

Electronic Supplementary Information

A theoretical and shock tube kinetic study on hydrogen abstraction from phenyl formate

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Cartesian coordinates of species for H-abstraction reactions PF + H/O/OH/HO₂ at the M062x/cc-pVTZ level.

PF				8	3.523490	0.139084	-0.104307
6	-2.091539	-0.939256	0.304304				
6	-0.772580	-1.308371	0.087116	PF-R2			
6	0.150311	-0.338782	-0.260615	6	1.386413	1.439014	0.000005
6	-0.211429	0.990503	-0.398949	6	0.114803	0.926231	0.000009
6	-1.533321	1.345841	-0.176486	6	-0.159559	-0.416089	0.000005
6	-2.473904	0.387779	0.175001	6	0.904252	-1.312033	-0.000002
1	-2.818940	-1.692108	0.574978	6	2.202008	-0.826377	-0.000007
1	-0.447865	-2.335419	0.176672	6	2.450624	0.541375	-0.000002
1	0.527832	1.730519	-0.664944	1	1.557737	2.507265	0.000007
1	-1.827277	2.381392	-0.278232	1	0.695498	-2.373346	-0.000003
1	-3.501852	0.674968	0.346683	1	3.027862	-1.523836	-0.000015
8	1.442407	-0.782174	-0.535328	1	3.467366	0.909728	-0.000009
6	2.499040	-0.154963	0.015320	8	-1.427009	-0.971999	0.000012
1	3.411395	-0.658684	-0.321520	6	-2.515969	-0.182413	-0.000004
8	2.464748	0.782527	0.746856	1	-3.404982	-0.821484	-0.000007
				8	-2.527855	1.007427	-0.000010
PF-R1				PF-R3			
6	-2.162371	-1.008892	-0.075203	6	1.495973	-1.380355	-0.194078
6	-0.806634	-1.285047	0.006999	6	0.184762	-1.040121	-0.391698
6	0.086922	-0.232684	0.089062	6	-0.112610	0.310166	-0.232976
6	-0.336838	1.084727	0.097244	6	0.866122	1.233123	0.099900
6	-1.697293	1.343844	0.007395	6	2.175624	0.816157	0.284934
6	-2.611407	0.304289	-0.078437	6	2.514993	-0.527842	0.139076
1	-2.868154	-1.825316	-0.140164	1	-0.578783	-1.760242	-0.644238
1	-0.429310	-2.297658	0.008156	1	0.587284	2.271769	0.203908
1	0.379606	1.889855	0.174626	1	2.936706	1.540093	0.543959
1	-2.040609	2.369100	0.011089	1	3.530476	-0.869794	0.281909
1	-3.669148	0.515946	-0.144551	8	-1.381744	0.827220	-0.470484
8	1.429562	-0.592173	0.200669	6	-2.475068	0.209441	0.018363
6	2.361487	0.289228	-0.160402				

1 -3.356055 0.788089 -0.277619
8 -2.495557 -0.788886 0.664354

PF-R4

6 -2.168499 -0.905066 0.326048
6 -0.849969 -1.285276 0.088192
6 0.081322 -0.323166 -0.263540
6 -0.253776 1.016038 -0.389482
6 -1.569200 1.404672 -0.149506
6 -2.464206 0.426132 0.196905
1 -2.914189 -1.638978 0.599462
1 -0.537249 -2.317549 0.165554
1 0.498463 1.742040 -0.659849
1 -1.857931 2.443201 -0.236037
8 1.363601 -0.784877 -0.556367
6 2.432478 -0.189315 0.006741
1 3.334900 -0.705207 -0.337960
8 2.414787 0.736425 0.753452

PF-OH-TS1

6 -2.153305 -0.701588 0.919659
6 -0.827765 -1.085636 0.778910
6 -0.092159 -0.573709 -0.275700
6 -0.647466 0.304988 -1.191430
6 -1.973053 0.685532 -1.037638
6 -2.725376 0.185141 0.016496
1 -2.738056 -1.092638 1.740556
1 -0.356923 -1.769245 1.471133
1 -0.040634 0.681070 -2.003553
1 -2.415510 1.375303 -1.742732
1 -3.757466 0.484183 0.133359

8 1.231149 -0.963740 -0.419285
6 2.191103 -0.088984 -0.040983

1 1.750068 0.880985 0.452675
8 3.343689 -0.293760 -0.179083
8 1.027910 1.933888 1.097421
1 0.104670 1.674783 0.940262

