

Supporting information

**Where does methanol lose hydrogen to trigger steam
reforming? A revisit of methanol dehydrogenation on the
PdZn alloy model obtained from kinetic Monte Carlo
simulations**

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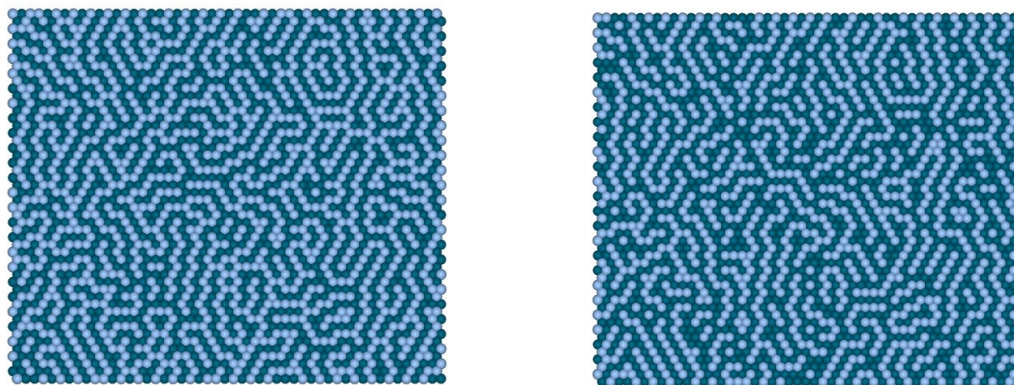


Figure S1 Atomic arrangement of the low-temperature alloy obtained from kMC simulation for the first layer (left) and second layer (right). The blue and white spheres denote Pd and Zn respectively.

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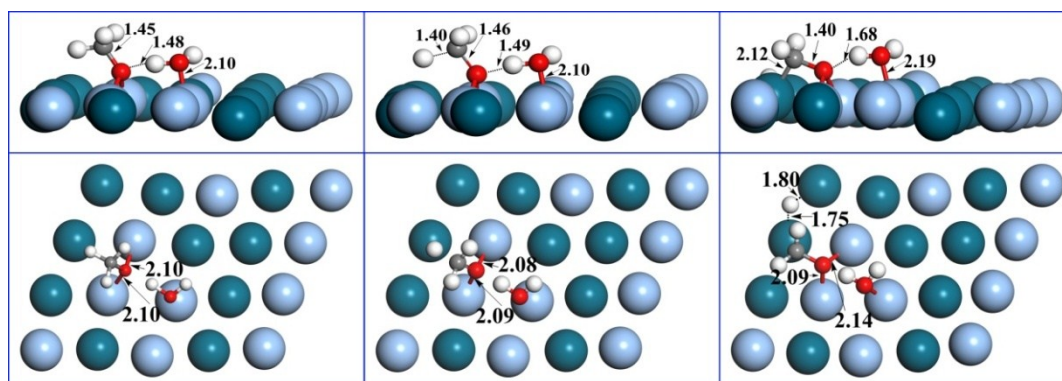


Figure S2 Dehydrogenation of CH_3O^* with co-adsorbed water on the kMC-model

Table S1 Reaction heats (in kJ/mol) and energy barriers (in eV) of methoxy dehydrogenation to formaldehyde*.

Reaction	kMC model		kMC model (co-adsorbed with H_2O)		Ideal model	
	$\Delta\text{H}(\Delta\text{H}_0)$	$E_a(E_{a,0})$	$\Delta\text{H}(\Delta\text{H}_0)$	$E_a(E_{a,0})$	$\Delta\text{H}(\Delta\text{H}_0)$	$E_a(E_{a,0})$
$\text{CH}_3\text{O} \rightarrow \text{CH}_2\text{O}$ +H	90(75)	1.29(1.17)	64(52)	0.87(0.73)	60(45)	1.13(0.93)

*: Values in parentheses are ZPE corrected.

Cartesian coordinates of the stationary points.

