Support Information for

Palladium-Atom Catalyzed Formic Acid Decomposition and the Switch of Reaction Mechanism with Temperature

Nan He[a] and Zhen Hua Li*[a]

Collaborative Innovation Center of Chemistry for Energy Material, Shanghai Key Laboratory of Molecular Catalysis & Innovative Materials, Department of Chemistry, Fudan University, Shanghai 200433, China

List of supporting materials:

Multireference character.

T_1-diagnostic value is a factor to indicate how strong the multireference character is for the wavefunction of a certain structure (see ref. 68, ref. 69 and ref. 70). If the multireference effects are strong, then the results of single-reference WFT methods would be doubtful. It is recommended that the T_1-diagnostic value should be less than 0.05 (ref. 68) or 0.04 (ref. 69) to ignore multireference effects. The results show that all T_1-diagnostic values are small enough in this work to use CCSD(T) as a standard.

Table S1 T_1-diagnostic values of some important structures. (CCSD/aug-cc-pVDZ)

Structure	***T*$_1$-diagnostics**
I1.11	0.033
I1.12	0.030
I1.31	0.026
I1.32	0.034
I1.13	0.028
I1.41	0.028
TS1.12	0.028
TS1.21	0.031
TS1.31	0.030
TS1.32	0.035
TS1.33	0.025
TS1.11	0.028
TS1.42	0.027

Energy barriers of twelve elementary steps.

Table S2 Potential-energy barriers of twelve elementary steps calculated with different methods. "-" denotes that a different step was obtained by that DFT method from that of the mPW2PLYP method so that a comparison on energy barrier of that step does not make sense. So they would not be used in error estimations (for example, calculating MUE for BLYP would use 10 barriers without EB4 and EB5).

DFT Methods	EB1 I1.11-TS1.11	EB2 I1.12-TS1.12a	EB3 I1.12-TS1.12b	EB4 I1.21-TS1.21a	EB5 I1.21-TS1.21b	EB6 I1.31-TS1.31	EB7 I1.32-TS1.32	EB8 I1.33-TS1.33	EB9 I1.31-TS1.40	EB10 I1.41b-TS1.41a	EB11 I1.41b-TS1.41b	EB12 I1.41b-TS1.41c
B2PLYP	27.97	22.70	22.20	34.37	1.53	20.90	7.66	8.84	7.32	17.20	22.05	31.69
B97D3	24.33	19.89	22.82	-	-	15.13	6.02	8.83	3.56	18.18	20.92	31.02
BLYP	20.41	22.64	23.76	-	-	12.97	6.74	9.31	4.41	15.41	21.88	30.03
BPW91	21.57	21.35	-	-	-	14.79	6.82	8.98	3.06	17.11	20.10	30.61
OLYP	22.16	20.48	24.35	27.84	0.01	17.22	6.16	9.00	3.54	20.48	21.21	32.07
HCTH-407	24.71	19.57	23.96	28.76	0.27	18.65	5.93	8.59	3.84	22.05	21.30	32.90
PBE	22.33	21.07	-	-	-	15.32	7.03	8.72	2.75	17.82	19.68	30.30
B3LYP	24.93	24.35	21.93	32.61	1.92	21.28	7.27	10.30	7.15	18.87	24.47	34.21
B3PW91	25.30	23.18	21.16	32.75	0.73	22.59	7.35	9.98	5.72	20.28	23.09	34.46
B3LYP-GD3	25.25	24.62	22.00	33.03	1.94	21.40	6.87	10.49	6.82	18.99	24.85	34.05
B3PW91-GD3	25.31	23.50	21.16	33.02	0.70	22.67	6.90	10.21	5.33	20.43	23.54	34.27
SOGGA-11x	31.09	25.09	20.07	42.04	5.71	30.22	8.00	10.67	10.51	21.63	25.09	36.81
LC-wPBE	25.78	28.50	19.47	41.47	2.58	28.75	10.02	11.75	7.84	18.42	24.17	36.85
wB97	28.32	28.63	19.54	43.29	4.61	28.74	10.23	11.29	9.46	17.47	25.19	36.84
N12SX	22.19	26.91	23.70	-	0.52	23.84	8.13	11.66	6.21	21.21	25.36	35.90
M06L	25.44	19.55	18.50	31.38	1.15	18.99	6.36	9.18	6.95	16.50	19.72	34.47
M11L	32.57	16.69	16.06	42.01	9.70	28.90	5.34	10.22	14.93	18.84	19.11	34.73
MN12L	6.76	42.38	17.74	-	-	18.99	11.99	20.20	9.83	13.37	34.79	43.79
TPSS	18.45	24.24	-	-	-	14.52	7.81	10.04	5.94	13.70	19.57	30.99
rev-TPSS	16.68	26.12	-	-	-	14.82	8.89	10.68	6.90	13.01	19.15	32.68
tHCTHhyb	22.22	23.79	21.40	30.38	0.24	19.87	7.46	10.20	3.78	18.85	23.46	33.94
MN12SX	19.26	31.15	19.72	29.37	0.74	24.70	8.00	14.65	4.66	18.22	30.47	39.15
M11	27.23	24.32	18.59	-	-	28.14	8.40	11.47	8.34	19.34	26.26	36.87
MPW2PLYP	28.06	23.97	22.00	35.57	1.66	22.20	7.99	9.38	7.54	19.36	24.92	36.49
CC/CBS	27.47	25.61	21.81	36.16	0.66	22.42	8.66	9.76	5.83	18.79	25.79	36.73

