Supplemental Information for:

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Inaccessibility of beta-hydride elimination from
-OH functional groups in Wacker-Type Oxidation

Tabulated by John A. Keith (johnk@wag.caltech.edu)

Supplemental Information is divided into 4 parts:

--Wacker type date ->
Contains calculation data used in table 1

--Phenyl-ketone data ->
Contains calculation data used in table 1

--Miscellaneous Data ->
Contains calculated structures mentioned in the
manuscript

--Structures ->
Contains calculated structures mentioned in the
manuscript

--*-*-*-*-*-*-*-*-WACKER TYPE DATA*-*-*-*-*-*-*-*-*-*-
The following data table contains energies,
solvation energy, ZPE's and cartesian coordinates
of species referenced in Table 1 of the manuscript.

B3LYP//LACVP**++ Gas phase geometries, energies, frequencies
B3LYP//LACVP** Solvent single point

(Wacker) - pre TS structure (ground state)

Gas Phase Energy = -817.87238999778 = Eh
Solvent Correction = -0.03070087825 = Eh
Zero Point Energy = 60.009 = kcal/mol

Geometry Coordinates

Pd1	-0.8167951159	1.7656805743	0.0873896638
C2	-1.7825849483	3.0633076031	-1.0370020442
H3	-1.3711006587	3.0734701665	-2.0511984781
C4	-1.9759027442	4.4161196033	-0.4073951660
H5	-2.3901245094	4.3266873300	0.6014653118

H6	-1.0119425948	4.9268950616	-0.3462952643
H7	-2.6651607435	5.0248168105	-1.0090933687
O8	-2.9406322374	2.2546522039	-0.9240955415
H9	-2.9901396652	1.6345018907	-1.6662217777
Cl10	1.3817360704	2.6373915861	0.0181879475
O11	0.1589321630	0.1766546023	1.5194716770
H12	0.3450790039	-0.6865323961	1.1264086735
H13	1.0022094648	0.6675855403	1.5003914304

(Wacker) - BHE Transition State

Gas Phase Energy = -817.81191564472 = Eh
Solvent Correction = -0.02625256705 = Eh
Zero Point Energy = 55.475 = kcal/mol

Imaginary Frequencies (cm^-1): -1081.39

Geometry Coordinates

Pd1	0.0145791581	-0.0028040254	-0.0029575011
H2	0.0207251735	-0.0981181156	1.5741008090
O3	1.4831368955	0.0109864056	1.6849076195
Cl4	0.0804499857	-0.0525607999	-2.4420692033
C5	2.0790566020	-0.2459876594	0.5542487916
H6	2.5382729988	0.6130484532	0.0477012913
C7	2.5650543646	-1.6271663694	0.2268756026
H8	1.9132546215	-2.3891263517	0.6624367056
H9	2.6273951784	-1.7627810129	-0.8554559509
H10	3.5721470866	-1.7543907371	0.6501577572
O11	-2.1756336686	0.0917207935	-0.4444555705
H12	-2.5821340458	0.9493255545	-0.2580267362
H13	-2.0165532813	0.0550988325	-1.4130918104

(Wacker) -- BHE IRC, forward and reverse paths

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Summary of IRC Reaction Path:
Major Components
of TS Vector
(units are
Angstroms/Degrees)
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point #	Rxn. Coord	Energy	Coord 1
1	0.00000	-817.811939	41.2539
2	0.10000	-817.812146	43.0591
3	0.19998	-817.812696	44.9093
4	0.29995	-817.813496	46.7707
5	0.39994	-817.814454	48.6464
6	0.49992	-817.815498	50.5273
7	0.59992	-817.816567	52.4094
8	0.69992	-817.817612	54.2873
9	0.79988	-817.818615	56.1335
10	0.89984	-817.819525	57.9382
11	0.99978	-817.820350	59.6758
12	1.09967	-817.821061	61.3141
13	1.19950	-817.821668	62.8039
14	1.29929	-817.822186	64.0931
15	1.39900	-817.822628	65.1215
16	1.49876	-817.823034	65.8953

Coord 1 = H2-Pd1-O3

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Summary of IRC Reaction Path:

Major Components of TS Vector (units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1
1	-1.49821	-817.843731	26.0299
2	-1.39821	-817.841764	26.1443
3	-1.29823	-817.839766	26.2558
4	-1.19826	-817.837734	26.3806
5	-1.09832	-817.835648	26.5447
6	-0.99854	-817.833474	26.8523
7	-0.89913	-817.831104	27.4720
8	-0.79958	-817.828340	28.4846
9	-0.69982	-817.825195	29.7511
10	-0.59991	-817.821943	31.1850
11	-0.49994	-817.818894	32.7207
12	-0.39996	-817.816303	34.3288
13	-0.29997	-817.814297	35.9949
14	-0.19999	-817.812936	37.7089
15	-0.10000	-817.812176	39.4487
16	0.00000	-817.811939	41.2539

Coord 1 = H2-Pd1-O3

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(Wacker) -- RE Transition State

Gas Phase Energy = -817.84053067499 = Eh
Solvent Correction = -0.02553024257 = Eh
Zero Point Energy = 55.523 = kcal/mol

Imaginary Frequencies (cm^-1): -456.65

Geometry Coordinates

Pd1	-0.0056224695	-0.0145216867	-0.0249139695
Cl2	-0.0120289601	0.0183151745	3.4067363187
C3	2.0174782604	0.0192134987	0.4330052669
H4	2.5496253623	-0.4207485266	-0.4214128136
O5	1.5624030051	-0.8643884755	1.2936913500
H6	0.9524955305	-0.4396484134	2.3331396385
C7	2.4375086873	1.3998248885	0.8685618049
H8	3.4489748012	1.3503918552	1.2973889627
H9	2.4748089031	2.0776330745	0.0105868230
H10	1.7675414800	1.8037376846	1.6321944709
O11	-2.1713174844	-0.0175923566	0.9313468268
H12	-1.8294152981	-0.0304196845	1.8496371552
H13	-2.7736043531	0.7347202986	0.8721044999

