	0.036218000	-6.447384000	-0.407454000		
		V	0.078561000	-3.345372000	-3.373396000		
		Pt	2.191517000	-2.350991000	-2.566396000		
		Pt	1.862430000	-4.964830000	-2.886310000		
		Pt	0.689354000	-3.570605000	-0.935709000		
2	reagent (a) – {H <sub>2</sub> +Pt <sub>2</sub> VPt–OC(H)N H <sub>2</sub> }_Td 	C	-0.345503000	-6.065183000	0.769357000	-1472.73617795	-1472.78316850
		O	-0.044899000	-4.890281000	0.972646000		
		N	-0.925480000	-6.824238000	1.697926000		
		H	-1.115648000	-6.442094000	2.610073000		
		H	-1.151866000	-7.783512000	1.508566000		
		H	-0.152770000	-6.547118000	-0.195978000		
		V	-0.080694000	-3.069701000	-2.701150000		
		Pt	2.313300000	-2.640197000	-2.362728000		
		Pt	1.325950000	-5.079812000	-2.837975000		
		Pt	1.010813000	-3.809002000	-0.533947000		
		H	-8.604222000	-4.468163000	-4.285954000		
		H	-8.121743000	-5.017989000	-4.431844000		
3	min1_Td (a) 	C	-0.260854000	-6.100014000	0.837205000	-1472.74606355	-1472.79017781
		O	-0.125860000	-4.884766000	0.967118000		
		N	-0.766258000	-6.869269000	1.800217000		
		H	-1.034714000	-6.459179000	2.679981000		
		H	-0.847586000	-7.861638000	1.673967000		
		H	0.026808000	-6.612750000	-0.087791000		
		V	-0.330366000	-3.303775000	-2.817753000		
		Pt	1.977092000	-2.541499000	-2.461839000		
		Pt	1.348424000	-5.109495000	-2.797691000		
		Pt	0.805507000	-3.763577000	-0.588266000		
		H	-2.128818000	-4.146285000	-2.968812000		
		H	-1.611481000	-4.736076000	-3.044654000		
4	TS1(a) (v=64i cm <sup>-1</sup> ) 	C	-0.040248000	-0.948842000	1.460753000	-1472.741542400	-1472.78517479
		O	0.068140000	0.273398000	1.513772000		
		N	-0.557662000	-1.663994000	2.460723000		
		H	-0.855360000	-1.199910000	3.303396000		
		H	-0.624631000	-2.663276000	2.398230000		
		H	0.279752000	-1.521804000	0.583578000		
		V	-0.093872000	1.845694000	-2.133130000		
		Pt	2.272493000	2.654714000	-1.818234000		
		Pt	1.760479000	0.399684000	-2.832280000		
		Pt	1.055605000	1.344196000	-0.017252000		
		H	-1.885829000	1.014807000	-2.339908000		
		H	-1.378867000	0.465333000	-2.579647000		
5	min2(a) flat	C	-1.595094000	-1.313015000	0.214418000	-1472.74976075	-1472.79469387
		O	-1.275059000	-0.128964000	0.295962000		

		N	-2.498948000	-1.864264000	1.023221000		
		H	-2.955095000	-1.299246000	1.721121000		
		H	-2.746261000	-2.832927000	0.935129000		
		H	-1.153097000	-1.984438000	-0.529188000		
		V	2.394484000	1.231520000	-0.587960000		
		Pt	1.477789000	1.698286000	-2.895856000		
		Pt	3.005049000	3.284541000	-1.738776000		
		Pt	0.025587000	0.775239000	-1.082498000		
		H	2.272216000	1.229086000	1.360858000		
		H	3.048430000	1.204181000	1.283569000		
6	TS2(a) ( $\nu=285i\text{ cm}^{-1}$ ) 	C	-1.267053000	-0.974751000	0.517742000	-1472.74008599	-1472.78363816
		O	-1.418474000	-0.322906000	-0.516036000		
		N	-2.270489000	-1.612688000	1.110176000		
		H	-3.194454000	-1.576448000	0.710668000		
		H	-2.117600000	-2.139912000	1.950837000		
		H	-0.290054000	-1.059884000	1.008837000		