CH_3OH	IS:			TS			FS		
C	0.409950	4.977250	10.673640	0.509960	4.908360	10.236590	0.858270	6.518640	9.613120
H	-0.542350	5.499130	10.534200	1.084900	5.274310	11.096240	-0.043550	6.013400	9.992620
H	1.109800	5.631460	11.209880	-0.457290	5.433320	10.210880	0.890580	7.542960	10.008470
H	0.240000	4.054530	11.246470	0.327120	3.828940	10.333370	1.745920	5.970340	9.951500
H	1.769680	4.193680	9.411670	2.347900	4.856460	8.851920	3.142190	3.185850	7.875870
O	0.917010	4.669310	9.352430	1.212680	5.231490	8.999200	0.833670	6.541860	8.167820
Pd	-0.904370	2.254340	6.648180	-0.857600	2.240820	6.641650	-0.870010	2.253220	6.623460
Pd	-2.789680	7.083240	6.985990	-2.806750	7.088690	6.993570	-2.949020	7.058150	6.987170
Pd	1.778550	2.392340	6.797380	1.824690	2.413190	6.804490	1.773330	2.445460	6.928650
Pd	-1.451280	9.995960	6.838330	-1.465910	10.022280	6.839970	-1.445780	10.076810	6.835780
Pd	4.476350	2.348960	6.927400	4.526930	2.364010	6.902870	4.513500	2.342410	6.956320
Pd	3.322280	4.836660	7.041310	3.385940	4.817700	7.188780	3.405290	4.833690	7.064700
Pd	1.331960	9.784740	6.976410	1.317710	9.784700	6.973650	1.341950	9.899950	6.969450
Pd	7.143270	2.406320	6.995320	7.193470	2.432440	6.972970	7.178020	2.475910	6.936050
Pd	5.022980	7.080020	6.840870	5.017860	7.072870	6.857650	4.943180	7.131980	6.838660
Pd	4.235360	9.845880	6.935980	4.224070	9.833640	6.930730	4.237700	9.888400	6.932800
Pd	1.381470	0.507030	4.782440	1.371310	0.520600	4.797240	1.374400	0.586090	4.814300
Pd	-0.865660	5.466500	5.134590	-0.778170	5.522070	5.065870	-0.788980	5.567620	4.989830

Pd	-1.591540	8.081240	4.704960	-1.613400	8.109420	4.708500	-1.660770	8.153810	4.738390
Pd	4.158070	0.810080	4.681120	4.158240	0.791810	4.685230	4.169030	0.810720	4.673540
Pd	1.879960	5.517190	4.847420	1.989450	5.501190	4.915400	1.973650	5.581000	4.816120
Pd	1.193030	8.119340	4.695300	1.176160	8.077780	4.699880	1.099680	8.130090	4.785160
Pd	6.908930	0.794750	4.820360	6.907860	0.791270	4.824430	6.909440	0.790340	4.833600
Pd	2.684280	10.533440	4.734330	2.673660	10.515930	4.728200	2.682100	10.510200	4.717900
Pd	7.039050	5.514100	4.883380	7.111070	5.531510	4.863950	7.105000	5.546120	4.824780
Pd	6.414680	8.261500	4.833280	6.393950	8.257770	4.835250	6.354360	8.280160	4.820270
Pd	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840
Pd	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840
Pd	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840
Pd	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840
Pd	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840
Pd	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840
Pd	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840
Pd	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840
Pd	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840
Pd	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840
Pd	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840
Pd	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840
Pd	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840
Pd	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pd	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000
Pd	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000
Pd	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000
Pd	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000
Pd	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000
Pd	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000
Pd	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000
Pd	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000
Pd	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000
Pd	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000
Pd	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000
Pd	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000
Pd	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000
Pd	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000
Zn	-5.148410	12.152890	7.061100	-5.140470	12.126950	7.067980	-5.130200	12.173400	7.099940
Zn	8.514440	4.562270	7.124860	8.591070	4.583270	7.056580	-2.086440	4.604740	7.018190
Zn	-3.972340	9.417950	7.194350	-3.981760	9.422280	7.194030	-3.959450	9.474180	7.147690
Zn	2.911380	0.081110	6.945610	2.918350	0.105270	6.954420	2.909940	0.141750	6.958950
Zn	0.627170	4.679980	7.113650	0.619880	4.669240	7.088570	0.680770	4.749050	7.017160
Zn	-0.248210	7.577700	6.853490	-0.277210	7.610980	6.853160	-0.423310	7.619350	6.931600
Zn	0.198090	12.207580	6.950250	0.203490	12.208050	6.949040	5.556950	-0.029730	6.966370
Zn	2.471510	7.354330	6.939730	2.479000	7.363130	6.943030	2.419620	7.355910	6.968130
Zn	2.871210	12.118620	6.967320	2.874880	12.112450	6.960110	2.893550	12.156170	6.968120

Zn	5.893510	4.680760	7.244330	5.972250	4.707770	7.258530	5.985860	4.773600	7.220610
Zn	0.462120	3.197900	4.609870	0.498650	3.212200	4.613820	0.482700	3.238360	4.620020
Zn	-2.650870	10.502080	4.628110	-2.665860	10.521640	4.628260	-2.685030	10.563520	4.630110
Zn	3.125500	3.232620	4.741090	3.166700	3.220440	4.734310	3.109150	3.223040	4.778030
Zn	0.036200	10.554830	4.660370	0.030890	10.535280	4.658250	0.026650	10.571350	4.655580
Zn	5.787840	3.158640	4.735490	5.831070	3.174810	4.725880	5.803190	3.168730	4.717500
Zn	4.486960	5.603410	4.720610	4.560020	5.610550	4.714890	4.552800	5.598760	4.718260
Zn	3.811860	8.161370	4.710560	3.797940	8.142230	4.707080	3.733030	8.133360	4.712470
Zn	9.489450	0.684650	4.596140	9.483910	0.681240	4.594920	9.482700	0.696850	4.593170
Zn	8.416720	3.220880	4.626460	8.459300	3.231020	4.619670	8.447940	3.245610	4.613850
Zn	5.281560	10.546500	4.662920	5.273480	10.547530	4.661490	5.276650	10.576990	4.660560
Zn	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840
Zn	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840
Zn	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840
Zn	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840
Zn	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840
Zn	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840
Zn	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840
Zn	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000
Zn	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000
Zn	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000
Zn	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000
Zn	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000