(Wacker) -- RE IRC, forward and reverse paths

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Summary of IRC Reaction Path:

point #	Rxn. Coord	Energy	Major Components of TS Vector (units are Angstroms/Degrees) Coord 1
1	0.00000	-817.840534	1.2730
2	0.09908	-817.840582	1.3170
3	0.19871	-817.840665	1.3532
4	0.29832	-817.840733	1.3786

5	0.39819	-817.840800	1.4000
6	0.49798	-817.840859	1.4185
7	0.59415	-817.840914	1.4354
8	0.68849	-817.840965	1.4489
9	0.78117	-817.841013	1.4619
10	0.87283	-817.841058	1.4723
11	0.96252	-817.841100	1.4829
12	1.04679	-817.841138	1.4900
13	1.13411	-817.841173	1.4995
14	1.21501	-817.841208	1.5044
15	1.30051	-817.841241	1.5109
16	1.38282	-817.841270	1.5190
17	1.47309	-817.841302	1.5257
18	1.56376	-817.841333	1.5327
19	1.65744	-817.841362	1.5390
20	1.74751	-817.841389	1.5450
21	1.83871	-817.841417	1.5504

Coord 1 = O5-H6

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Summary of IRC Reaction Path:

point #	Rxn. Coord	Energy	Major Components of TS Vector (units are Angstroms/Degrees) Coord 1
1	-1.92329	-817.842384	1.0641
2	-1.82827	-817.842319	1.0656
3	-1.73246	-817.842304	1.0681
4	-1.63701	-817.842233	1.0703
5	-1.54117	-817.842160	1.0727
6	-1.44632	-817.842086	1.0752
7	-1.35557	-817.842017	1.0778
8	-1.26067	-817.841931	1.0807
9	-1.16990	-817.841855	1.0837
10	-1.07438	-817.841759	1.0869
11	-0.98291	-817.841677	1.0906
12	-0.88632	-817.841586	1.0945
13	-0.78844	-817.841487	1.0997
14	-0.69079	-817.841386	1.1028
15	-0.59351	-817.841284	1.1097
16	-0.49536	-817.841172	1.1160
17	-0.39555	-817.841050	1.1258

18	-0.29719	-817.840924	1.1443
19	-0.19913	-817.840771	1.1802
20	-0.09969	-817.840620	1.2253
21	0.00000	-817.840534	1.2730

Coord 1 = O5-H6

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(Wacker) -- pre-TS structure with explicit water (ground state)

Gas Phase Energy = -894.32083098753 = Eh
Solvent Correction = -0.03663368801 = Eh
Zero Point Energy = 74.949 = kcal/mol

Geometry Coordinates

Pd1	-0.0589378772	0.1696612700	-0.1243451714
O2	0.3494821547	-0.0718246615	2.1661186101
H3	1.3307465171	-0.1121810173	2.2222589135
C4	-0.1189481829	-1.1223709144	1.3667193378
H5	0.6228671720	-1.9142663322	1.2222613819
C6	-1.5015183072	-1.5864800482	1.7378042717
H7	-2.1827942738	-0.7391198874	1.8591273868
H8	-1.8898506282	-2.2401453579	0.9528924304
H9	-1.4762701965	-2.1454599045	2.6840149661
Cl10	-0.6127684131	-1.1171484813	-2.0462948774
O11	-0.0353538434	1.9128007234	-1.7386275958
H12	0.8369789530	2.1900772169	-2.0474958303
H13	-0.3553927723	1.2601026329	-2.3921955792
O14	3.0821477032	-0.3679712975	2.1786854622
H15	3.5761183794	-0.2982281022	1.3520378107
H16	3.6900661994	-0.1437795685	2.8940028315

(Wacker) -- BHE Transition State with explicit water

Gas Phase Energy = -894.27547542596 = Eh
Solvent Correction = -0.03617068228 = Eh
Zero Point Energy = 71.206 = kcal/mol

Imaginary Frequencies (cm^-1): -596.33

Geometry Coordinates

Pd1	0.0136125193	-0.0046311788	-0.0053967048
O2	0.0470756463	-0.0448646162	2.1898098569
H3	1.6615696739	-0.0209297929	2.0160705477
C4	-0.3582422701	-1.1909857358	1.7025633950
H5	0.3612498983	-2.0215070968	1.6757971456
C6	-1.8112762914	-1.5744556496	1.7948027558
H7	-2.4579359530	-0.7007942750	1.6764371479
H8	-2.0628032519	-2.3276913860	1.0433126423
H9	-2.0025181979	-2.0067925169	2.7875786388
Cl10	0.1150382847	-0.9034896479	-2.1924432786
O11	0.0529972943	2.1044515064	-1.4262017163
H12	0.7714021805	2.7342923871	-1.5664264603
H13	0.0764767905	1.4799889311	-2.1763112385
O14	2.4502693209	-0.1576844688	1.3763584792
H15	1.6215732644	-0.2127207444	0.3743030517
H16	2.9745018892	0.6573968675	1.3318801574

(Wacker) -- BHE IRC with explicit water, forward and reverse paths

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Summary of IRC Reaction Path:

Major Components of TS Vector
(units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1	Coord 2	Coord 3
1	0.00000	-894.275470	1.3015	1.6252	1.6649
2	0.09972	-894.275532	1.3437	1.6444	1.6339
3	0.19908	-894.275679	1.3837	1.6624	1.6075
4	0.29878	-894.275846	1.4180	1.6798	1.5896
5	0.39851	-894.276031	1.4516	1.6954	1.5726
6	0.49719	-894.276227	1.4781	1.7118	1.5640
7	0.59652	-894.276427	1.5060	1.7264	1.5535
8	0.69344	-894.276625	1.5294	1.7413	1.5475
9	0.79147	-894.276838	1.5540	1.7547	1.5405
10	0.88955	-894.277049	1.5769	1.7687	1.5356
11	0.98910	-894.277250	1.5993	1.7820	1.5311
12	1.08872	-894.277439	1.6221	1.7954	1.5265
13	1.18836	-894.277870	1.6431	1.8089	1.5237
14	1.28790	-894.278063	1.6640	1.8217	1.5205
15	1.38743	-894.278245	1.6845	1.8341	1.5173
16	1.48706	-894.278418	1.7051	1.8469	1.5146
17	1.58604	-894.278581	1.7248	1.8590	1.5126