		V	2.229971000	1.524419000	-0.008416000		
		Pt	2.074623000	1.879805000	-2.573685000		
		Pt	2.468084000	3.780852000	-1.052810000		
		Pt	0.225765000	0.679882000	-1.424196000		
		H	2.286754000	-0.061878000	0.805105000		
		H	1.272927000	-0.116490000	-0.528222000		
7	min 3(a) 	C	-1.553002000	-1.227406000	0.233860000	-1472.76430959	-1472.80772712
		O	-1.161093000	-0.069415000	0.104661000		
		N	-2.506731000	-1.564107000	1.096021000		
		H	-2.933056000	-0.855740000	1.671627000		
		H	-2.809132000	-2.517437000	1.182965000		
		H	-1.133646000	-2.047788000	-0.358451000		
		V	2.603257000	1.239879000	-0.389460000		
		Pt	2.099785000	1.514566000	-2.762669000		
		Pt	1.107368000	3.034089000	-0.787249000		
		Pt	0.357721000	0.488782000	-1.288058000		
		H	3.843005000	0.815569000	0.713178000		
		H	0.454144000	-0.977446000	-1.841277000		
8	TS3(a) ( $\nu=135i\text{ cm}^{-1}$ ) 	6	-0.926522000	-1.202512000	0.467684000	-1472.71735833	-1472.75980009
		8	-0.577773000	0.025149000	1.026719000		
		7	-2.330678000	-1.472053000	0.375379000		
		1	-2.808563000	-0.688894000	-0.054956000		
		1	-2.716851000	-1.581986000	1.305560000		
		1	-0.450008000	-2.024881000	1.018441000		
		23	2.793935000	1.409016000	-0.392254000		
		78	1.726307000	1.842923000	-2.504705000		
		78	1.101067000	3.239675000	-0.420329000		
		78	0.398957000	0.795979000	-0.496239000		
		1	4.294985000	0.942273000	0.253559000		
		1	-0.504856000	-1.284690000	-0.578858000		
9	min 4(a) 	C	-1.326512000	-1.230694000	0.418785000	-1472.73267577	-1472.77582014
		O	-1.435776000	0.119168000	0.010194000		
		N	-2.580647000	-1.777728000	0.817210000		
		H	-3.245592000	-1.742279000	0.054817000		
		H	-2.969802000	-1.254910000	1.591605000		
		H	-0.628925000	-1.302858000	1.260768000		
		V	2.311166000	0.741230000	-0.816073000		
		Pt	1.381911000	2.183970000	-2.585847000		
		Pt	1.786111000	3.076190000	-0.246030000		
		Pt	-0.056500000	1.267621000	-0.617847000		
		H	3.431209000	-0.508687000	-0.538953000		
		H	-0.929971000	-1.829957000	-0.408540000		

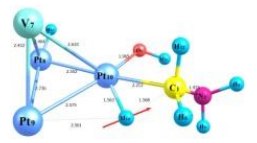
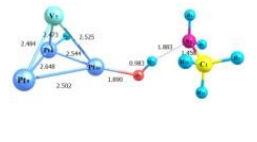
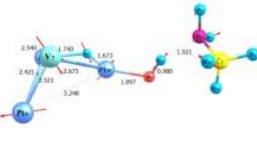
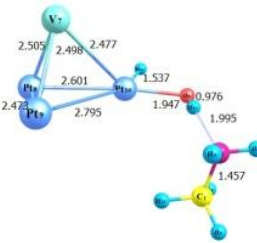
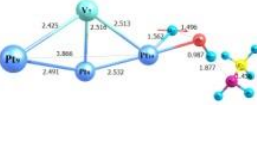
10	<div>TS4(a) (<math>\nu = 591 i \text{ cm}^{-1}</math>)</div> <div>C -0.780587000 -0.987812000 0.757116000 O -0.883234000 0.332848000 0.273529000 N -2.034890000 -1.672697000 0.749644000 H -2.400351000 -1.726997000 -0.193183000 H -2.713390000 -1.171961000 1.310037000 H -0.410716000 -0.953211000 1.789336000 V 2.935732000 0.931890000 -1.145105000 Pt 1.655808000 2.573959000 -2.479849000 Pt 2.346101000 3.111242000 -0.098339000 Pt 0.501810000 1.390251000 -0.510842000 H 1.847298000 -0.268983000 -0.609550000 H -0.063582000 -1.558528000 0.157206000</div>	-1472.71865104	-1472.76169316