CH ₃ O	IS:			TS			FS		
C	0.851270	6.524530	9.616480	2.489210	5.447320	9.229580	2.795760	5.487130	9.345500
H	-0.048180	6.021640	9.995090	3.569830	4.702220	8.955900	2.507470	4.578460	9.892200
H	0.888410	7.548120	10.008120	1.960210	4.723870	9.856580	3.704060	6.002520	9.687620
H	1.742320	5.973770	9.956210	2.940840	6.249740	9.840280	3.136700	3.049190	7.925960
O	0.830920	6.543580	8.169320	1.568060	6.033290	8.313620	1.834390	6.196100	8.805740
Pd	-0.875110	2.263970	6.639220	-0.853820	2.265350	6.641900	-0.873010	2.233840	6.622600
Pd	-2.945940	7.055980	6.990430	-2.843140	7.090780	6.999950	-2.849630	7.102690	6.989250
Pd	1.787250	2.445620	6.881470	1.815730	2.425110	6.819540	1.772790	2.389810	6.916100
Pd	-1.442990	10.077750	6.832650	-1.482250	10.048350	6.841780	-1.458580	10.036600	6.837520
Pd	4.507510	2.350720	6.929280	4.527110	2.309730	6.907670	4.511730	2.361710	6.916530
Pd	3.408360	4.818060	7.012380	3.518720	4.786960	7.144310	3.356870	4.802640	7.380950
Pd	1.340180	9.905290	6.967180	1.295780	9.838650	6.949570	1.317920	9.812030	6.965710
Pd	7.172650	2.480550	6.950630	7.194210	2.462010	6.935430	7.187230	2.449910	6.939140
Pd	4.949450	7.132940	6.851080	5.008240	7.147640	6.846810	4.975910	7.067460	6.808330
Pd	4.237110	9.886460	6.932150	4.204840	9.862010	6.936670	4.227520	9.843470	6.922370
Pd	1.375610	0.571480	4.809960	1.375760	0.528500	4.794920	1.390730	0.563950	4.797100
Pd	-0.794620	5.561430	4.995300	-0.757830	5.555790	5.010880	-0.755460	5.547400	5.029400

Pd	-1.660290	8.146360	4.737140	-1.634280	8.124800	4.698230	-1.634480	8.127050	4.703250
Pd	4.161240	0.816650	4.680940	4.163030	0.796530	4.676930	4.191570	0.762940	4.679990
Pd	1.966130	5.577840	4.814990	2.022620	5.512010	4.901910	2.031900	5.481380	4.948150
Pd	1.100560	8.126820	4.782990	1.148040	8.066980	4.709630	1.163460	8.046000	4.727210
Pd	6.915450	0.790620	4.830320	6.916800	0.775250	4.825960	6.924670	0.778070	4.832080
Pd	2.682680	10.506760	4.715430	2.676240	10.492230	4.713050	2.675840	10.489980	4.718990
Pd	7.107570	5.546040	4.824580	7.130030	5.550130	4.843920	7.118570	5.536060	4.859120
Pd	6.350410	8.275170	4.824580	6.390270	8.279990	4.822390	6.380620	8.274540	4.819350
Pd	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840
Pd	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840
Pd	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840
Pd	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840
Pd	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840
Pd	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840
Pd	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840
Pd	3.392640	6.543340	2.502840	3.392630	6.543340	2.502840	3.392640	6.543340	2.502840
Pd	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840
Pd	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840
Pd	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840
Pd	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840
Pd	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840
Pd	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pd	-2.140170	4.907540	0.000000	8.567630	4.907540	0.000000	-2.140170	4.907540	0.000000
Pd	-3.210260	7.361300	0.000000	7.497540	7.361300	0.000000	-3.210260	7.361300	0.000000
Pd	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000
Pd	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000
Pd	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000
Pd	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000
Pd	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000
Pd	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000
Pd	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000
Pd	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000
Pd	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000
Pd	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000
Pd	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000
Pd	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000
Zn	-5.129120	12.172390	7.098980	-5.148680	12.145480	7.067730	-5.129580	12.141580	7.067860
Zn	8.623540	4.606160	7.028420	8.632120	4.605910	7.047740	-2.101390	4.603120	7.047640
Zn	-3.959670	9.471910	7.148190	-3.993800	9.449670	7.169840	-3.974230	9.463670	7.154950
Zn	2.909500	0.142440	6.961850	2.905190	0.119160	6.953160	2.922480	0.110430	6.952040
Zn	0.691650	4.746850	7.020270	0.622600	4.684670	7.031990	0.615070	4.656950	7.042710
Zn	-0.426110	7.620590	6.933860	-0.341150	7.669380	6.845130	-0.322650	7.622680	6.841700
Zn	0.203330	12.250390	6.964430	0.199990	12.219010	6.952410	0.212980	12.219260	6.952020
Zn	2.418880	7.351290	6.968020	2.425520	7.405290	6.940650	2.426450	7.407210	7.063940
Zn	2.895470	12.159770	6.961640	2.876980	12.134520	6.955140	2.883440	12.117700	6.967880