18	1.68460	-894.278736	1.7440	1.8709	1.5105
19	1.78281	-894.278884	1.7623	1.8823	1.5090
20	1.88019	-894.279022	1.7791	1.8932	1.5082
21	1.97858	-894.279155	1.7970	1.9042	1.5061

Coord 1 = O14-H15
Coord 2 = O2-H3
Coord 3 = Pd1-H15

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Summary of IRC Reaction Path:

Major Components of TS Vector
(units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1	Coord 2	Coord 3
1	-1.99426	-894.307699	0.9858	1.0018	2.1517
2	-1.89432	-894.306901	0.9871	1.0038	2.1320
3	-1.79440	-894.306025	0.9886	1.0062	2.1113
4	-1.69454	-894.305050	0.9903	1.0092	2.0894
5	-1.59476	-894.303944	0.9924	1.0138	2.0663
6	-1.49622	-894.302615	0.9965	1.0283	2.0429
7	-1.39800	-894.300691	1.0020	1.0625	2.0226
8	-1.29838	-894.297779	1.0090	1.1085	2.0061
9	-1.19844	-894.294231	1.0163	1.1584	1.9918
10	-1.09847	-894.290573	1.0242	1.2091	1.9777
11	-0.99850	-894.287227	1.0332	1.2600	1.9628
12	-0.89855	-894.284316	1.0437	1.3104	1.9462
13	-0.79863	-894.282015	1.0560	1.3596	1.9271
14	-0.69875	-894.280280	1.0709	1.4065	1.9046
15	-0.59890	-894.278893	1.0897	1.4501	1.8782
16	-0.49911	-894.277819	1.1133	1.4896	1.8478
17	-0.39939	-894.276943	1.1425	1.5245	1.8134
18	-0.29958	-894.276268	1.1774	1.5551	1.7762
19	-0.19974	-894.275827	1.2170	1.5811	1.7376
20	-0.09987	-894.275561	1.2589	1.6043	1.7000
21	0.00000	-894.275470	1.3015	1.6252	1.6649

Coord 1 = O14-H15
Coord 2 = O2-H3
Coord 3 = Pd1-H15

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(Wacker) -- RE Transition State with explicit water

Gas Phase Energy = -894.29708664998 = Eh
Solvent Correction = -0.02786000199 = Eh
Zero Point Energy = 71.696 = kcal/mol

Imaginary Frequencies (cm^-1): -241.10

Geometry Coordinates

Pd1	0.0085253063	0.0403763852	-0.0320582568
Cl2	-0.0462816333	-0.0244864124	3.5170928803
C3	2.0514820494	-0.0390824502	-0.4062430662
H4	2.1595973915	0.2656776256	-1.4575882029
O5	1.6990401224	-1.2851818282	-0.2182507354
H6	1.5321522507	-1.7750439361	1.2001624736
C7	2.9019986234	0.7124664198	0.5892628079
H8	3.9533144154	0.4120408887	0.4686212278
H9	2.8433984513	1.7883906674	0.4010946134
H10	2.5976065759	0.5210417857	1.6214689016
O11	1.2762261291	-2.0609240472	2.1666388136
H12	2.0571479714	-2.3573069360	2.6544450750
H13	0.6939508398	-1.1859815914	2.7573186003
O14	-1.4502981028	1.3720715309	1.0289310486
H15	-1.1724491665	1.1357061800	1.9432285753
H16	-1.4011828418	2.3324754487	0.9468115175

(Wacker) -- RE IRC with explicit water, forward and reverse paths

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Summary of IRC Reaction Path:

Major Components of TS Vector
(units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1	Coord 2	Coord 3	Coord 4
1	0.00000	-894.297089	1.5000	1.5859	1.0428	1.1937
2	0.09968	-894.297096	1.5172	1.5588	1.0370	1.2192
3	0.19568	-894.297124	1.5337	1.5288	1.0304	1.2497
4	0.29303	-894.297190	1.5489	1.5053	1.0260	1.2761
5	0.39001	-894.297248	1.5640	1.4830	1.0210	1.3024
6	0.48776	-894.297332	1.5766	1.4679	1.0184	1.3234
7	0.58475	-894.297407	1.5896	1.4540	1.0148	1.3437
8	0.68249	-894.297494	1.6004	1.4420	1.0133	1.3623

9	0.77711	-894.297561	1.6111	1.4356	1.0108	1.3755
10	0.87592	-894.297637	1.6216	1.4268	1.0090	1.3914
11	0.97456	-894.297702	1.6310	1.4221	1.0078	1.4035
12	1.07277	-894.297772	1.6405	1.4150	1.0063	1.4172
13	1.17126	-894.297835	1.6488	1.4103	1.0053	1.4292
14	1.26797	-894.297886	1.6572	1.4059	1.0039	1.4398
15	1.36432	-894.297936	1.6647	1.4022	1.0033	1.4491
16	1.45466	-894.297974	1.6718	1.3985	1.0020	1.4581
17	1.54386	-894.298018	1.6777	1.3962	1.0015	1.4658
18	1.63578	-894.298058	1.6834	1.3934	1.0006	1.4739
19	1.72315	-894.298095	1.6887	1.3903	1.0003	1.4819
20	1.80558	-894.298126	1.6933	1.3889	0.9997	1.4872
21	1.88848	-894.298153	1.6982	1.3865	0.9991	1.4932

Coord 1 = O5-H6
Coord 2 = Cl2-H13
Coord 3 = H6-O11
Coord 4 = O11-H13

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Summary of IRC Reaction Path:

Major Components of TS Vector
(units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1	Coord 2	Coord 3	Coord 4
1	0.00000	-894.298486	186.7049	1.2997	172.1626	110.3559
2	0.09837	-894.298729	187.0396	1.3201	171.8692	110.3892
3	0.19737	-894.298953	187.4118	1.3355	171.7349	110.3357
4	0.29667	-894.299162	187.7004	1.3493	171.6896	110.2680
5	0.39638	-894.299368	187.9430	1.3614	171.6345	110.2245
6	0.49543	-894.299552	188.1573	1.3728	171.6546	110.1622
7	0.59355	-894.299726	188.3845	1.3812	171.6572	110.1224
8	0.69231	-894.299887	188.5211	1.3918	171.7005	110.0735
9	0.79162	-894.300041	188.7274	1.4000	171.7394	110.0431
10	0.88895	-894.300180	188.8634	1.4084	171.7879	109.9820
11	0.98716	-894.300314	189.0359	1.4157	171.8574	109.9514
12	1.08325	-894.300427	189.1614	1.4227	171.9253	109.8882
13	1.18125	-894.300541	189.3148	1.4288	172.0261	109.8473
14	1.27701	-894.300644	189.4341	1.4347	172.1089	109.7813
15	1.37466	-894.300742	189.5732	1.4397	172.2385	109.7393
16	1.46975	-894.300829	189.6770	1.4448	172.3275	109.6715
17	1.56710	-894.300920	189.8091	1.4489	172.4633	109.6338
18	1.66195	-894.301002	189.9007	1.4532	172.5566	109.5599

19	1.75866	-894.301076	190.0297	1.4564	172.6908	109.5166
20	1.85266	-894.301142	190.1080	1.4600	172.7827	109.4357
21	1.94851	-894.301210	190.2211	1.4626	172.9173	109.4028

Coord 1 = O5-H6-O11
Coord 2 = H6-O11
Coord 3 = O5-H6-O11
Coord 4 = O5-O11-H13

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MPW1K//LACVP**++ Gas phase geometries, energies, frequencies
MPW1K//LACVP** Solvent single point

(Wacker) - pre TS structure (ground state)

Gas Phase Energy = -817.98026581806 = Eh
Solvent Correction = -0.03394475425 = Eh
Zero Point Energy = 61.902 = kcal/mol

Geometry Coordinates

Pd1	-0.8152500000	1.7640210000	0.0872720000
C2	-1.7581600000	3.0401630000	-1.0223770000
H3	-1.3495560000	3.0565700000	-2.0305480000
C4	-1.9435360000	4.3799090000	-0.3900740000
H5	-2.3468160000	4.2831140000	0.6151880000
H6	-0.9834890000	4.8837740000	-0.3333680000
H7	-2.6330270000	4.9884090000	-0.9774320000
O8	-2.8947710000	2.2378490000	-0.9062950000
H9	-2.9737620000	1.6496610000	-1.6557930000
Cl10	1.3386240000	2.6584840000	0.0058410000
O11	0.1473170000	0.2068100000	1.4996120000
H12	0.3416430000	-0.6526980000	1.1328480000
H13	0.9776200000	0.6959570000	1.4976340000

(Wacker) - BHE Transition State

Gas Phase Energy = -817.91398212048 = Eh
Solvent Correction = -0.02874361200 = Eh
Zero Point Energy = 57.628 = kcal/mol

Imaginary Frequencies (cm^-1): -1082.61

Geometry Coordinates

Pd1	0.0000089306	-0.0002294477	-0.0000527095
H2	0.0006969699	0.0058367204	1.5527628951
O3	1.4562109605	-0.0011834353	1.6605102090
Cl4	0.1653056594	-0.0840646823	-2.3980155266
C5	2.0369645919	-0.2265153361	0.5394566706
H6	2.4776392450	0.6370694213	0.0385017643
C7	2.5047627319	-1.5919960810	0.1740696728
H8	1.8673652537	-2.3527285635	0.6159363100
H9	2.5272211241	-1.7053422299	-0.9054305713
H10	3.5176162831	-1.7269750218	0.5588294325
O11	-2.1451024277	0.1003818841	-0.4682367533
H12	-2.5720715723	0.9365402035	-0.2938190066
H13	-1.9967232046	0.0462836000	-1.4232357669

(Wacker) - RE Transition State

Gas Phase Energy = -817.94583693146 = Eh
Solvent Correction = -0.02567891403 = Eh
Zero Point Energy = 57.594 = kcal/mol

Imaginary Frequencies (cm^-1): -150.31

Geometry Coordinates

Pd1	-0.0002859160	0.0014424211	0.0002902639
Cl2	0.0004785074	-0.0024544258	3.3836343318
C3	1.9962578050	-0.0006617457	0.4136182173
H4	2.5108154870	-0.4347170213	-0.4466680020
O5	1.5446375270	-0.8610155592	1.2670459038
H6	0.9187178963	-0.4385405151	2.3386254284
C7	2.4200534202	1.3695079726	0.8405602525
H8	3.4310984305	1.3205408458	1.2498727124
H9	2.4407171469	2.0473623451	-0.0089698661
H10	1.7651942070	1.7651632147	1.6126221893
O11	-2.1760388794	-0.0315829746	0.8889231140
H12	-1.8770138256	-0.0823104871	1.8048152642
H13	-2.7764621900	0.7074300568	0.8368526920

(Wacker) -- pre-TS structure with explicit water (ground state)

Gas Phase Energy = -894.42625637798 = Eh
Solvent Correction = -0.03940073497 = Eh
Zero Point Energy = 77.769 = kcal/mol

Geometry Coordinates

Pd1	-0.0671774661	0.1745143040	-0.1192891611
O2	0.3117165053	-0.0410398101	2.1338267687
H3	1.2786120560	-0.0634680923	2.2137738032
C4	-0.1144011189	-1.0930553243	1.3467155917
H5	0.6391664970	-1.8675945310	1.2200544529
C6	-1.4839221114	-1.5790591770	1.6898542087
H7	-2.1771742596	-0.7475385181	1.7901732944
H8	-1.8400565801	-2.2386965410	0.9043778062
H9	-1.4688327895	-2.1267583756	2.6337668095
Cl10	-0.5326032382	-1.1613095799	-1.9913444523
O11	-0.0637158972	1.8703790927	-1.7222684744
H12	0.7847128830	2.1914386594	-2.0176365892
H13	-0.3497155275	1.2197592788	-2.3750026699
O14	3.0236078639	-0.3202852812	2.1145818859
H15	3.4940401221	-0.4090462613	1.2895178676
H16	3.6715165799	-0.2405641851	2.8092541723