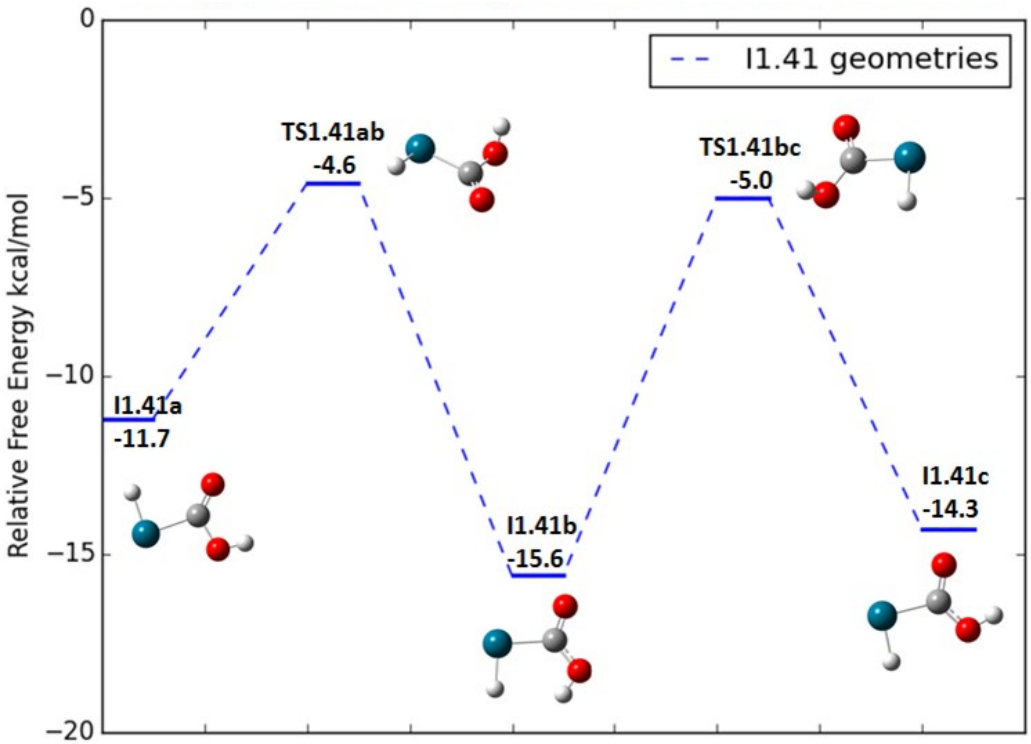

Figure S1 Free-energy profiles for the inter-conversion among three I1.41 intermediates.