11	<div>min 5(a)</div> <div>C -0.907383000 -0.832637000 0.730988000 O -0.665230000 0.263574000 -0.096866000 N -2.261521000 -1.270438000 0.493346000 H -2.331634000 -1.804803000 -0.362295000 H -2.603910000 -1.834716000 1.258732000 H -0.836239000 -0.563585000 1.795515000 V 2.587906000 0.764828000 -2.144643000 Pt 1.330077000 2.907654000 -2.313120000 Pt 3.116126000 2.669148000 -0.611809000 Pt 1.080317000 1.122764000 -0.190651000 H 1.646666000 0.197339000 0.901142000 H -0.155175000 -1.619127000 0.539660000</div>	-1472.737236529	-1472.78036555
12	<div>TS5(a) (<math>\nu = 1070 i \text{ cm}^{-1}</math>)</div> <div>C -1.024527000 -0.831687000 0.267473000 O -0.740989000 0.441934000 0.826637000 N -2.012966000 -1.477090000 1.059993000 H -2.853383000 -1.737157000 0.575304000 H -1.683079000 -2.207064000 1.667126000 H -0.097907000 -1.421211000 0.210863000 V 2.786751000 0.601467000 -1.154257000 Pt 3.051002000 2.086176000 -3.052506000 Pt 2.589940000 3.088331000 -0.820647000 Pt 0.742469000 1.544194000 -0.044375000 H 0.640538000 0.612376000 1.218564000 H -1.397850000 -0.700268000 -0.754174000</div>	-1472.70755776	-1472.75140326
13	<div>min 6(a)</div> <div>C -0.921026000 -1.065434000 0.695417000 O -0.889743000 0.097240000 -0.160846000 N -2.272782000 -1.415528000 0.945129000 H -2.652091000 -2.113338000 0.324875000 H -2.470874000 -1.639822000 1.906129000 H -0.413749000 -0.833664000 1.633879000 V 2.118229000 1.413505000 -2.484289000 Pt 3.059774000 3.658524000 -2.578424000 Pt 3.099504000 2.436535000 -0.405493000 Pt 0.916666000 1.208837000 -0.353668000 H -1.635483000 0.653673000 0.098889000 H -0.338385000 -1.809428000 0.149277000</div>	-1472.73776152	-1472.78164

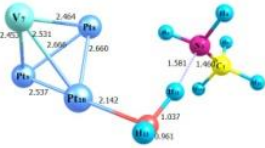
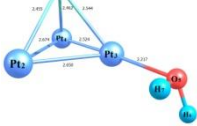
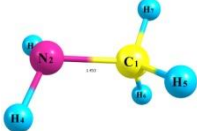
		N -0.515370000 H -1.468537000 H -0.010884000 H 0.506285000 V 2.147920000 Pt 2.960167000 Pt 0.396817000 Pt 0.197349000 H 0.350276000 H -1.236199000	-1.475473000 -1.743977000 -1.313301000 0.163472000 1.354930000 2.187644000 1.533992000 0.158635000 -1.818873000 0.211754000	2.784909000 2.974346000 3.640883000 2.054216000 -1.732575000 -3.674806000 -3.357474000 -1.226645000 0.626107000 1.702679000			
16	reagent (b) – {Pt <sub>2</sub> VPt–O(H)CH <sub>2</sub> NH <sub>2</sub> }		C -1.608108000 O -1.637838000 N -1.723852000 H -1.103479000 H -2.665828000 H -2.425975000 V 0.807048000 Pt 1.612433000 Pt -0.963016000 Pt -1.219646000 H -1.156183000 H -0.664017000 H 6.518546000 H 7.040856000	0.638609000 -0.057445000 -0.306549000 -0.139805000 -0.468466000 1.357544000 1.923542000 2.694367000 2.108634000 0.952130000 -0.885307000 1.180397000 -2.587204000 -3.116004000	1.995823000 0.732824000 3.046832000 3.821872000 3.367290000 1.919443000 -1.770814000 -3.740241000 -3.377023000 -1.123952000 0.852447000 2.082408000 -0.704898000 -0.642360000	-1473.89748179	-1473.94575633