(Wacker) -- BHE Transition State with explicit water

Gas Phase Energy = -894.37112816206 = Eh
Solvent Correction = -0.04087734689 = Eh
Zero Point Energy = 73.790 = kcal/mol

Imaginary Frequencies (cm^-1): -494.82

Geometry Coordinates

Pd1	0.0014155338	-0.0004695318	-0.0000324164
O2	0.0005420244	-0.0012334517	2.1389956921
H3	1.7091874277	-0.0030010032	1.9877174990
C4	-0.3662625952	-1.1523949822	1.6917881087
H5	0.3644643834	-1.9651666467	1.6950415786
C6	-1.8028872967	-1.5582589814	1.7430745699
H7	-2.4536898611	-0.7006189996	1.5972141240
H8	-2.0163677849	-2.3171521646	0.9958424681

H9	-2.0151094573	-1.9806614971	2.7271811868
Cl10	0.2103674936	-0.9097092363	-2.1445597058
O11	0.0008520684	2.0614829812	-1.4065546480
H12	0.6592424652	2.7398955551	-1.5288920531
H13	0.0749792778	1.4532030960	-2.1506322186
O14	2.4249705100	-0.2087846278	1.3294135136
H15	1.5601817299	-0.2714280323	0.3685722579
H16	2.9978575197	0.5527999239	1.2293912230

(Wacker) -- RE Transition State with explicit water

Gas Phase Energy = -894.39869956414 = Eh
Solvent Correction = -0.02827392880 = Eh
Zero Point Energy = 74.382 = kcal/mol

Imaginary Frequencies (cm^-1): -89.42

Geometry Coordinates

Pd1	0.0000000000	0.0000000000	0.0000000000
Cl2	0.0000000000	0.0000000000	3.4713710000
C3	2.0044280000	0.0000000000	-0.4096670000
H4	2.0924190000	0.3392640000	-1.4453350000
O5	1.6947450000	-1.2410760000	-0.2495270000
H6	1.5325620000	-1.7683960000	1.1991880000
C7	2.8273970000	0.7473900000	0.5947230000
H8	3.8804550000	0.4900560000	0.4611550000
H9	2.7288630000	1.8186640000	0.4420350000
H10	2.5362810000	0.5139530000	1.6149190000
O11	1.2888200000	-2.0300520000	2.1447030000
H12	2.0594840000	-2.3489200000	2.6105450000
H13	0.6994790000	-1.1186700000	2.7501370000
O14	-1.4002350000	1.4311900000	0.9780190000
H15	-1.1558710000	1.2233980000	1.8913630000
H16	-1.2978480000	2.3714540000	0.8575430000

--*-*-*-*-*-*-*-Phenyl-ketone Data*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-*-
The following data table contains energies,
solvation energy, ZPE's and cartesian coordinates
of species referneced in Table 1 of the manuscript.

B3LYP//LACVP**++ Gas phase geometries, energies, frequencies
B3LYP//LACVP** Solvent single point

(Phenyl-ketone) -- pre-TS structure (ground state)

Gas Phase Energy = -1048.93827741806 = Eh
Solvent Correction = -0.02753097826 = Eh
Zero Point Energy = 110.824 = kcal/mol

Geometry Coordinates

Pd1	-0.9274592693	1.6037381222	0.1497671493
C2	-1.4317701330	3.0447426085	-1.1293909301
C3	-1.5002791297	4.3942256089	-0.4441197981
H4	-2.0410370272	4.3242447415	0.5033251912
H5	-0.4883776890	4.7536056373	-0.2455029193
H6	-2.0114543901	5.1204011299	-1.0912232865
O7	-2.7055820140	2.4134926342	-1.1121944185
H8	-2.7708897300	1.7966746727	-1.8595770103
Cl9	1.3063984922	2.0594811250	0.8682707415
O10	-0.6865098250	-0.1399537145	1.7113108332
H11	-0.5165294197	-1.0072984692	1.3200879607
H12	0.1872188177	0.2138666637	1.9684394296
C13	0.5064039385	2.9845997470	-4.9844888946
C14	-0.8870812119	3.0085450254	-4.9013283149
C15	-1.5133978661	3.0231907850	-3.6519717111
C16	-0.7519244552	2.9992771289	-2.4684401712
C17	0.6501721154	2.9855202560	-2.5622523574
C18	1.2695531894	2.9791082758	-3.8118627102
H19	0.9950063557	2.9742300841	-5.9545717831
H20	-1.4893576866	3.0306771009	-5.8051895428
H21	-2.5979764628	3.0932212985	-3.6059970389
H22	1.2429514485	2.9465199171	-1.6535655079
H23	2.3540583693	2.9583081719	-3.8688926551

(Phenyl-ketone) -- BHE Transition State

Gas Phase Energy = -1048.90429802943 = Eh
Solvent Correction = -0.02693161056 = Eh
Zero Point Energy = 107.088 = kcal/mol

Imaginary Frequencies (cm^-1): -516.54

Geometry Coordinates

Pd1	0.0382626192	0.0801670302	0.0140540648
O2	0.0512248346	0.0950082315	2.2119653507
H3	1.6370188704	-0.0445483765	2.0513994449
O4	2.4386776940	-0.1820104617	1.4342953529
H5	1.6375185368	-0.1708346102	0.4171025627
C6	-0.7107819104	-0.8975498993	1.8673685512
Cl7	0.3668943514	-0.0137438424	-2.2596122968
H8	2.9754242901	0.6269140680	1.4145240877
C9	-0.1869535734	-2.3142511386	1.9697684332
H10	-0.5602118480	-2.9490034346	1.1639147115
H11	0.9032611693	-2.3264846032	1.9411226660
H12	-0.5180164452	-2.7481388129	2.9231936186
C13	-4.9345314766	-0.1267537573	1.6844986276
C14	-4.4483789482	-1.3936310513	1.3484704786
C15	-3.0805211422	-1.6578651752	1.4071679609
C16	-2.1775273750	-0.6521456014	1.8003631956
C17	-2.6781892343	0.6208227253	2.1380084040
C18	-4.0454360752	0.8780992998	2.0815253872
H19	-6.0002863908	0.0771626304	1.6366681626
H20	-5.1342759426	-2.1753625916	1.0361364861
H21	-2.7201431806	-2.6427202288	1.1312581715
H22	-1.9814413686	1.3917271186	2.4483990853
H23	-4.4194922090	1.8627819238	2.3458420656