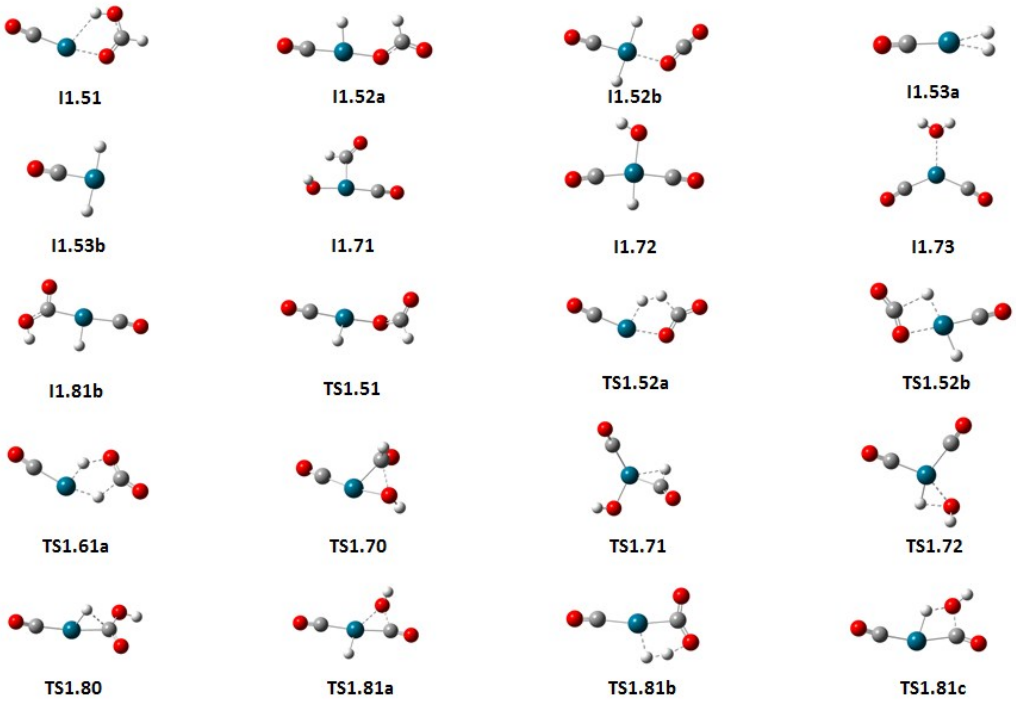

Figure S2 Geometries of ISs and TSs in PdCO catalyzed FAD reaction routes

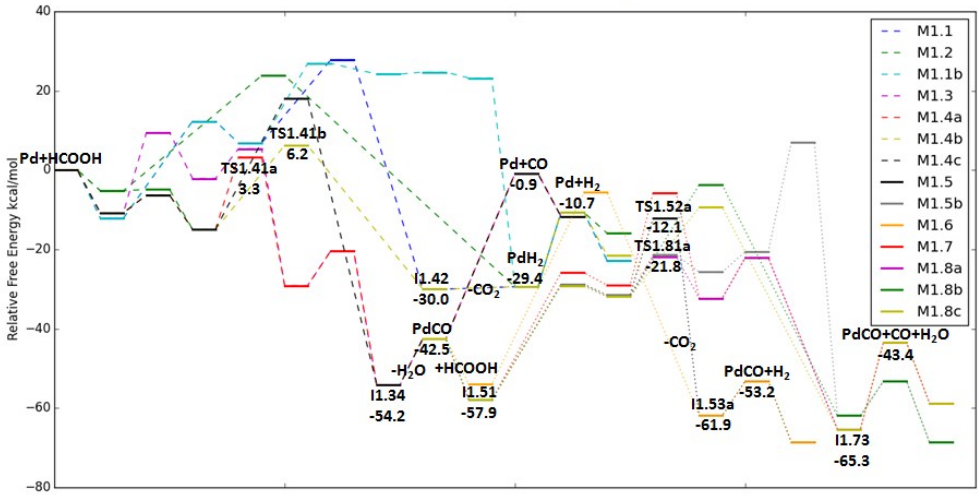

Figure S3 Free-energy profiles of the PdCO catalyzed FAD reaction pathways at room temperature

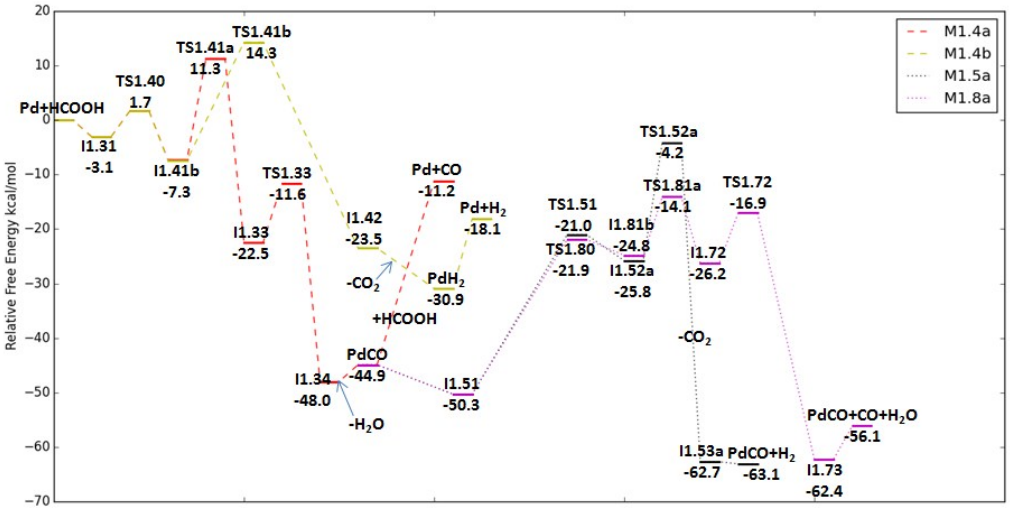

Figure S4 Free-energy profiles of the PdCO catalyzed FAD reaction pathways at 600 K. Only the four low-energy pathways are presented.