PF-OH-TS1-RC

6 2.117508 -0.953833 -0.610641
6 0.763379 -1.243108 -0.637432
6 -0.092900 -0.553993 0.209260
6 0.388690 0.404920 1.089682
6 1.749141 0.688940 1.104882
6 2.614008 0.017593 0.254746
1 2.789428 -1.486825 -1.269202
1 0.351792 -1.984609 -1.307077
1 -0.290920 0.910598 1.761913
1 2.128068 1.437680 1.786270
1 3.671831 0.238715 0.271158
8 -1.430195 -0.877774 0.170153
6 -2.333718 0.133635 0.045302
1 -1.860778 1.106231 -0.145128
8 -3.498352 -0.067660 0.121435
8 0.058538 1.866954 -1.349310
1 0.934000 1.441131 -1.370946

PF-OH-TS1-PC

6 -2.261983 0.560369 0.860837
6 -0.932146 0.410402 1.221498
6 -0.109365 -0.369110 0.429674
6 -0.579047 -1.003141 -0.707743

6	-1.911512	-0.835868	-1.061479
6	-2.754251	-0.057170	-0.281471
1	-2.912612	1.170814	1.471610
1	-0.516562	0.895282	2.092759
1	0.084786	-1.618924	-1.298526
1	-2.290482	-1.325870	-1.947784
1	-3.791115	0.065575	-0.560684
8	1.208485	-0.505403	0.851723
6	2.158419	-0.502336	-0.082548
1	1.896871	1.987069	-1.457492
8	3.316343	-0.582878	0.091603
8	1.157092	2.080802	-0.852545
1	0.413073	1.667002	-1.298740

PF-OH-TS2

6	2.057035	0.761446	0.296169
6	0.707406	0.933036	0.079692
6	-0.113841	-0.116933	-0.267367
6	0.411661	-1.393407	-0.396531
6	1.767471	-1.581735	-0.170303
6	2.589489	-0.517537	0.174047
1	2.682621	1.603075	0.558439
1	0.194783	2.048101	0.196569
1	-0.230793	-2.219658	-0.661512
1	2.184524	-2.574411	-0.267580
1	3.644628	-0.679545	0.345522
8	-1.445113	0.180637	-0.544466
6	-2.425588	-0.554795	0.026272
1	-3.390061	-0.151481	-0.298642
8	-2.275447	-1.480351	0.754917
8	-0.512502	3.062568	0.065076

1	-1.183009	2.690633	-0.528884
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PF-OH-TS2-RC

6	1.706219	1.256380	0.657106
6	0.393358	0.883665	0.413660
6	0.155823	-0.296238	-0.270494
6	1.187038	-1.101192	-0.716451
6	2.496312	-0.713982	-0.469132
6	2.757471	0.461929	0.218474
1	1.907390	2.173630	1.193111
1	-0.439673	1.487229	0.744836
1	0.954847	-2.012277	-1.249713
1	3.311453	-1.335184	-0.813656
1	3.778315	0.760231	0.412500
8	-1.145258	-0.678436	-0.598300
6	-2.041342	-0.848923	0.405601
1	-3.012783	-1.088649	-0.036933
8	-1.807894	-0.760803	1.566104
8	-2.602074	1.527149	-0.963922
1	-1.987013	1.461909	-1.713779

PF-OH-TS2-PC

6	1.552686	1.173674	0.844259
6	0.329884	0.560539	0.751677
6	0.117423	-0.613611	0.075217
6	1.201402	-1.220414	-0.550569
6	2.452135	-0.627671	-0.475647
6	2.636205	0.563734	0.215702
1	1.673559	2.100903	1.388521
1	-1.824631	1.640388	-0.734251
1	1.042429	-2.146052	-1.086916

1	3.291786	-1.102654	-0.963390
1	3.616314	1.017486	0.269463
8	-1.095781	-1.260593	-0.043392
6	-2.215659	-0.709879	0.446998
1	-3.058048	-1.367095	0.212780
8	-2.296013	0.317629	1.048105
8	-1.666813	1.395145	-1.651166
1	-0.717010	1.481343	-1.760406

PF-OH-TS3

6	-1.721566	-0.047850	0.136481
6	-0.609121	-0.835184	-0.070451
6	0.596926	-0.192486	-0.302956
6	0.684655	1.190283	-0.340524
6	-0.460261	1.944797	-0.133113
6	-1.684987	1.330353	0.105617
1	-2.774748	-0.603365	0.371846
1	-0.653886	-1.914817	-0.050882
1	1.636176	1.666719	-0.519218
1	-0.396147	3.024066	-0.158245
1	-2.580076	1.913343	0.269119
8	1.690245	-1.010183	-0.566002
6	2.868028	-0.781924	0.050801
1	3.584515	-1.536308	-0.290096
8	3.099970	0.082705	0.833081
8	-3.896493	-1.200559	0.280903
1	-4.007658	-1.173276	-0.681508