(Phenyl-ketone) -- RE Transition State

Gas Phase Energy = -1048.92556154538 = Eh
Solvent Correction = -0.01535505866 = Eh
Zero Point Energy = 107.412 = kcal/mol

Imaginary Frequencies (cm^-1): -33.45

Geometry Coordinates

Pd1	-0.0045566229	-0.0236707007	-0.0144159355
Cl2	-0.0240508050	0.0231722839	3.9623284922
C3	2.1723101894	0.0044197861	1.1584200280
O4	2.0050382012	-0.8395682483	2.0792533242
H5	1.0157240698	-0.4048848432	3.1702534911
C6	2.5661315816	1.4219022525	1.5265774217
H7	3.6520507882	1.4492011372	1.6884929758
H8	2.3082893552	2.1557103918	0.7614970480
H9	2.0892889631	1.6956870252	2.4702867794

O10	-1.6910649809	0.8544271383	1.2394632376
H11	-1.3994609449	0.6461519490	2.1491197905
H12	-1.8408649303	1.8074379663	1.2053909674
C13	2.0814203397	-1.3354699779	-2.9366249661
C14	2.7172702111	-0.1160502461	-2.6214995526
C15	2.7347639204	0.3541571243	-1.3194535579
C16	2.1503381938	-0.4119658010	-0.2662862754
C17	1.5119450262	-1.6499349471	-0.5931008524
C18	1.4815329004	-2.0882364123	-1.9376948437
H19	2.0668707802	-1.6850810331	-3.9649188867
H20	3.1899873827	0.4642456364	-3.4086191477
H21	3.2250167919	1.2956623797	-1.0948969480
H22	1.2368932185	-2.3269354040	0.2101967719
H23	1.0049345514	-3.0348575251	-2.1750942071

MPW1K//LACVP**++ Gas phase geometries, energies, frequencies
MPW1K//LACVP** Solvent single point

(Phenyl-ketone) -- pre-TS structure (ground state)

Gas Phase Energy = -1049.08649512569 = Eh
Solvent Correction = -0.03123481139 = Eh
Zero Point Energy = 113.778 = kcal/mol

Geometry Coordinates

Pd1	-0.9244642956	1.6030548802	0.1361494788
C2	-1.4211334262	3.0159574010	-1.1174577725
C3	-1.4871506665	4.3531325415	-0.4380597808
H4	-2.0251370554	4.2813140212	0.5033289002
H5	-0.4798935211	4.7042441364	-0.2384189607
H6	-1.9934406446	5.0757733444	-1.0799111318
O7	-2.6707948815	2.3863464294	-1.1093373868
H8	-2.7411938335	1.7957564316	-1.8619338314
Cl9	1.2640137978	2.1175887009	0.8471284988
O10	-0.6737263497	-0.1041982724	1.6756814052
H11	-0.4943533436	-0.9696721981	1.3153158283
H12	0.1774218556	0.2558600098	1.9517169740
C13	0.5003814693	2.9744840990	-4.9427281772
C14	-0.8819618728	3.0137585818	-4.8592960316
C15	-1.5015790249	3.0225959609	-3.6183600512
C16	-0.7441335839	2.9781924124	-2.4474221048

C17	0.6456365449	2.9486007599	-2.5393644299
C18	1.2590325351	2.9480502098	-3.7804670832
H19	0.9850206198	2.9685721163	-5.9073225354
H20	-1.4803785704	3.0513530608	-5.7570831942
H21	-2.5791222640	3.1039994913	-3.5693550183
H22	1.2327652485	2.8979120518	-1.6341654638
H23	2.3364329089	2.9162497267	-3.8389382536

(Phenyl-ketone) -- BHE Transition State

Gas Phase Energy = -1049.02628957279 = Eh
Solvent Correction = -0.03020646450 = Eh
Zero Point Energy = 109.610 = kcal/mol

Imaginary Frequencies (cm^-1): -1089.41

Geometry Coordinates

Pd1	0.0068467659	0.0418416724	-0.0453662268
H2	0.0910762058	0.4660919158	1.4429259252
O3	1.4645866002	0.0719115834	1.6732102149
Cl4	0.0485751324	-0.7074420238	-2.3688730201
C5	2.0827387366	-0.1182705637	0.5619974258
C6	2.5218407460	-1.5144163672	0.2379879521
H7	1.9034422411	-2.2229518088	0.7788622650
H8	2.4592206754	-1.7237385382	-0.8241518485
H9	3.5569372573	-1.6343933672	0.5601282128
O10	-2.1295306215	0.2662967047	-0.5318169520
H11	-2.4350296949	1.1678358033	-0.6069312662
H12	-1.9950368658	-0.0669578921	-1.4319773538
C13	3.7741744166	3.2905716136	-1.3445154912
C14	3.7407381418	2.0749966687	-2.0138358696
C15	3.1922487708	0.9605786588	-1.4060278168
C16	2.6698956679	1.0561889262	-0.1154463474
C17	2.6998904263	2.2833695560	0.5498921270
C18	3.2521010352	3.3936215057	-0.0627637126
H19	4.2041883621	4.1573497815	-1.8234074984
H20	4.1311639888	1.9978530850	-3.0167587232
H21	3.1295767314	0.0319737974	-1.9497854223
H22	2.3033134338	2.3470998520	1.5510344134
H23	3.2799269138	4.3376145773	0.4596289630

(Phenyl-ketone) -- RE Transition State

Gas Phase Energy = -1049.07041985708 = Eh
Solvent Correction = -0.01661415455 = Eh
Zero Point Energy = 109.933 = kcal/mol