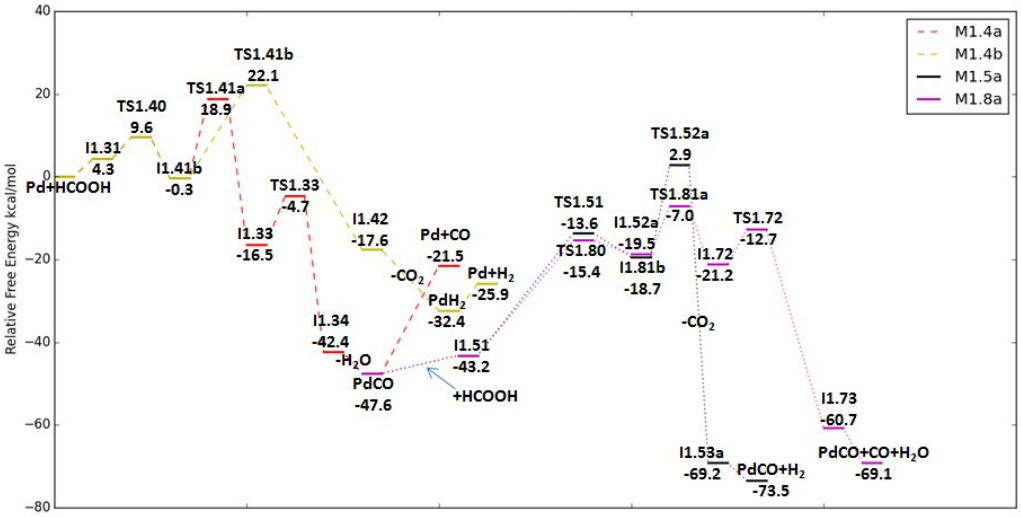

Figure S5 Free-energy profiles of the PdCO catalyzed FAD reaction pathways at 900 K. Only the four low-energy pathways are presented.

Cartesian coordinates for all optimized structures.

The structures with * are structures with an open-shell singlet wavefunction.

Vacuum:

I1.11

C	-1.98207500	0.33913000	0.00033600
O	-0.98872100	1.04708300	0.00024600
H	-2.98951400	0.74720600	0.00055700
O	-1.95569800	-0.97251100	0.00018200
H	-0.98138200	-1.21238500	-0.00000700
Pd	0.85692800	-0.04709100	-0.00013000

I1.12

C	1.93607000	0.33168400	-0.01835200
O	3.06438000	-0.08085300	-0.04512400
H	1.68374000	1.39505600	-0.10848100
O	0.89444800	-0.48200300	0.13165500
H	-0.74219700	1.38580600	0.47683400
Pd	-0.96149100	-0.00582900	-0.02066300

I1.13a

C	-1.48512000	0.03879600	-0.00001100
O	-1.06378000	1.17469500	0.00008000
H	1.76086000	-1.24036800	-0.42228800
O	-2.26929200	-0.82988800	-0.00004100
H	1.75960900	-1.24132000	0.42279300
Pd	0.69684400	-0.01107700	-0.00001600

I1.13b*

C	-1.98283600	0.17199200	0.00005100
O	-1.07031600	0.91158200	0.00043300
H	0.10899400	-1.52551100	0.00161600
O	-2.92142500	-0.49591000	-0.00033600
H	1.68215400	1.32227200	-0.00164200
Pd	0.91390900	-0.09030600	-0.00002300
I1.14			
H	0.00000000	0.42975400	-1.54539800
H	0.00000000	-0.42975400	-1.54539800
Pd	0.00000000	0.00000000	0.06719100
I1.14b*			
H	-0.05672074	0.00175793	1.63771080
H	-0.05445507	0.00170478	-1.65889836
Pd	-0.04128895	0.00128543	0.00476677
I1.21			
C	-1.27951700	-0.13323400	0.22318900
O	-1.72318900	-1.20271300	-0.09386100
H	-0.52647100	0.00767600	1.13219700
O	-1.89035300	1.02611900	-0.13421600
H	-1.38360600	1.76803200	0.21298300
Pd	0.83685900	0.00948800	-0.01868900
I1.31			
C	1.29842400	0.19438900	0.42782500
O	0.92218800	1.20140500	-0.21303900
H	1.33593900	0.15492400	1.51679300
O	2.11317100	-0.75061400	-0.10915400
H	2.15998800	-0.58146100	-1.05924300
Pd	-0.77324700	-0.09448100	-0.00971600
I1.32			
C	1.32085500	0.79945700	-0.01585100
O	2.16695100	-0.05231400	0.01354900
H	1.45938100	1.88398100	-0.05792900
O	-1.95421800	0.53698100	-0.10547600
H	-2.20124600	0.90766600	0.74801900
Pd	-0.19315500	-0.24925500	0.00305300
I1.33			
C	-1.60491900	-0.04594300	0.00889100
O	-2.74203900	-0.00663800	0.02712000
H	0.06088100	1.46080500	-0.20239200
O	2.15673400	-0.09552200	-0.04489200
H	2.64046000	0.44555600	0.58369700
Pd	0.25240500	-0.01768300	-0.00635800
I1.34			
C	1.64385300	0.00000100	0.02036300