Zn	5.979960	4.774970	7.227470	6.042470	4.771380	7.193190	5.968220	4.721510	7.226270
Zn	0.484650	3.237340	4.620520	0.512060	3.222310	4.610800	0.498730	3.212910	4.609280
Zn	-2.680700	10.556190	4.626770	-2.671450	10.533500	4.624970	-2.673670	10.543670	4.629760
Zn	3.120590	3.235400	4.776920	3.176070	3.227560	4.758640	3.133720	3.161590	4.754860
Zn	0.027350	10.575070	4.653570	0.025670	10.542620	4.650210	0.033070	10.511710	4.651040
Zn	5.806540	3.169560	4.724160	5.838970	3.168640	4.716140	5.825800	3.160600	4.710290
Zn	4.553380	5.600360	4.718700	4.572050	5.570950	4.750520	4.569050	5.566880	4.715500
Zn	3.734310	8.127430	4.712860	3.783450	8.109470	4.708330	3.772380	8.106830	4.721600
Zn	9.488280	0.698020	4.593920	9.490020	0.690140	4.596760	9.494570	0.684520	4.592300
Zn	8.447290	3.239910	4.615920	8.470320	3.242790	4.613450	8.461470	3.243390	4.616800
Zn	5.273410	10.575270	4.659530	5.264170	10.556840	4.662390	5.275010	10.561690	4.656490
Zn	-1.961260	6.543340	2.502840	-1.961270	6.543340	2.502840	-1.961260	6.543340	2.502840
Zn	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840
Zn	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840
Zn	0.715690	6.543340	2.502840	0.715680	6.543340	2.502840	0.715690	6.543340	2.502840
Zn	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840
Zn	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840
Zn	6.069590	6.543340	2.502840	6.069580	6.543340	2.502840	6.069590	6.543340	2.502840
Zn	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000
Zn	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000
Zn	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000
Zn	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000
Zn	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000

CH₂O

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C	2.434600	5.235820	9.238170	2.501710	4.368600	9.125280	2.867510	4.949930	9.405620
H	2.691390	4.217890	9.587160	2.689750	3.345660	8.132420	3.789480	4.857480	10.021920
H	3.003040	6.055000	9.707530	3.205080	4.225290	9.971890	3.131820	3.047410	7.911110
O	1.189870	5.497300	8.910440	1.336670	4.712950	9.372820	1.758740	4.985060	9.871600
Pd	-0.899950	2.273620	6.648370	-0.899950	2.273620	6.648370	-0.886320	2.240840	6.620820
Pd	-2.805650	7.109650	6.996790	-2.805650	7.109650	6.996790	-2.833400	7.107790	6.980100
Pd	1.784040	2.404910	6.771950	1.784040	2.404910	6.771950	1.763000	2.408730	6.912590
Pd	-1.476510	10.035890	6.834080	-1.476510	10.035890	6.834080	-1.471730	10.042310	6.843380
Pd	4.464930	2.458120	6.883970	4.464930	2.458120	6.883970	4.497030	2.401960	6.944150
Pd	3.286390	4.946180	7.285270	3.286390	4.946180	7.285270	3.222560	4.910670	7.455310
Pd	1.289770	9.872530	6.977860	1.289770	9.872530	6.977860	1.310420	9.812240	6.967170
Pd	7.141070	2.428790	6.963780	7.141070	2.428790	6.963780	7.167000	2.477890	6.951190
Pd	5.017660	7.103730	6.843570	5.017660	7.103730	6.843570	4.954040	7.095490	6.831190
Pd	4.210070	9.868240	6.937330	4.210070	9.868240	6.937330	4.216480	9.882300	6.939280
Pd	1.374260	0.505610	4.774520	1.374260	0.505610	4.774520	1.371670	0.567590	4.815020
Pd	-0.767140	5.510950	5.161240	-0.767140	5.510950	5.161240	-0.799070	5.551120	4.979130
Pd	-1.610900	8.086470	4.702540	-1.610900	8.086470	4.702540	-1.620540	8.151960	4.718150
Pd	4.156310	0.806860	4.692590	4.156310	0.806860	4.692590	4.172700	0.802070	4.681500
Pd	1.989570	5.508280	4.906880	1.989570	5.508280	4.906880	1.999230	5.499700	4.909100
Pd	1.168200	8.086310	4.706600	1.168200	8.086310	4.706600	1.164270	8.090160	4.698350