Imaginary Frequencies (cm^-1): -86.61

Geometry Coordinates

Pd1	0.0000000000	0.0000000000	0.0000000000
Cl2	0.0000000000	0.0000000000	3.9425983933
C3	2.2070109346	0.0000000000	1.2062159870
O4	2.0296965028	-0.8585852579	2.0823992109
H5	1.0190138253	-0.4352301283	3.1718188128
C6	2.6105296189	1.3900616938	1.6068885561
H7	3.6991417631	1.4271046938	1.6659723740
H8	2.2767025630	2.1456591896	0.9042586187
H9	2.2191951064	1.6084372625	2.5949879680
O10	-1.6435376676	0.9562137365	1.2364932724
H11	-1.3774179657	0.7396365565	2.1368431077
H12	-1.7693155742	1.9005749031	1.2002485167
C13	1.9848889711	-1.1330655050	-2.9076242407
C14	2.6558504765	0.0468617716	-2.5533828608
C15	2.7160620733	0.4486844628	-1.2431653006
C16	2.1349750585	-0.3447294185	-0.2229418017
C17	1.4679135771	-1.5432875209	-0.5840695434
C18	1.3996606621	-1.9148443629	-1.9406807483
H19	1.9371546213	-1.4299003551	-3.9444606316
H20	3.1234523934	0.6471851616	-3.3189721253
H21	3.2343106173	1.3592143078	-0.9854261383
H22	1.2152044874	-2.2545932532	0.1895159425
H23	0.9039773555	-2.8353029310	-2.2094019123

--*-*-*-*-*-*-*-*-Miscellaneous Data*-*-*-*-*-*-*-*-*-*-
The following species were referenced in the manuscript.

The following calculations are B3LYP//LACVP**++ with B3LYP//LACVP** solvent corrections unless noted otherwise

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H2O

Gas Phase Energy = -76.43321063266 = Eh
Solvent Phase Energy = -0.01233895178 = Eh
Zero Point Energy = 13.359 = kcal/mol

Geometry Coordinates

O1	0.0000000000	0.0000000000	0.0000000000
H2	0.0000000000	0.0000000000	0.9649004762
H3	0.9288188358	0.0000000000	-0.2613971840

(Wacker) -- pre TS structure with saturated Pd with one explict water

Gas Phase Energy = -894.32462672815 = Eh
Solvent Phase Energy = -0.03121903671 = Eh
Zero Point Energy = 76.348 = kcal/mol

Geometry Coordinates

Pd1	-0.1189248153	-0.0795798869	-0.0023209653
C2	-0.0171901371	0.0457057232	2.0172624319
H3	1.0220102936	0.3594931088	2.1683972368
O4	-0.0883621532	-1.2968820870	2.5146428204
H5	-1.0166738565	-1.5103288806	2.6895368020
C6	-1.0122675088	0.9537174581	2.7048806162
H7	-0.8556205973	0.9131380369	3.7924226140
H8	-0.8910353927	1.9820015645	2.3618167192
H9	-2.0453141744	0.6618475765	2.4842288158
Cl12	-1.2408142833	1.9575088079	-0.4203413590
O14	0.9768013686	-2.0211384829	0.1786596217
H15	0.7146587257	-2.2383372162	1.0970347906
H16	0.6119104034	-2.6951266469	-0.4098859583
O17	-0.2572779420	-0.2435474949	-2.3717160401
H18	-0.8403839533	0.5399400588	-2.3734757096
H19	0.5709696278	0.0527300230	-2.7738503807

Hydride shifting reaction TS (MPW1K//LACVP**++)

Compare to pre TS with one explicit water

Gas Phase Energy = -894.35264359895 = Eh
Zero Point Energy = 74.705 = kcal/mol

Imaginary Frequencies (cm^-1): -434.40

Geometry Coordinates

Pd1	0.0144049503	0.0022612703	-0.0059930591
C2	-0.0271481699	0.0155978998	2.2435836815
H3	0.9863522930	0.0078954169	1.2066374497
C4	0.2959086465	1.1552046501	2.9620756579
O5	0.2853581026	2.3678238136	2.5504232634
H6	-0.9709617379	0.0917061809	1.6275344048
H7	0.0476711442	-0.9136848272	2.7847379993
Cl8	1.2585334790	0.8854141158	-1.8947931693
H9	0.6198937516	1.0602347860	3.9918576413
H10	0.1821911873	2.5325351077	1.5536804160
O11	-1.6706719044	-0.0713971584	-1.6823727375
H12	-1.0391103608	0.3731690382	-2.2599097971
H13	-1.7240296310	-0.9637689237	-2.0167358641
O14	0.2422269129	3.1075891817	0.1313736942
H15	0.5479210350	2.4842030494	-0.5519083777
H16	0.7954060358	3.8812808651	0.0511777785

--*-*-*-*-*-*-*-*-Beta-Hydride Elimination*-*-*-*-*-*-*-*-*-*-
The following data was referenced in the manuscript

(Wacker) - pre TS structure for BHE with Pd-C-C-H

Gas Phase Energy = -817.85075754112 = Eh
Solvent Phase Energy = -0.03203406745 = Eh
Zero Point Energy = 59.140 = kcal/mol

Geometry Coordinates

Pd1	0.0038427143	-0.0110800804	0.0489046284
Cl2	0.0240983389	0.0313764822	2.4003852126
C3	1.9733185044	0.0269918777	-0.3494887940
C4	1.5879227679	-0.0075024576	-1.7859686087
H5	0.4036751389	-0.0351565524	-1.8130481244
O6	1.9945960095	1.1476757412	-2.4801233073
H7	2.4302685650	0.9583740448	-0.0159806260

H8	2.4415911438	-0.8675259197	0.0596000367
H9	1.8612515834	-0.9373064350	-2.3000190353
H10	1.6431607525	1.1337415743	-3.3804545867
O11	-2.2916808292	0.0169259687	0.3635139098
H12	-2.7147403447	-0.8463129522	0.2600530900
H13	-2.1836731985	0.1476638536	1.3256262355

(Wacker) - BHE TS with Pd-C-C-H

Gas Phase Energy = -817.84155716217 = Eh
Solvent Phase Energy = -0.03525494715 = Eh
Zero Point Energy = 57.536 = kcal/mol