O	2.79009700	0.00000400	0.05239400
H	-2.71158400	-0.77030500	0.40153800
O	-2.33516200	0.00000400	-0.03305800
H	-2.71157400	0.77032400	0.40152500
Pd	-0.17564000	-0.00000200	-0.02347700
I1.41b			
C	-1.13924800	0.11184600	0.00001300
O	-1.48751200	1.25897300	0.00002100
O	-1.96698600	-0.92833800	0.00002100
H	-1.42732700	-1.72783900	0.00001300
Pd	0.76218300	-0.00104200	-0.00000900
H	0.83839200	-1.54040600	-0.00002900
TS1.11			
C	1.92233800	-0.25039900	0.30095000
O	2.74752800	0.51319900	-0.12162300
H	2.02697100	-0.73222500	1.28439400
O	0.84284800	-0.66412700	-0.37631400
H	-0.42319700	1.44295700	-0.10449700
Pd	-0.91001800	0.04345800	0.02169400
TS1.12a			
C	-1.86054200	-0.07914900	0.00022100
O	-3.03354600	-0.24598500	0.00017700
H	-1.17923800	-1.24522100	0.00026200
O	-1.01266200	0.83394500	0.00019600
H	-0.14750800	-1.19708600	0.00000400
Pd	0.97521000	-0.03883600	-0.00010000
TS1.12b*			
C	-1.69486500	0.09991300	-0.00018000
O	-0.95254300	1.04819700	0.00014900
H	-0.37037000	-1.28418700	0.00069900
O	-2.69586600	-0.48805900	-0.00002000
H	1.85396000	1.09424200	-0.00032900
Pd	0.82332300	-0.10631800	-0.00000700
TS1.14*			
H	-0.00000000	1.61952628	-0.17550632
H	-0.00000000	-1.61952628	-0.17550632
Pd	-0.00000000	0.00000000	0.00763071
TS1.21a			
C	1.76961600	-0.01816400	0.00003100
O	2.62878200	-0.81970900	-0.00003500
H	0.51959500	-0.78604700	0.00028900
O	1.52936300	1.19594400	-0.00000500
H	0.10364100	1.08437800	-0.00000900
Pd	-0.96752400	-0.06954800	-0.00000300

TS1.21b

O	1.84487000	1.04370100	-0.07320600
H	1.22433700	1.75968300	0.10425100
Pd	-0.81182100	0.00255700	-0.01907800
H	0.22337800	0.03120900	1.19997800
C	1.19468900	-0.13362300	0.09228800
O	1.74612200	-1.18205000	-0.04934000

TS1.31

C	-1.28440200	-0.13356400	0.41821900
O	-2.10809100	-0.56557500	-0.31445800
H	-1.41167500	0.19569300	1.45582900
O	-0.25890800	1.63123200	0.01327300
H	-0.45258800	1.86960900	-0.90126600
Pd	0.61971000	-0.21280800	-0.01422600

TS1.32

C	-1.41046200	0.10906400	0.41803700
O	-2.25375900	0.50258300	-0.31589200
H	-1.55450100	-0.11268000	1.49476300
O	1.31838100	1.32995500	0.14292900
H	1.07587600	1.90059800	-0.59466000
Pd	0.35474300	-0.36851700	-0.04390300

TS1.33

C	-1.62525700	0.03554500	0.00011300
O	-2.75096800	0.20913400	0.00171000
H	0.92091900	1.25716300	-0.15267800
O	2.18135900	0.21431200	-0.10018300
H	2.54131500	0.51917500	0.73997200
Pd	0.23578700	-0.11689500	0.00434400

TS1.40

C	1.15761400	0.13056900	0.08676500
O	1.74769300	1.16782600	-0.04578900
O	1.75299700	-1.08323800	-0.01893400
H	2.67965100	-0.91576300	-0.25317700
Pd	-0.82115300	-0.01100600	-0.02134600
H	0.14217400	-0.03807400	1.23230200

TS1.41a

C	-1.15666400	-0.36782500	-0.00007800
O	-2.25156900	-0.69086800	0.00060900
O	-0.67735800	1.52707200	-0.11299700
H	-0.91592000	1.85597500	0.76243900
Pd	0.65352800	-0.10433900	0.00272200
H	1.22503100	-1.53907600	0.01193900

TS1.41b

C	1.24658900	-0.05835900	0.00001700

O	1.69777300	-1.16088500	0.00002700
O	1.60021400	1.15525100	0.00001600
H	0.34529200	1.54364300	-0.00001200
Pd	-0.72843500	-0.06033800	-0.00000900
H	-0.70071000	1.62715600	-0.00003900

TS1.41c

C	-0.41928900	-1.10421600	0.00000000
O	-1.20319000	-1.96753000	0.00000000
O	1.15559600	-1.50385700	0.00000000
H	1.54705600	-2.40179300	0.00000000
Pd	0.00000000	0.80477300	0.00000000
H	1.34943300	-0.22137400	0.00000000

Aqueous solution:

I1.11

C	1.96827500	0.32423700	0.00000200
O	0.98128400	1.05134400	-0.00000300
H	2.98062100	0.71555600	0.00001000
O	1.89555100	-0.98215500	-0.00000100
H	0.89029800	-1.16978500	-0.00000700
Pd	-0.84120100	-0.04445000	0.00000000

I1.12

C	1.93546100	0.31124400	-0.02292200
O	3.10232700	-0.05862500	-0.05039600
H	1.68230800	1.37178700	-0.14038700
O	0.93381100	-0.49450500	0.14662200
H	-0.68191500	1.30680800	0.60369500
Pd	-0.97613600	-0.00263100	-0.02381700

I1.13b*

C	-2.06989500	0.17501700	-0.00031100
O	-1.14740300	0.89341900	-0.00036800
H	0.19827600	-1.54097200	-0.02768800
O	-3.00143200	-0.50725900	0.00006200
H	1.67722400	1.36722800	0.02798100
Pd	0.95123700	-0.08603300	-0.00045000

I1.14

Pd	0.00000000	0.00000000	0.06293682
H	-0.00000000	0.48562117	-1.44754681
H	-0.00000000	-0.48562117	-1.44754681