Pd	6.909980	0.789850	4.812690	6.909980	0.789850	4.812690	6.907700	0.812420	4.828070
Pd	2.671990	10.513260	4.723570	2.671990	10.513260	4.723570	2.671400	10.532480	4.733050
Pd	7.118110	5.537260	4.871010	7.118110	5.537260	4.871010	7.085120	5.543000	4.861150
Pd	6.400630	8.259740	4.823980	6.400630	8.259740	4.823980	6.380760	8.274950	4.831460
Pd	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840
Pd	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840
Pd	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840
Pd	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840
Pd	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840
Pd	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840
Pd	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840
Pd	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840
Pd	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840
Pd	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840
Pd	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840
Pd	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840
Pd	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840
Pd	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pd	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000
Pd	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000
Pd	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000
Pd	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000
Pd	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000
Pd	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000
Pd	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000
Pd	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000
Pd	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000
Pd	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000
Pd	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000
Pd	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000
Pd	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000
Pd	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000
Zn	-5.160320	12.168420	7.056070	-5.160320	12.168420	7.056070	-5.146170	12.160740	7.106540
Zn	-2.189270	4.588190	7.101990	8.518530	4.588190	7.101990	-2.111530	4.614000	7.054240
Zn	-3.995190	9.440250	7.171880	-3.995190	9.440250	7.171880	-3.992710	9.445920	7.186580
Zn	2.900320	0.112270	6.945810	2.900320	0.112270	6.945810	2.911660	0.120190	6.957180
Zn	0.549390	4.610510	7.198070	0.549390	4.610510	7.198070	0.573300	4.672700	6.988840
Zn	-0.269850	7.639320	6.865150	-0.269850	7.639320	6.865150	-0.290770	7.610360	6.858620
Zn	5.526650	0.022700	6.953730	5.526650	0.022700	6.953730	0.197450	12.229070	6.950110
Zn	2.502290	7.522940	6.910520	2.502290	7.522940	6.910520	2.428120	7.404460	6.962900
Zn	2.858560	12.140740	6.965190	2.858560	12.140740	6.965190	2.858230	12.146810	6.978270
Zn	5.900310	4.718370	7.239640	5.900310	4.718370	7.239640	5.932550	4.758890	7.221230
Zn	0.489560	3.226650	4.614440	0.489560	3.226650	4.614440	0.481020	3.207330	4.604160
Zn	-2.663020	10.508600	4.620850	-2.663020	10.508600	4.620850	-2.681830	10.555730	4.634060
Zn	3.150550	3.232790	4.713260	3.150550	3.232790	4.713260	3.115860	3.190430	4.772130

Zn	0.026790	10.553020	4.659000	0.026790	10.553020	4.659000	0.025290	10.546150	4.659210
Zn	5.827090	3.180390	4.716720	5.827090	3.180390	4.716720	5.788000	3.187540	4.729900
Zn	4.559720	5.616190	4.717540	4.559720	5.616190	4.717540	4.544710	5.611060	4.707930
Zn	3.803560	8.143960	4.681300	3.803560	8.143960	4.681300	3.778940	8.159570	4.706840
Zn	9.485710	0.689140	4.600110	9.485710	0.689140	4.600110	9.479930	0.685970	4.593430
Zn	8.453320	3.242000	4.621130	8.453320	3.242000	4.621130	8.432450	3.247450	4.619640
Zn	5.267930	10.548220	4.662130	5.267930	10.548220	4.662130	5.275040	10.569650	4.669380
Zn	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840
Zn	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840
Zn	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840
Zn	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840
Zn	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840
Zn	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840
Zn	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840
Zn	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000
Zn	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000
Zn	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000
Zn	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000
Zn	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000