17	min1(b)		C -0.510095000 O -0.014529000 N -1.124371000 H -0.890757000 H -2.119836000 H -1.175210000 V 1.109006000 Pt 1.808132000 Pt 3.076095000 Pt 1.329577000 H 0.332367000 H 0.322946000 H -0.647318000 H -0.625988000	-0.249574000 -0.919948000 -1.205036000 -1.101707000 -1.302524000 0.519403000 -0.059670000 2.084678000 1.173479000 0.095117000 -1.774550000 2.229895000 -0.072191000 -0.812691000	2.223780000 1.044628000 3.073513000 4.047142000 2.949484000 1.826790000 -2.696111000 -3.618988000 -1.685009000 -0.256734000 1.330348000 2.742246000 -3.538516000 -3.290782000	-1473.90619708	-1473.95157129
18	TS1_b ( $\nu=297\text{ i cm}^{-1}$ )		C -0.508159000 O -0.202422000 N -1.230146000 H -0.930319000 H -2.232805000 H -1.050823000 V 0.758621000 Pt 1.806542000 Pt 3.044997000 Pt 1.239748000 H 0.024173000 H 0.422788000 H -0.487346000 H -0.654850000	0.007198000 -0.632605000 -0.901067000 -0.916661000 -0.818821000 0.908176000 0.737162000 2.892983000 1.211481000 0.277928000 -1.550131000 0.294784000 -0.753230000 -0.757196000	1.860765000 0.602392000 2.678071000 3.638935000 2.615617000 1.569523000 -3.070654000 -3.457318000 -2.118214000 -0.673989000 0.800156000 2.353568000 -3.779080000 -3.019774000	-1473.89964613	-1473.94429004
19	min2(b)		C -0.491256000 O -0.333996000 N -1.237981000 H -0.877172000 H -2.230583000 H -0.965328000 V 0.413859000 Pt 1.652719000 Pt 2.826159000 Pt 1.080392000	0.014937000 -0.620045000 -0.842355000 -0.907382000 -0.667118000 0.969119000 0.940600000 3.036051000 1.061210000 0.199606000	1.853993000 0.566796000 2.703611000 3.641153000 2.711744000 1.617470000 -3.096694000 -3.308735000 -2.363047000 -0.802665000	-1473.90221089	-1473.94712509

		H	-0.188084000	-1.560088000	0.731622000		
		H	0.494083000	0.203412000	2.285072000		
		H	-0.179918000	-0.872755000	-3.650131000		
		H	0.037105000	-0.955192000	-2.890191000		
20	TS2 $(\nu = 447 \text{ i cm}^{-1})$ 	C	-0.506697000	-0.082975000	1.924040000	-1473.89595865	-1473.94078491
		O	-0.267882000	-0.688439000	0.643404000		
		N	-1.359913000	-0.922272000	2.687126000		
		H	-1.104382000	-0.994037000	3.658460000		
		H	-2.343039000	-0.720977000	2.588430000		
		H	-0.915790000	0.900728000	1.679957000		
		V	0.395907000	1.126848000	-3.145438000		
		Pt	1.575173000	2.786010000	-4.194596000		
		Pt	2.744508000	1.159873000	-2.536020000		
		Pt	1.099454000	0.174102000	-0.903511000		
		H	-0.207473000	-1.641512000	0.782398000		
		H	0.442481000	0.046614000	2.451608000		
		H	-0.088029000	-0.518966000	-3.463667000		
		H	0.535682000	-0.624996000	-2.172190000		
21	min3(b) 	C	-1.021829000	-0.475696000	1.174397000	-1473.92667636	-1473.97121521
		O	0.340611000	-0.940925000	0.900997000		
		N	-1.145218000	-0.230064000	2.556175000		
		H	-1.498327000	0.681282000	2.794263000		
		H	-1.583995000	-0.957556000	3.096110000		
		H	-1.649808000	-1.281087000	0.792486000		
		V	0.770497000	1.394389000	-1.808844000		
		Pt	2.033822000	2.235210000	-3.626646000		
		Pt	1.462362000	-0.230573000	-3.592145000		
		Pt	1.086613000	-0.913655000	-1.055244000		
		H	0.906960000	-0.505617000	1.551284000		
		H	-1.185659000	0.434328000	0.594539000		
		H	-0.478130000	2.177950000	-0.935441000		