I1.14b*

H	0.00000000	-0.00000000	-1.63472365
H	0.00000000	-0.00000000	1.63360345
Pd	-0.00000000	0.00000000	0.00002435

I1.21

C	-2.27907800	-0.27862500	0.00096400

O	-3.48690800	-0.26842000	-0.00108500
H	-1.68853200	-1.20164800	0.00346500
O	-1.55406400	0.82948400	0.00037100
H	-0.55642400	0.58410700	0.00128700
Pd	1.22276500	-0.04780900	-0.00010500
I1.31			
C	1.20604800	0.18157400	0.43306200
O	0.91454400	1.23968000	-0.21527000
H	1.31375700	0.18334900	1.51926400
O	2.05261700	-0.76680400	-0.10588100
H	2.04574200	-0.64703600	-1.06433200
Pd	-0.74637100	-0.09584300	-0.01052400
I1.32			
C	1.20265200	0.76291100	-0.02637900
O	2.27602600	0.22250200	0.01098100
H	1.04388700	1.84796600	-0.08371500
O	-1.69029000	0.98828100	-0.09339600
H	-1.61735300	1.52394800	0.70248400
Pd	-0.24626800	-0.38338400	0.00432200
I1.33			
C	-1.60863000	-0.02127300	0.00000800
O	-2.73980600	0.11384900	-0.00005900
H	0.11273000	1.41814100	-0.00009300
O	2.19652400	0.03452700	-0.00013600
H	2.55411700	0.92460100	0.00034400
Pd	0.24633000	-0.07395900	0.00002700
I1.34			
C	-1.62623700	0.00000900	0.00597900
O	-2.78201700	-0.00003700	0.00233800
H	2.75373700	0.76838100	0.31280100
O	2.33371000	-0.00005900	-0.08648900
H	2.75394600	-0.76822400	0.31291800
Pd	0.17035200	0.00001200	0.00025300
I1.41b			
C	-1.11916400	-0.11620700	-0.00000600
O	-1.59222200	-1.23195900	-0.00000900
O	-1.94328300	0.95194600	-0.00001100
H	-1.39116400	1.74259200	-0.00000700
Pd	0.77674700	-0.00699500	0.00000400
H	0.65982500	1.51652100	0.00004000
TS1.11			
C	1.93990500	-0.28755800	0.27138500
O	2.71651000	0.58233700	-0.09536800
H	2.13725900	-0.83059200	1.20946100

O	0.89178500	-0.70681800	-0.37759100
H	-0.36444000	1.39522200	-0.19457900
Pd	-0.91910000	0.04688200	0.02479300
TS1.12a			
C	1.93990500	-0.28755800	0.27138500
O	2.71651000	0.58233700	-0.09536800
H	2.13725900	-0.83059200	1.20946100
O	0.89178500	-0.70681800	-0.37759100
H	-0.36444000	1.39522200	-0.19457900
Pd	-0.91910000	0.04688200	0.02479300
TS1.12b*			
C	1.70785500	0.10904300	-0.00004100
O	0.98391600	1.06196700	-0.00009500
H	0.36123400	-1.27332000	-0.00051900
O	2.69341200	-0.51082400	0.00011500
H	-1.88095100	1.09594400	0.00059300
Pd	-0.82926200	-0.10621800	0.00000000
TS1.14*			
H	1.46634003	0.15660029	0.00000000
H	-1.46634003	-1.05417688	0.00000000
Pd	-0.00000000	0.01951253	0.00000000
TS1.21			
C	1.76152100	-0.06875300	0.00368700
O	2.75732600	-0.78228300	-0.00281800
H	0.75830900	-0.68612800	0.01745400
O	1.63730900	1.18039300	-0.00025200
H	-0.19863800	1.16703000	-0.00227900
Pd	-1.00621500	-0.07072300	-0.00027700
TS1.31			
C	-1.20676800	-0.22169300	0.42114300
O	-2.03659100	-0.70172900	-0.30533100
H	-1.34937100	-0.00525100	1.48876300
O	-0.54312400	1.57422500	0.02061300
H	-0.80948100	1.72282600	-0.89432600
Pd	0.65298200	-0.16016000	-0.01833800
TS1.32			
C	-1.33137300	0.12720900	0.38436900
O	-2.20672000	0.47931400	-0.35125100
H	-1.42832500	0.08262900	1.48488600
O	1.25543600	1.27658700	0.18229500
H	0.89831900	1.89216100	-0.46474800
Pd	0.34294100	-0.49689900	-0.13427600
TS1.33			
C	-1.60857900	0.05721700	0.00304600

O	-2.72378500	0.30990300	-0.00017700
H	0.87233400	1.22740700	-0.08716800
O	2.19212000	0.37208100	-0.10766900
H	2.50469800	0.57883900	0.78061400
Pd	0.22886400	-0.16533500	0.00328400

TS1.40a

C	1.16382700	0.12893400	0.31191500
O	1.58876700	1.20582100	-0.13113600
O	1.76238200	-1.06549900	-0.03771800
H	2.38912300	-0.86439200	-0.74707000
Pd	-0.80139500	-0.02293300	-0.02417600
H	0.68289200	0.02311300	1.33852000