Imaginary Frequencies (cm^-1): -558.90

Geometry Coordinates

Pd1	0.0057029172	0.0410757351	0.0268506070
Cl2	-0.0004016135	-0.1274087293	2.4387823744
C3	2.0579691263	0.0005849621	-0.2813181581
O4	1.8715454879	1.5672114465	-2.0672499653
H5	2.5126927574	0.7908686384	0.3106448878
H6	2.3655923005	-1.0168350199	-0.0552249554
H7	1.6750626589	-0.4857866026	-2.3649903827
H8	1.4846047819	1.6848238452	-2.9454948571
O9	-2.2101461178	0.1612985754	0.4160930323
H10	-2.6623932507	-0.6782487741	0.2005174592
H11	-2.0537380914	0.1446793521	1.3936058193
C12	1.6749466343	0.3008071377	-1.6134603865
H13	-0.0050519700	0.1290869743	-1.5590676708

(Wacker) - BHE IRC with Pd-C-C-H

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Summary of IRC Reaction Path:

			Major Components of TS Vector (units are Angstroms/Degrees)
point #	Rxn. Coord	Energy	Coord 1
1	0.00000	-817.841726	82.5655

2	0.10000	-817.841769	84.0377
3	0.19910	-817.841883	85.4609
4	0.29847	-817.842041	86.8420
5	0.39777	-817.842215	88.1534
6	0.49713	-817.842388	89.3605
7	0.59628	-817.842534	90.3936
8	0.69540	-817.842660	91.2347
9	0.79395	-817.842774	91.9113
10	0.89271	-817.842879	92.3710
11	0.99115	-817.842977	92.7598
12	1.09004	-817.843066	93.0833
13	1.18892	-817.843149	93.3981
14	1.28626	-817.843223	93.6733
15	1.38505	-817.843294	93.9015
16	1.48379	-817.843362	94.1392

Coord 1 = C3-Pd1-H13

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Summary of IRC Reaction Path:

Major Components of TS Vector
(units are Angstroms/Degrees)

point #	Rxn. Coord	Energy	Coord 1
1	-1.49688	-817.849838	68.4891
2	-1.39702	-817.849575	68.7457
3	-1.29721	-817.849269	68.9909
4	-1.19743	-817.848889	69.2386
5	-1.09780	-817.848432	69.5240
6	-0.99839	-817.847866	69.9652
7	-0.89894	-817.847157	70.6688
8	-0.79921	-817.846316	71.6240
9	-0.69928	-817.845372	72.7859
10	-0.59933	-817.844435	74.0469
11	-0.49935	-817.843577	75.3845
12	-0.39937	-817.842874	76.7721
13	-0.29941	-817.842342	78.1960
14	-0.19958	-817.841983	79.6555
15	-0.10000	-817.841788	81.0934
16	0.00000	-817.841726	82.5655

Coord 1 = C3-Pd1-H13

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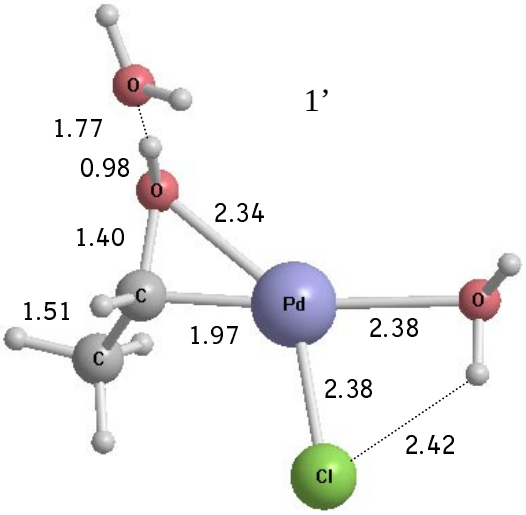
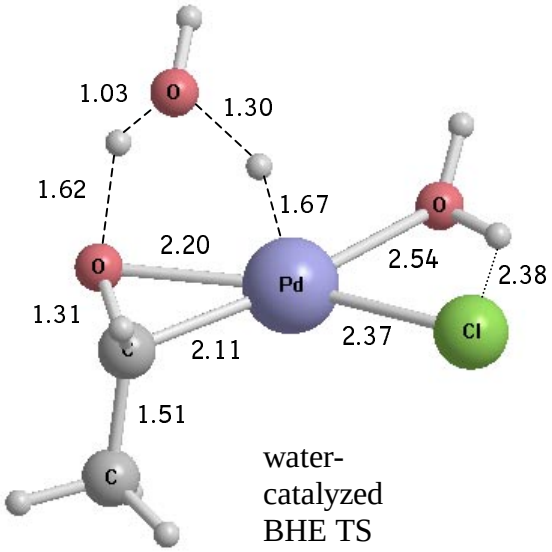
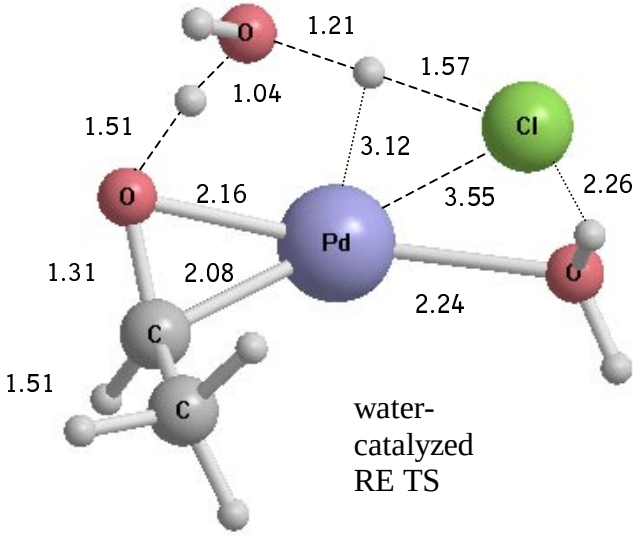
Contact John A. Keith (johnk@wag.caltech.edu) for unabridged output files.





water-catalyzed BHE TS



water-catalyzed RE TS