		H	1.962102000	-1.387988000	-2.441932000		
22	TS3 $(\nu = 574 \text{ i cm}^{-1})$ 	C	-0.914438000	-0.633538000	1.318683000	-1473.90819343	-1473.95307784
		O	0.473197000	-0.590681000	0.902612000		
		N	-0.984894000	-0.409734000	2.712920000		
		H	-1.674376000	0.265654000	2.997038000		
		H	-1.023834000	-1.239816000	3.282211000		
		H	-1.253232000	-1.616166000	0.986235000		
		V	0.557586000	1.606865000	-2.416570000		
		Pt	2.864317000	1.729216000	-2.132265000		
		Pt	1.840879000	-0.213164000	-3.549861000		
		Pt	0.988779000	-0.527495000	-1.202531000		
		H	0.903581000	0.077659000	1.451432000		
		H	-1.465170000	0.139557000	0.780212000		
		H	-0.672218000	2.756299000	-2.726931000		
		H	0.359823000	-1.344655000	-2.403187000		
23	min4(b) 	C	-0.700821000	-1.052012000	1.790218000	-1473.92186545	-1473.96580420
		O	0.537935000	-0.387671000	1.443140000		
		N	-1.194575000	-0.505269000	2.997360000		
		H	-2.174782000	-0.279013000	2.986337000		
		H	-0.940546000	-1.006814000	3.833185000		
		H	-0.423507000	-2.106602000	1.832960000		
		V	0.527559000	0.736584000	-2.440146000		
		Pt	2.363742000	1.749560000	-1.329698000		
		Pt	2.581946000	-0.549426000	-2.711950000		
		Pt	1.405582000	-0.632858000	-0.507187000		
		H	0.435326000	0.544176000	1.674387000		
		H	-1.418099000	-0.901446000	0.981741000		
		H	-0.955439000	1.191619000	-3.166275000		
		H	0.858274000	-2.099935000	-0.588853000		

24	TS4 $(\nu = 483 \text{ i cm}^{-1})$ 	C	-0.771400000	-0.710135000	1.332203000	-1473.91103329	-1473.95480159
		O	0.326966000	0.096257000	0.866924000		
		N	-1.299138000	-0.135964000	2.516249000		
		H	-2.304528000	-0.127867000	2.560751000		
		H	-0.900478000	-0.489761000	3.371737000		
		H	-0.332131000	-1.703370000	1.443766000		
		V	0.241210000	0.633697000	-3.162538000		
		Pt	1.878053000	2.105926000	-2.089229000		
		Pt	2.566603000	-0.177630000	-3.174732000		
		Pt	1.271113000	-0.253256000	-1.043621000		
		H	0.076980000	1.022633000	0.971875000		
		H	-1.542585000	-0.746666000	0.559595000		
		H	-0.185206000	2.282128000	-3.225640000		
		H	0.974540000	-1.795995000	-0.927340000		
25	min5(b) 	C	-0.726278000	-1.032421000	1.792949000	-1473.95349046	-1473.99715562
		O	0.494800000	-0.373286000	1.413388000		
		N	-1.177388000	-0.501420000	3.028518000		
		H	-2.170608000	-0.344981000	3.072966000		
		H	-0.851690000	-0.995604000	3.844440000		
		H	-0.455402000	-2.090212000	1.805129000		
		V	0.539879000	0.767656000	-2.539427000		
		Pt	2.361056000	1.740888000	-1.228939000		
		Pt	2.606305000	-0.549533000	-2.706691000		
		Pt	1.358979000	-0.618280000	-0.548694000		
		H	0.402920000	0.566042000	1.619415000		
		H	-1.479836000	-0.867918000	1.019565000		
		H	1.806287000	2.881574000	-0.311892000		
		H	0.853114000	-2.100417000	-0.636264000		
26	TS5(b) $(\nu = 260 \text{ i cm}^{-1})$ 	C	-1.151063000	-0.673909000	0.723215000	-1473.90454214	-1473.94737332
		O	1.117382000	-1.404904000	1.133864000		
		N	-1.157376000	0.503316000	1.272109000		
		H	-0.993613000	1.322321000	0.660697000		