CHO	IS:			TS			FS		
C	2.867510	4.949930	9.405620	3.107340	5.017310	9.436610	3.014740	3.196440	8.571110
H	3.789480	4.857480	10.021920	4.030860	4.175900	9.220950	5.877840	2.423790	8.276960
O	1.758740	4.985060	9.871600	2.686570	5.245610	10.539320	2.873300	3.220520	9.747770
Pd	-0.886320	2.240840	6.620820	-0.877700	2.243320	6.643480	-0.901060	2.237070	6.588440
Pd	-2.833400	7.107790	6.980100	-2.831690	7.108220	6.986100	-2.831490	7.093510	6.978210
Pd	1.763000	2.408730	6.912590	1.794480	2.443920	6.808550	1.758090	2.408400	7.047410
Pd	-1.471730	10.042310	6.843380	-1.477410	10.046780	6.841430	-1.447170	10.028360	6.835030
Pd	4.497030	2.401960	6.944150	4.491390	2.481070	6.883280	4.454860	2.350290	7.231590
Pd	3.222560	4.910670	7.455310	3.175400	4.965030	7.511620	3.217340	4.870350	7.298930
Pd	1.310420	9.812240	6.967170	1.296140	9.815780	6.957780	1.329710	9.804260	6.978000
Pd	7.167000	2.477890	6.951190	7.172180	2.461960	6.955970	7.168180	2.417810	7.122180
Pd	4.954040	7.095490	6.831190	4.979440	7.101720	6.836960	4.964320	7.063150	6.815370
Pd	4.216480	9.882300	6.939280	4.199270	9.859360	6.928960	4.238920	9.845570	6.922180
Pd	1.371670	0.567590	4.815020	1.377370	0.537410	4.798350	1.406300	0.625450	4.839380
Pd	-0.799070	5.551120	4.979130	-0.751820	5.541870	4.993220	-0.836610	5.550270	4.966830
Pd	-1.620540	8.151960	4.718150	-1.616950	8.127700	4.717370	-1.622360	8.155820	4.717330
Pd	4.172700	0.802070	4.681500	4.169700	0.777600	4.702610	4.215230	0.860010	4.723170
Pd	1.999230	5.499700	4.909100	2.051020	5.449630	4.968340	1.962710	5.522360	4.862870
Pd	1.164270	8.090160	4.698350	1.168940	8.045080	4.692320	1.162120	8.114020	4.696710
Pd	6.907700	0.812420	4.828070	6.914120	0.794640	4.820740	6.966020	0.846600	4.858940
Pd	2.671400	10.532480	4.733050	2.665830	10.508820	4.721710	2.673150	10.543920	4.740090
Pd	7.085120	5.543000	4.861150	7.145730	5.569630	4.825020	7.048790	5.508800	4.884230

Pd	6.380760	8.274950	4.831460	6.383640	8.280630	4.834070	6.383450	8.270960	4.827130
Pd	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840
Pd	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840
Pd	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840
Pd	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840
Pd	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840
Pd	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840
Pd	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840
Pd	3.392640	6.543340	2.502840	3.392630	6.543340	2.502840	3.392640	6.543340	2.502840
Pd	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840
Pd	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840
Pd	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840
Pd	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840
Pd	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840
Pd	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pd	-2.140170	4.907540	0.000000	8.567630	4.907540	0.000000	-2.140170	4.907540	0.000000
Pd	-3.210260	7.361300	0.000000	7.497540	7.361300	0.000000	-3.210260	7.361300	0.000000
Pd	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000
Pd	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000
Pd	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000
Pd	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000
Pd	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000
Pd	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000
Pd	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000
Pd	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000
Pd	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000
Pd	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000
Pd	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000
Pd	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000
Zn	-5.146170	12.160740	7.106540	-5.152730	12.137950	7.071750	-5.138410	12.147670	7.105940
Zn	8.596270	4.614000	7.054240	8.613950	4.613810	7.049480	-2.111200	4.593820	7.044330
Zn	-3.992710	9.445920	7.186580	-4.000990	9.455640	7.173860	-3.966670	9.449590	7.166760
Zn	2.911660	0.120190	6.957180	2.904000	0.132020	6.950110	2.913870	0.085280	6.952110
Zn	0.573300	4.672700	6.988840	0.585950	4.673350	7.043880	0.576190	4.703290	6.958620
Zn	-0.290770	7.610360	6.858620	-0.291330	7.621670	6.866390	-0.288450	7.596630	6.859110
Zn	0.197450	12.229070	6.950110	0.185020	12.267060	6.950140	0.217510	12.217230	6.978930
Zn	2.428120	7.404460	6.962900	2.431440	7.424790	6.957480	2.424470	7.378120	6.945220
Zn	2.858230	12.146810	6.978270	2.855350	12.138480	6.964070	2.889530	12.110780	7.013990
Zn	5.932550	4.758890	7.221230	5.967290	4.757930	7.122390	5.931590	4.733950	7.224070
Zn	0.481020	3.207330	4.604160	0.495390	3.204590	4.600860	0.484730	3.222060	4.602130
Zn	-2.681830	10.555730	4.634060	-2.671970	10.530330	4.628240	-2.679510	10.565130	4.633900
Zn	3.115860	3.190430	4.772130	3.164660	3.187050	4.715000	3.099790	3.193890	4.838130
Zn	0.025290	10.546150	4.659210	0.031350	10.525030	4.657630	0.026470	10.566540	4.661700
Zn	5.788000	3.187540	4.729900	5.836800	3.184200	4.713180	5.760590	3.156910	4.788670
Zn	4.544710	5.611060	4.707930	4.582730	5.598810	4.713730	4.510170	5.576870	4.728210