PF-OH-TS3-RC

6	-1.884425	0.073657	1.142231
6	-0.651035	-0.560677	1.133372

6	0.312717	-0.161588	0.221193
6	0.067110	0.853421	-0.690732
6	-1.173639	1.475879	-0.673349
6	-2.149592	1.094032	0.239311
1	-2.640496	-0.241396	1.847512
1	-0.425677	-1.370972	1.811775
1	0.826151	1.150004	-1.396554
1	-1.374819	2.268851	-1.380446
1	-3.110859	1.588235	0.244228
8	1.489475	-0.896518	0.228241
6	2.684035	-0.293320	0.074651
1	3.461994	-1.062744	0.112853
8	2.877696	0.871421	-0.070466
8	-1.634125	-1.996891	-1.237869
1	-1.831682	-1.044505	-1.278681

PF-OH-TS3-PC

6	-1.703461	0.563953	0.037740
6	-0.817284	-0.452776	-0.199710
6	0.511991	-0.074543	-0.346469
6	0.902982	1.253077	-0.257807
6	-0.051576	2.229498	-0.012811
6	-1.396363	1.894359	0.141522
1	-3.504357	-1.356449	1.051049
1	-1.116723	-1.489475	-0.274462
1	1.943292	1.515955	-0.369921
1	0.254470	3.264716	0.057700
1	-2.144540	2.651767	0.328608
8	1.410861	-1.088656	-0.655069
6	2.573925	-1.188893	0.020859
1	3.123452	-2.051384	-0.370106

8	2.946675	-0.474090	0.894695
8	-3.718394	-1.789369	0.220942
1	-3.790012	-1.066259	-0.407343

PF-OH-TS4

6	1.389140	1.258330	0.157934
6	0.017812	1.463043	0.079366
6	-0.807630	0.405278	-0.262676
6	-0.305541	-0.857660	-0.534657
6	1.066136	-1.062057	-0.454071
6	1.881034	-0.000281	-0.118476
1	2.052700	2.069654	0.422007
1	-0.421196	2.431846	0.273018
1	-0.971593	-1.665921	-0.794488
1	1.485393	-2.037483	-0.657857
1	3.083364	-0.178976	-0.079653
8	-2.161295	0.703193	-0.387804
6	-3.085854	-0.104167	0.168723
1	-4.075921	0.315806	-0.036854
8	-2.876819	-1.100337	0.783787
8	4.266984	-0.456085	0.286170
1	4.085709	-0.724008	1.199743

PF-OH-TS4-RC

6	1.910869	0.959953	0.820105
6	0.581421	1.339028	0.699905
6	-0.188006	0.752808	-0.284927
6	0.325167	-0.194377	-1.152035
6	1.653138	-0.570834	-1.014931
6	2.445154	0.005259	-0.031736
1	2.525662	1.408181	1.588088

1	0.139127	2.076478	1.354644
1	-0.310428	-0.636016	-1.906938
1	2.062642	-1.325090	-1.671590
1	3.477247	-0.296916	0.074510
8	-1.519245	1.169245	-0.419618
6	-2.474306	0.317262	-0.034240
1	-3.455047	0.773213	-0.197020
8	-2.303658	-0.774456	0.421849
8	0.161334	-2.369834	0.752213
1	-0.667276	-1.854073	0.709904

PF-OH-TS4-PC

6	1.039690	1.728397	0.313405
6	-0.338059	1.639633	0.131324
6	-0.895404	0.433205	-0.258568
6	-0.125990	-0.698983	-0.478607
6	1.252229	-0.622586	-0.296497
6	1.765977	0.588303	0.091163
1	1.498240	2.659558	0.616401
1	-0.983587	2.493710	0.283204
1	-0.594414	-1.624803	-0.777736
1	1.888966	-1.482198	-0.455936
1	4.236406	-0.216764	-0.426245
8	-2.269105	0.437379	-0.488799
6	-3.040727	-0.522019	0.060110
1	-4.079911	-0.335332	-0.229956
8	-2.669575	-1.419664	0.746118
8	4.435329	-1.011930	0.074880
1	4.114816	-0.816150	0.958691