		H	-0.842648000	0.593927000	2.226649000		
		H	-1.084023000	-1.561437000	1.332244000		
		V	-0.536508000	0.389284000	-2.563976000		
		Pt	0.655157000	1.982891000	-1.127616000		
		Pt	1.835801000	0.378835000	-2.945311000		
		Pt	1.100174000	-0.698526000	-0.775035000		
		H	1.504547000	-0.675063000	1.630001000		
		H	-1.483670000	-0.766864000	-0.302719000		
		H	-0.230355000	2.790634000	-0.086371000		
		H	1.266192000	-2.180505000	-1.177750000		
27	min6(b) 	C	-0.740118000	-1.068808000	0.657552000	-1473.94998454	-1473.99309949
		O	0.845997000	1.108157000	1.315720000		
		N	-1.366050000	-0.450511000	1.799642000		
		H	-2.232102000	0.014432000	1.572505000		
		H	-1.519361000	-1.091448000	2.564699000		
		H	-0.162217000	-1.933591000	0.993655000		
		V	-0.280744000	1.532818000	-2.177028000		
		Pt	2.136615000	1.462016000	-2.162646000		
		Pt	0.701688000	-0.707623000	-2.878517000		
		Pt	0.645042000	0.121486000	-0.323854000		
		H	0.111141000	0.818309000	1.881182000		
		H	-1.449430000	-1.399578000	-0.106443000		
		H	2.592384000	2.903429000	-1.779079000		
		H	0.717155000	-1.309089000	-1.357387000		
28	TS6(b) $(\nu = 862 \text{ i cm}^{-1})$	C	-1.058072000	-0.806687000	0.497793000	-1473.91493732	-1473.95821022
		O	0.470636000	1.517643000	0.980984000		
		N	-0.883228000	-0.788660000	1.922462000		
		H	-1.766326000	-0.733952000	2.412554000		
		H	-0.363977000	-1.584427000	2.264997000		
		H	-1.401461000	-1.762588000	0.084381000		
		H					



		V 0.018125000 0.902939000 -2.958745000 Pt 2.248958000 1.434557000 -2.056896000 Pt 1.350568000 -1.095986000 -2.578854000 Pt 0.612138000 0.240841000 -0.505423000 H 0.008418000 1.038655000 1.685161000 H -1.779980000 -0.047170000 0.198972000 H 2.320570000 2.941371000 -1.664493000 H 0.223630000 -1.256537000 -0.282891000		
29	min7(b) 	C -2.121448000 -1.520302000 1.904028000 O 0.851893000 -0.056110000 0.954218000 N -1.767106000 -0.113369000 2.052504000 H -2.543965000 0.484047000 1.800454000 H -1.535654000 0.096875000 3.015666000 H -2.971240000 -1.840826000 2.519068000 V -0.092710000 1.758370000 -2.485503000 Pt 2.350759000 2.136656000 -2.503342000 Pt 1.285713000 -0.207457000 -3.122196000 Pt 1.331263000 0.597168000 -0.753335000 H -0.088462000 0.056828000 1.216177000 H -2.358693000 -1.723646000 0.858471000 H 2.648170000 3.481495000 -1.760213000 H -1.256835000 -2.133296000 2.161748000	-1473.94307462	-1473.98902095
30	TS7 ( $\nu=57i\text{ cm}^{-1}$ ) 	C -1.668729000 -1.526552000 1.530649000 O 1.247027000 -0.148444000 0.380859000 N -1.289334000 -0.129563000 1.698383000 H -2.089993000 0.480464000 1.596390000 H -0.912924000 0.029361000 2.624780000 H -2.386659000 -1.896331000 2.273406000 V 0.408883000 1.028929000 -3.117585000 Pt 2.502358000 2.472570000 -3.152788000 Pt 2.425978000 0.145344000 -4.128899000 Pt 1.799790000 0.913531000 -1.091998000 H 0.338206000 0.044765000 0.690586000 H -2.104987000 -1.665245000 0.539691000 H 2.502320000 2.397345000 -1.419853000 H -0.771937000 -2.146174000 1.576379000	-1473.92064308	-1473.96649044