Zn	3.778940	8.159570	4.706840	3.780640	8.131010	4.702380	3.779380	8.158610	4.704620
Zn	9.479930	0.685970	4.593430	9.486770	0.687410	4.599620	9.515560	0.672570	4.579560
Zn	8.432450	3.247450	4.619640	8.464730	3.243880	4.619900	8.419050	3.244900	4.612880
Zn	5.275040	10.569650	4.669380	5.261180	10.561610	4.660550	5.289950	10.574200	4.663570
Zn	-1.961260	6.543340	2.502840	-1.961270	6.543340	2.502840	-1.961260	6.543340	2.502840
Zn	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840
Zn	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840
Zn	0.715690	6.543340	2.502840	0.715680	6.543340	2.502840	0.715690	6.543340	2.502840
Zn	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840
Zn	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840
Zn	6.069590	6.543340	2.502840	6.069580	6.543340	2.502840	6.069590	6.543340	2.502840
Zn	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000
Zn	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000
Zn	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000
Zn	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000
Zn	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000

	CH ₃ O_H ₂ O			IS:			TS			FS		
C	1.169340	8.151730	10.342410	1.091330	8.075240	9.767600	1.038920	8.988260	8.952210			
H	1.272190	9.203140	10.159940	1.199820	9.388850	9.295730	1.894710	9.119160	9.625720			
H	2.022660	7.788770	10.935650	1.967120	7.750600	10.348500	0.094290	9.338780	9.385510			
H	0.286250	7.964920	10.981250	0.183110	7.893360	10.360730	0.892180	6.172870	9.180350			
H	0.923530	5.945930	9.520910	0.920370	5.902070	8.998560	1.644440	4.812270	9.499380			
H	1.836940	4.439320	9.053910	1.547420	4.445820	9.413490	2.978400	10.510270	7.938380			
O	0.900710	4.777080	8.945740	0.727350	4.880920	9.101950	0.955000	7.680340	8.452880			
O	1.066750	6.717560	8.433810	1.023360	7.310590	8.541460	0.783880	5.173020	9.200440			
Pd	-0.902660	2.233040	6.630960	-0.878390	2.230280	6.626820	-0.867220	2.296910	6.644670			
Pd	-2.848760	7.080930	6.986850	-2.882200	7.040290	6.998650	-2.955580	7.036940	7.008240			
Pd	1.780950	2.412560	6.839290	1.827900	2.336970	6.757880	1.821470	2.363130	6.793190			
Pd	-1.467030	10.043810	6.846890	-1.418030	10.042860	6.820940	-1.282830	10.082000	6.783800			
Pd	4.499220	2.372840	6.914660	4.507480	2.409920	6.908730	4.515780	2.387080	6.919090			
Pd	3.387950	4.838090	7.006380	3.360830	4.856750	6.983960	3.355160	4.817180	6.994070			
Pd	1.312850	9.905640	6.954130	1.360120	10.046500	6.963500	1.474540	10.048640	7.165380			
Pd	7.162060	2.513820	6.959640	7.171030	2.442620	6.968020	7.171510	2.469480	6.973410			
Pd	5.008040	7.132460	6.850350	4.991650	7.115820	6.857030	4.944620	7.112890	6.852580			
Pd	4.214120	9.888250	6.947740	4.248520	9.878030	6.927290	4.361730	9.916990	6.959390			
Pd	1.358590	0.541370	4.809850	1.380330	0.487500	4.762780	1.430850	0.526680	4.747020			
Pd	-0.838510	5.549910	5.000090	-0.809300	5.527920	5.166380	-0.808660	5.502230	5.151760			
Pd	-1.614280	8.154380	4.731830	-1.632070	8.095630	4.736890	-1.677580	8.084260	4.729590			
Pd	4.142760	0.817570	4.686160	4.148370	0.845930	4.685200	4.190720	0.860650	4.676000			
Pd	1.924590	5.563940	4.827060	1.921110	5.615190	4.824300	1.923720	5.638870	4.813960			
Pd	1.154060	8.129020	4.752500	1.110750	8.180570	4.833090	1.077260	8.223820	4.836910			
Pd	6.896220	0.814800	4.834740	6.911340	0.788620	4.820600	6.947390	0.789310	4.833770			
Pd	2.678400	10.539900	4.727480	2.702330	10.517170	4.706770	2.699850	10.515910	4.738350			
Pd	7.058540	5.531600	4.869230	7.103620	5.521030	4.844340	7.097500	5.553770	4.822660			