PF-H-TS1

6	2.163972	-0.971060	0.275559
6	0.832045	-1.317286	0.107668
6	-0.081714	-0.329436	-0.209712
6	0.294417	0.992116	-0.369812
6	1.630917	1.322386	-0.195862
6	2.565001	0.348808	0.126914
1	2.886857	-1.736175	0.522568
1	0.490161	-2.337059	0.213423
1	-0.437139	1.745949	-0.616250
1	1.940217	2.351488	-0.314958
1	3.603409	0.617699	0.260328
8	-1.398631	-0.762447	-0.423887
6	-2.423577	-0.063895	0.060246
1	-3.512639	-0.728586	-0.284139
8	-2.423670	0.944431	0.676094
1	-4.278815	-1.258986	-0.568638

PF-H-TS2

6	2.084632	-0.983050	0.274203
6	0.770121	-1.338337	0.001693
6	-0.145700	-0.349991	-0.319405
6	0.265115	0.961173	-0.362713
6	1.557707	1.337383	-0.091583
6	2.481064	0.345726	0.232592
1	2.801786	-1.753249	0.521571
1	0.443373	-2.369196	0.028818
1	-0.692385	1.984299	-0.732746
1	1.851679	2.378173	-0.129789
1	3.506199	0.613726	0.449258
8	-1.440317	-0.735805	-0.650222
6	-2.466406	-0.207465	0.051396

1	-3.401894	-0.608885	-0.351329
8	-2.376567	0.557138	0.956278
1	-1.252893	2.591823	-0.951315

PF-H-TS3

6	-2.021305	-1.100159	0.281831
6	-0.684058	-1.399060	0.066334
6	0.205306	-0.383974	-0.246007
6	-0.209295	0.937782	-0.353182
6	-1.543902	1.178787	-0.128483
6	-2.471084	0.213031	0.186636
1	-2.714386	-1.894535	0.524456
1	-0.315435	-2.412817	0.130827
1	0.489227	1.726702	-0.589731
1	-2.011052	2.533470	-0.239000
1	-3.510494	0.460513	0.353967
8	1.512606	-0.774394	-0.518964
6	2.548890	-0.090953	0.006070
1	3.477205	-0.563814	-0.331159
8	2.482264	0.859695	0.717421
1	-2.321330	3.335349	-0.316209

PF-H-TS4

6	1.998418	-1.013568	0.284757
6	0.662934	-1.343345	0.080152
6	-0.234211	-0.348401	-0.268527
6	0.155947	0.972617	-0.421859
6	1.490277	1.305004	-0.214521
6	2.366680	0.302388	0.132363
1	2.717354	-1.775208	0.555716
1	0.308330	-2.359885	0.180935

1	-0.569747	1.726587	-0.688164
1	1.820430	2.329269	-0.324411
1	3.754976	0.635727	0.346206
8	-1.540258	-0.758028	-0.527914
6	-2.572113	-0.103952	0.040365
1	-3.502257	-0.583811	-0.281803
8	-2.500290	0.832470	0.770120
1	4.587705	0.807322	0.477498

PF-O-TS1

6	2.469829	-1.165677	0.273869
6	1.096326	-1.330672	0.184473
6	0.315414	-0.240800	-0.150113
6	0.858150	1.004682	-0.405918
6	2.234709	1.152455	-0.310539
6	3.040444	0.075171	0.028784
1	3.091922	-2.010005	0.536197
1	0.623218	-2.285676	0.363530
1	0.226443	1.839109	-0.669039
1	2.676308	2.120087	-0.504372
1	4.111380	0.203126	0.100521
8	-1.060380	-0.499087	-0.283699
6	-1.946199	0.354355	0.204687
1	-3.096581	-0.138396	-0.030720
8	-1.790402	1.382209	0.764792
8	-4.154808	-0.736289	-0.324540

PF-O-TS2

6	2.477034	-0.755441	0.084927
6	1.253748	-1.353068	-0.186737
6	0.120289	-0.563331	-0.295030

6	0.246835	0.796681	-0.128309
6	1.437756	1.416886	0.151134
6	2.574927	0.617257	0.257324
1	3.361497	-1.371923	0.163994
1	1.159993	-2.422132	-0.321461
1	-0.905702	1.534349	-0.294334
1	1.493161	2.488683	0.282079
1	3.531183	1.074284	0.471061
8	-1.079700	-1.166840	-0.625899
6	-2.164640	-0.909359	0.142795
1	-3.024160	-1.428972	-0.290337
8	-2.178410	-0.245442	1.127781
8	-1.903348	1.990776	-0.522835

PF-O-TS3

6	-1.117881	2.025608	0.256056
6	0.228475	1.791872	0.021704
6	0.672087	0.506317	-0.244448
6	-0.207837	-0.569510	-0.287779
6	-1.527177	-0.273489	-0.046304
6	-2.031069	0.975420	0.227520
1	-1.459756	3.030470	0.463687
1	0.948922	2.597109	0.037248
1	0.132284	-1.573218	-0.490876
1	-2.414656	-1.313331	-0.085639
1	-3.083706	1.135651	0.410977
8	2.022578	0.372380	-0.536587
6	2.739207	-0.641664	-0.006530
1	3.771078	-0.551993	-0.360588
8	2.332035	-1.487472	0.722370
8	-3.158237	-2.161409	-0.122799