31	min8 	C -1.754690000 -1.559916000 1.621304000 O 0.715716000 0.838002000 1.588750000 N -2.051472000 -0.143317000 1.786062000 H -2.867604000 0.122610000 1.250734000 H -2.247666000 0.072671000 2.755199000 H -2.566444000 -2.235943000 1.920146000 V 0.779277000 2.347633000 -1.981099000 Pt 2.057381000 0.321834000 -2.715029000 Pt -0.376150000 0.156677000 -2.304542000 Pt 1.408293000 0.715984000 -0.227059000 H -0.241184000 0.655647000 1.533209000 H -1.510724000 -1.756435000 0.574981000 H 2.695101000 1.291201000 0.384915000 H -0.866182000 -1.805716000 2.204473000	-1473.92283821	-1473.96922723
32	TS 8 ( $\nu=1026i\text{ cm}^{-1}$ ) 	C -0.981616000 -1.799536000 1.989504000 O 0.543743000 1.160109000 0.505587000 N -1.481030000 -0.783681000 1.071257000 H -1.835525000 -1.207831000 0.222928000 H -2.248768000 -0.269664000 1.485397000 H -1.727561000 -2.545898000 2.288765000 V 2.831275000 2.476568000 -2.428883000 Pt 1.429983000 1.057433000 -3.962236000 Pt 1.917114000 3.450107000 -4.453297000 Pt 0.888388000 1.187814000 -1.492191000 H -0.154665000 0.479470000 0.659190000	-1473.90069561	-1473.94786959

		H	-0.143192000	-2.322800000	1.526698000		
		H	1.565236000	0.432087000	-0.303238000		
		H	-0.603382000	-1.314177000	2.890518000		
33	product (b)– {VPt <sub>2</sub> Pt–OH <sub>2</sub> ···NH <sub>2</sub> C H <sub>3</sub> }	C	1.741404000	-0.108747000	0.465937000	-1473.93550851	-1473.98023194
		O	-1.065441000	-1.290325000	-1.079796000		
		N	0.479322000	-0.685773000	0.920121000		
		H	0.625004000	-1.299197000	1.712936000		
		H	-0.164891000	0.056500000	1.219995000		
		H	2.271774000	0.445398000	1.246827000		
		V	-3.999011000	0.635800000	1.116583000		
		Pt	-1.928036000	1.960600000	1.276388000		
		Pt	-3.826811000	2.444423000	-0.530973000		
		Pt	-2.381561000	0.378068000	-0.812753000		
		H	-0.413663000	-1.202809000	-0.278191000		
		H	2.396449000	-0.898489000	0.094193000		
		H	-1.547170000	-2.116697000	-0.991361000		
		H	1.538378000	0.575215000	-0.358921000		
34	{VPt <sub>2</sub> Pt–OH <sub>2</sub> }	V	-0.269795000	0.052021000	1.652247000	-1378.19547325	-1378.23612039
		Pt	-0.125380000	1.310054000	-0.451238000		
		Pt	-1.016356000	-1.185139000	-0.441825000		
		Pt	1.423191000	-0.803525000	0.082872000		
		O	-3.170165000	-1.341360000	-0.941724000		
		H	-3.255112000	-1.626206000	-1.858337000		
		H	-3.387331000	-0.401059000	-0.934942000		
35	H <sub>2</sub> O	8	-2.589176000	0.000000000	-1.780898000	-76.35599466	-76.37363020
		1	-2.589176000	0.761560000	-1.197205000		
		1	-2.589176000	-0.761560000	-1.197205000		
36	CH <sub>3</sub> NH <sub>2</sub>	C	-1.734606000	-5.602295000	0.440637000	-95.71332225	-95.73624500
		N	-0.711863000	-6.623370000	0.592077000		
		H	0.141392000	-6.222347000	0.959196000		
		H	-1.009178000	-7.331239000	1.250987000		
		H	-2.641020000	-6.055111000	0.032359000		
		H	-2.011421000	-5.072060000	1.363596000		
		H	-1.397483000	-4.856917000	-0.283217000		