Pd	6.393550	8.283200	4.830860	6.369280	8.229860	4.813480	6.329010	8.291580	4.859060
Pd	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840	0.178910	1.635800	2.502840
Pd	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840	-0.891180	4.089570	2.502840
Pd	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840	-3.031350	8.997110	2.502840
Pd	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840	1.785770	4.089570	2.502840
Pd	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840	-0.354400	8.997110	2.502840
Pd	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840	-1.424490	11.450880	2.502840
Pd	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840	4.462720	4.089570	2.502840
Pd	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840	3.392640	6.543340	2.502840
Pd	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840	1.252460	11.450880	2.502840
Pd	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840	8.209760	1.635800	2.502840
Pd	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840	7.139670	4.089570	2.502840
Pd	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840	4.999500	8.997110	2.502840
Pd	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840	3.929410	11.450880	2.502840
Pd	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
Pd	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000	-2.140170	4.907540	0.000000
Pd	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000	-3.210260	7.361300	0.000000
Pd	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000	-4.280350	9.815070	0.000000
Pd	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000	2.676950	0.000000	0.000000
Pd	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000	1.606860	2.453770	0.000000
Pd	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000	0.536780	4.907540	0.000000
Pd	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000	-0.533310	7.361300	0.000000
Pd	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000	5.353900	0.000000	0.000000
Pd	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000	4.283810	2.453770	0.000000
Pd	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000	2.143640	7.361300	0.000000
Pd	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000	1.073550	9.815070	0.000000
Pd	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000	8.030850	0.000000	0.000000
Pd	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000	5.890680	4.907540	0.000000
Pd	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000	4.820590	7.361300	0.000000
Zn	-5.150530	12.166020	7.105800	-5.104290	12.151880	7.069960	-5.032440	12.233940	7.078040
Zn	8.583690	4.612150	7.081350	8.567750	4.563620	7.121360	8.575150	4.593220	7.134850
Zn	-3.987620	9.447080	7.185560	-3.944410	9.436400	7.141270	-3.823880	9.518770	7.125240
Zn	2.900160	0.120040	6.958010	2.927410	0.074100	6.951740	2.969320	0.093000	6.941100
Zn	0.654610	4.699760	6.912070	0.663460	4.551650	7.024230	0.682100	4.614050	7.089160
Zn	-0.301650	7.575910	6.948360	-0.355390	7.613150	6.985030	-0.435010	7.525630	6.902650
Zn	0.173480	12.255410	6.953430	5.545440	0.055090	6.982620	5.607070	0.051150	7.005730
Zn	2.458180	7.387580	7.008790	2.475200	7.457530	7.032440	2.419820	7.298580	6.940350
Zn	2.857450	12.162860	6.970070	2.925030	12.188930	6.970780	8.357220	0.020900	6.955950
Zn	5.952280	4.761210	7.233420	5.941080	4.736750	7.236960	5.942560	4.756900	7.237160
Zn	0.463130	3.204070	4.604000	0.478300	3.224690	4.600330	0.491110	3.234660	4.605730
Zn	-2.676090	10.545860	4.629210	-2.657650	10.497580	4.618660	-2.639430	10.503370	4.624370
Zn	3.112430	3.248960	4.760770	3.133690	3.289790	4.722160	3.126330	3.285480	4.727880
Zn	0.021940	10.569510	4.659660	0.034470	10.620010	4.655330	0.064810	10.650610	4.635530
Zn	5.785390	3.182870	4.722710	5.815480	3.169790	4.721160	5.816740	3.179310	4.726210
Zn	4.504440	5.611680	4.738780	4.544930	5.620880	4.711840	4.541060	5.616370	4.710100

Zn	3.778870	8.167450	4.720170	3.736820	8.126950	4.722740	3.714810	8.132200	4.713110
Zn	9.471770	0.693690	4.591560	9.492300	0.677890	4.582930	9.522940	0.705800	4.585750
Zn	8.423780	3.245430	4.625420	8.452590	3.236390	4.622600	8.450340	3.252100	4.617990
Zn	5.270200	10.566850	4.667680	5.286350	10.532150	4.650910	5.292170	10.582530	4.636600
Zn	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840	-1.961260	6.543340	2.502840
Zn	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840	-4.101440	11.450880	2.502840
Zn	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840	2.855860	1.635800	2.502840
Zn	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840	0.715690	6.543340	2.502840
Zn	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840	5.532810	1.635800	2.502840
Zn	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840	2.322550	8.997110	2.502840
Zn	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840	6.069590	6.543340	2.502840
Zn	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000	-1.070090	2.453770	0.000000
Zn	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000	-1.603400	9.815070	0.000000
Zn	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000	3.213730	4.907540	0.000000
Zn	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000	6.960760	2.453770	0.000000
Zn	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000	3.750500	9.815070	0.000000