PF-O-TS4

6	-1.458722	1.226975	0.204571
6	-0.092629	1.449284	0.072129
6	0.741015	0.391963	-0.254014
6	0.257451	-0.891950	-0.457035
6	-1.107484	-1.123479	-0.323213
6	-1.909362	-0.055341	0.002345
1	-2.132486	2.033535	0.456685
1	0.334176	2.432745	0.212173
1	0.931442	-1.697277	-0.705495
1	-1.516590	-2.112967	-0.471150
1	-3.258390	-0.283367	0.133492
8	2.081783	0.711231	-0.438079
6	3.044245	-0.063365	0.103548
1	4.016573	0.370605	-0.151206
8	2.878251	-1.046762	0.750558
8	-4.362761	-0.457944	0.241960

PF-HO₂-TS1

6	-2.661667	1.303863	-0.233209
6	-1.315362	0.996473	-0.371350
6	-0.921352	-0.315090	-0.181799
6	-1.821689	-1.317104	0.126887
6	-3.163235	-0.992836	0.259056
6	-3.584435	0.317311	0.082424
1	-2.987294	2.324805	-0.376154
1	-0.592629	1.759921	-0.614783
1	-1.463136	-2.328536	0.254572
1	-3.877628	-1.767673	0.500135
1	-4.630517	0.568362	0.187446

8	0.412433	-0.727574	-0.355832
6	1.406533	0.007217	0.119228
1	2.605716	-0.574223	-0.137786
8	1.382543	1.034043	0.707162
8	4.319396	0.437102	-0.092507
1	4.442225	0.556884	0.858499
8	3.744440	-0.810889	-0.193743

PF-HO₂-TS2

6	-1.323483	1.593078	-0.079179
6	-0.367284	0.658012	-0.377258
6	-0.591312	-0.696571	-0.337036
6	-1.855779	-1.154438	-0.004285
6	-2.853509	-0.234099	0.288240
6	-2.595406	1.128582	0.255827
1	-1.101811	2.651340	-0.103607
1	1.026770	1.080041	-0.726978
1	-2.039874	-2.220060	0.018954
1	-3.841005	-0.588411	0.548279
1	-3.377955	1.837399	0.489414
8	0.388473	-1.619869	-0.687391
6	1.508710	-1.677476	0.050234
1	2.190171	-2.405309	-0.398301
8	1.725980	-1.057753	1.046654
8	2.079875	1.195788	-0.791799
8	2.443825	1.625864	0.484920
1	2.506871	0.790233	0.973910

PF-HO₂-TS3

6	0.319065	2.580249	0.255724
6	1.390491	1.731849	0.020173

6	1.162670	0.393953	-0.256685	6	-0.807749	-0.662670	-0.449177
6	-0.125848	-0.126575	-0.310735	6	0.579536	-0.697478	-0.554808
6	-1.141134	0.761415	-0.063158	6	1.301701	0.445899	-0.249901
6	-0.986841	2.096891	0.221254	6	0.686521	1.620382	0.149931
1	0.500047	3.624630	0.471768	6	-0.700295	1.664783	0.255863
1	2.408525	2.093328	0.042573	6	-1.388552	0.514904	-0.046439
1	-0.315217	-1.167811	-0.529055	1	-1.407191	-1.533249	-0.680120
1	-2.442840	0.139736	-0.086953	1	1.088803	-1.598840	-0.860910
1	-1.828933	2.746882	0.411383	1	1.294652	2.486742	0.370671
8	2.280563	-0.377594	-0.548745	1	-1.200948	2.571566	0.565052
6	2.422134	-1.599120	0.005837	1	-2.824247	0.448281	0.048046
1	3.360587	-2.032028	-0.354704	8	2.684720	0.498957	-0.399000
8	1.668399	-2.123815	0.761161	6	3.454693	-0.472446	0.130911
8	-3.319564	-0.506187	-0.057980	1	4.501379	-0.240299	-0.090279
8	-2.780384	-1.788999	-0.149836	8	3.075105	-1.421399	0.738843
1	-2.717512	-2.063946	0.773723	8	-3.884440	0.209884	0.129828
				8	-3.908065	-1.183844	0.060318
PF-HO ₂ -TS4				1	-3.946128	-1.443231	0.989344