TS1.40b

O	-1.83749900	-0.98865900	-0.17805500
H	-1.45955300	-1.76860600	0.24426200
Pd	0.79072300	-0.02233200	-0.02004400
H	-0.74359500	-0.01088200	1.33474800
C	-1.17839900	0.13414000	0.29163600
O	-1.54996400	1.23890200	-0.12279700

TS1.41a

C	1.11249800	-0.39010200	0.00199500
O	2.19683000	-0.77305400	0.00120200
O	0.82748100	1.51484000	-0.11216200
H	0.98824300	1.81158800	0.79243700
Pd	-0.66725800	-0.08401400	0.00095700
H	-1.16385500	-1.54063900	0.03927400

TS1.41b

C	-1.19934600	-0.06637900	-0.00000600
O	-1.73960300	-1.14292000	-0.00000500
O	-1.61997900	1.14744300	-0.00001200
H	-0.35028900	1.53466900	0.00002000
Pd	0.73391100	-0.06070500	0.00000200
H	0.66312500	1.61986300	0.00007000

TS1.41c

C	-0.51733500	-1.03443300	0.00000000
O	-1.28422000	-1.90136400	0.00000000
O	1.28998200	-1.58491900	0.00000000
H	1.75977900	-2.43953200	0.00000000
Pd	0.00000000	0.79661600	0.00000000
H	1.29814000	-0.10793200	0.00000000

PdCO routes:

I1.51

C	2.53109900	0.15130500	0.00003600
O	1.75617900	-0.79341300	0.00001800

H	3.60887900	0.01294500	0.00010300
O	2.18038100	1.41237600	-0.00002000
H	1.19002200	1.44500000	-0.00006100
Pd	-0.31743500	-0.33105300	-0.00001100
C	-2.02653300	0.32209000	-0.00000600
O	-3.08959800	0.74730300	0.00004000
I1.52a			
C	2.57874400	0.41311400	-0.00000800
O	3.70392700	-0.00974400	-0.00029900
H	2.35523400	1.48964400	0.00013300
O	1.50157900	-0.35616600	0.00018800
H	-0.47314800	1.40274400	0.00072400
Pd	-0.40091600	-0.09722400	0.00005700
C	-2.25416900	0.05805400	-0.00012000
O	-3.37893200	0.21002400	-0.00022900
I1.52b*			
C	2.55307400	0.08659200	0.00003500
O	1.73584600	-0.75737400	-0.00005400
H	0.11856900	1.40094300	-0.00106500
O	3.39727300	0.86757700	0.00018700
H	-0.91281500	-1.69003000	0.00087800
Pd	-0.37150500	-0.16516300	-0.00006100
C	-2.12098700	0.29902000	0.00008800
O	-3.22175000	0.58641000	0.00015100
I1.53a			
H	0.00000000	0.39442100	2.27824200
H	0.00000000	-0.39442100	2.27824200
Pd	0.00000000	0.00000000	0.51451700
C	0.00000000	0.00000000	-1.36534500
O	0.00000000	0.00000000	-2.50402500
I1.53b*			
H	0.00000000	1.62607600	0.50716700
H	0.00000000	-1.62607600	0.50716700
Pd	0.00000000	0.00000000	0.55569500
C	0.00000000	0.00000000	-1.24860400
O	0.00000000	0.00000000	-2.38558200
I1.71			
C	0.15007300	1.57577600	0.23663600
O	-0.67884300	2.28556600	-0.20859000
H	1.00862800	1.87436200	0.85348600
O	2.24448600	-0.34572800	0.01526900
H	2.64711600	-0.11363000	-0.82607700
Pd	0.30281100	-0.38011100	-0.00108900
C	-1.56857700	-0.59887900	0.01834100

O	-2.69989700	-0.70696700	0.00492500
I1.72			
C	-1.91758500	-0.27216600	0.00001600
O	-3.03821600	-0.42638700	0.00015800
O	0.21651400	1.89452500	0.00004100
H	-0.62471700	2.35596200	0.00001900
Pd	-0.02043800	-0.10763400	-0.00006300
H	-0.08396100	-1.66191100	-0.00013000
C	1.91408800	-0.32810400	0.00002200
O	3.03042700	-0.48579600	0.00015000
I1.73			
C	-1.75981300	-0.69408300	0.00771000
O	-2.73058900	-1.29567300	0.02788800
O	-0.00011600	2.51938900	-0.05884200
H	-0.76644900	2.95859300	0.31672200
Pd	0.00000600	0.06490700	-0.01524700
C	1.75986200	-0.69399100	0.00771200
O	2.73066600	-1.29553700	0.02789100
H	0.76621000	2.95868600	0.31662600
I1.81b			
C	2.17614500	0.05421000	-0.00006000
O	3.30652300	-0.02637700	0.00004300
O	-2.78065300	-0.74176700	0.00026700
H	-2.44592800	-1.64448200	0.00037800
Pd	0.22052800	-0.03677100	-0.00004400
H	0.23273000	-1.57603100	0.00019300
C	-1.73342300	0.07640400	0.00005600
O	-1.84929800	1.28418400	-0.00012300
TS1.51			
C	2.57993600	-0.03779800	0.29555100
O	3.11441500	0.97815800	-0.06687200
H	2.96650500	-0.63196300	1.13600100
O	1.51886800	-0.59463500	-0.27691900
H	-0.67507800	-0.66564500	1.32240400
Pd	-0.34921100	-0.16521800	-0.05220700
C	-2.14107000	0.27857100	0.01852000
O	-3.24089700	0.54809900	0.10112900
TS1.52a			
C	2.31014900	0.39851800	0.00004200
O	3.42339100	0.79749200	-0.00015100
H	1.40661100	1.38355200	0.00011500
O	1.67494700	-0.68120100	0.00016900
H	0.41040900	1.12571000	0.00006300
Pd	-0.40607400	-0.32880200	-0.00000300

C	-2.10942600	0.38884200	-0.00005200
O	-3.14108100	0.87014500	-0.00001700
TS1.52b*			
C	-2.15372600	0.25582500	0.00003200
O	-1.72576000	-0.87764100	-0.00000200
H	-0.61913300	1.18407300	-0.00006700
O	-2.97990300	1.07546600	0.00001200
H	1.06362900	-1.61626500	0.00022800
Pd	0.28974300	-0.23262600	-0.00001700
C	2.01162500	0.36961300	0.00007800
O	3.09065400	0.72472100	-0.00001300
TS1.61a			
C	2.33472100	0.35395000	0.00041000
O	3.36209400	-0.20361800	0.00203000
H	1.27008000	-0.81224200	0.00042400
O	1.72046400	1.41385400	-0.00151400
H	0.35293300	0.92319500	-0.00278300
Pd	-0.40634000	-0.46095500	-0.00043400
C	-2.12299300	0.34041900	0.00028600
O	-3.10777300	0.90561000	0.00175200
TS1.71			
C	1.09058300	1.13800500	0.41730900
O	1.29730600	2.02020000	-0.32918800
H	1.38213400	1.03787300	1.46631800
O	1.90172400	-0.87906000	0.06815800
H	2.31244300	-0.86982300	-0.80311700
Pd	-0.04587400	-0.47600500	-0.02823000
C	-1.80704000	0.16415000	0.00765200
O	-2.85973200	0.59826500	0.02173400
TS1.72			
C	1.92360500	-0.32887300	0.08008200
O	2.89824400	-0.79569500	0.42193200
H	-0.95340100	-1.21850600	-1.14323300
O	-0.86488600	1.87285500	0.43840400
H	-0.25730000	2.30702000	1.04383100
Pd	0.00735200	0.20612600	-0.23252100
C	-1.44795300	-0.94052000	-0.11756800
O	-2.28103300	-1.44640100	0.51719700
TS1.73			
C	-1.73643100	0.47464200	0.00359300
O	-2.78636200	0.91294700	0.01279200
H	-0.41789400	-1.83449700	-0.05964900
O	1.13016300	-2.04956400	-0.08264600
H	1.10585100	-2.53968700	0.74488400

Pd	-0.01831700	-0.32490300	-0.00567700
C	1.31727200	1.30754900	0.00220200
O	1.98989400	2.21494100	0.01249800
TS1.80			
C	-2.21516100	0.02548700	0.02236400
O	-3.33027500	0.12949500	0.19950500
O	2.37567500	1.12870500	0.02865600
H	3.32538900	0.94458000	-0.05803900
Pd	-0.26099700	-0.04875900	-0.10482600
H	0.39161300	0.38480900	1.23609600
C	1.74994300	-0.06509500	0.11949100
O	2.33961900	-1.11430600	0.12094200
TS1.81a			
C	-2.07309400	0.10651100	0.02432900
O	-3.20300400	0.17889900	0.05055500
O	1.34571600	1.40414600	-0.11586400
H	1.61967300	1.82092800	0.71085900
Pd	-0.16727000	-0.17368300	-0.01772900
H	-0.55283900	-1.65263900	-0.03366200
C	1.78485900	-0.22411000	-0.00670800
O	2.90191400	-0.51720300	0.06938700
TS1.81b			
C	-2.19851100	0.08804700	-0.00004600
O	-3.32987300	0.07113800	-0.00010300
O	2.48537700	-0.89664900	0.00014100
H	1.34000100	-1.50879400	0.00016100
Pd	-0.17607600	-0.05691500	0.00000900
H	0.31406100	-1.70672100	0.00013700
C	1.81092300	0.17083000	0.00001600
O	1.94086700	1.36055400	-0.00010700
TS1.81c			
C	1.79154800	-0.12581000	-0.02135000
O	2.84380400	-0.60549800	0.18139100
O	1.73509500	1.44416700	-0.10756300
H	2.42877800	1.89088300	0.41250900
Pd	-0.25621000	-0.29284700	-0.05076800
H	0.33739000	1.21825700	0.09466300
C	-2.12493100	0.11401200	0.05195300
O	-3.20142700	0.46540900	0.13173700