Supplementary Material

Quantum chemical study of the (Z)-2-penten-1-ol ($\text{HOCH}_2\text{-CH=CHCH}_2\text{CH}_3$) + OH + O₂ reactions

Weichao Zhang* and Benni Du

College of Chemistry and Chemical Engineering and Jiangsu Key Laboratory of Green Synthetic Chemistry for Functional Materials, Jiangsu Normal University, Xuzhou, Jiangsu 221116, People's Republic of China

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* Corresponding author. Tel.: +86 516 83403165; fax: +86 516 83403164.
E-mail address: zwc@jsnu.edu.cn

Figure S1. Optimized geometries for the reactant, reactant complexes (RC), intermediates (IM), transition states (TS), and products (P) involved in the reaction of OH+(Z)-PO21 at the BH&HLYP/6-311++G(d,p) level. Bond lengths are given in Angstroms.

Figure S1. Continued.

Figure S2 Optimized geometries of all stationary points involved in the reaction of IM1+O₂ at the BH&HLYP/6-311++G(d,p) level. Bond lengths are given in Angstroms.

Figure S3. Optimized geometries of all stationary points involved in the reaction of IM2+O₂ at the BH&HLYP/6-311++G(d,p) level. Bond lengths are given in Angstroms.

Table S1. Zero-point energies (ZPE, hartree), *T1* diagnostic values, total energies (*E*, hartree), and ZPE corrected relative energies (ΔE , kJ/mol) of the various species involved in the OH+(*Z*)-PO21 reaction

Species	ZPE, BHandHLYP/ 6-311++G(d,p)	<i>T1</i> Diag	<i>E</i> [CCSD(T)/6-311+G(d,p)]	<i>E</i> [CCSD(T)+ 0.9335×ZPE]	ΔE
(<i>Z</i>)-PO21+OH	0.155755	0.010, 0.010	-346.702886	-346.557489	0.00
TS1	0.152804	0.022	-346.6951214	-346.552479	13.15
TS2	0.152305	0.022	-346.6946454	-346.552469	13.18
RC3	0.158466	0.011	-346.7135755	-346.565647	-21.42
TS3	0.154134	0.023	-346.7009402	-346.557056	1.14
RC3A	0.156386	0.010	-346.7046881	-346.558702	-3.18
TS3A	0.154746	0.024	-346.7024877	-346.558032	-1.43
RC4	0.158466	0.011	-346.7135755	-346.565647	-21.42
TS4	0.153621	0.021	-346.7016591	-346.558254	-2.01
RC4A	0.158645	0.010	-346.7142998	-346.566205	-22.88
TS4A	0.152716	0.023	-346.6996201	-346.557060	1.13
TS5	0.152209	0.022	-346.6943672	-346.552280	13.68
TS6	0.152577	0.016	-346.694664	-346.552233	13.80
TS6A	0.152537	0.017	-346.6942766	-346.551883	14.72
TS6B	0.152961	0.016	-346.6960928	-346.553304	10.99
RC1	0.158834	0.015	-346.712952	-346.564680	-18.88
TSRC1-1	0.159522	0.026	-346.7129757	-346.564062	-17.26
IM1	0.161670	0.012	-346.7536453	-346.602726	-118.77
TSRC1-2	0.158718	0.024	-346.7117324	-346.563569	-15.96
IM2	0.161283	0.012	-346.7558405	-346.605283	-125.48
RC2	0.157658	0.014	-346.708331	-346.561157	-9.63
TSRC2-3	0.157739	0.025	-346.7024738	-346.555224	5.95
IM3	0.160652	0.012	-346.7504727	-346.600504	-112.94
TSRC2-4	0.158327	0.025	-346.7082674	-346.560469	-7.82
IM4	0.160998	0.012	-346.7526084	-346.602317	-117.70
P1+H2O	0.155053	0.023, 0.010	-346.713715	-346.568973	-30.15
P2+H2O	0.155184	0.023, 0.010	-346.716367	-346.571503	-36.79
P3+H2O	0.154513	0.021, 0.010	-346.746283	-346.602045	-116.98
P3A+H2O	0.154266	0.021, 0.010	-346.750775	-346.606768	-129.38
P4+H2O	0.154730	0.022, 0.010	-346.754694	-346.610254	-138.53
P4A+H2O	0.154063	0.022, 0.010	-346.755406	-346.611588	-142.04
P5+H2O	0.154427	0.015, 0.010	-346.719885	-346.575727	-47.88
P6+H2O	0.153548	0.012, 0.010	-346.723832	-346.580495	-60.40

Table S2. The variations in Gibbs free energy (ΔG) of various species at different temperatures calculated at the CCSD(T)/6-311+G(d,p)//BH&HLYP/ 6-311++G(d,p) +TCG levels of theory

Species	$\Delta G(220K)$	$\Delta G(260K)$	$\Delta G(298K)$	$\Delta G(340K)$	$\Delta G(380K)$	$\Delta G(420K)$	$\Delta G(460K)$	$\Delta G(500K)$
Z-trans-PO21+OH	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
RC3	-2.94	0.62	4.00	7.67	11.16	14.61	18.04	21.43
TS3	28.03	33.70	39.13	45.09	50.80	56.50	62.19	67.87
RC3A	8.97	10.92	12.72	14.61	16.36	18.06	19.72	21.33
TS3A	24.97	30.53	35.87	41.75	47.38	53.00	58.62	64.24
RC4	-2.94	0.62	4.00	7.67	11.16	14.61	18.04	21.43
TS4	20.52	25.22	29.71	34.63	39.33	44.02	48.70	53.36
RC4A	-3.19	0.61	4.22	8.16	11.89	15.59	19.26	22.91
TS4A	23.60	28.21	32.61	37.42	42.01	46.57	51.12	55.65
RC1	5.82	10.59	15.13	20.06	24.76	29.41	34.04	38.63
TSRC1-1	10.49	16.24	21.77	27.86	33.71	39.57	45.44	51.32
IM1	-90.93	-85.28	-79.84	-73.86	-68.13	-62.40	-56.66	-50.94
TSRC1-2	10.27	15.64	20.80	26.47	31.91	37.35	42.79	48.24
IM2	-99.80	-94.59	-89.59	-84.09	-78.82	-73.55	-68.29	-63.03
RC2	12.60	16.70	20.56	24.73	28.68	32.57	36.42	40.24
TSRC2-3	29.53	34.22	38.72	43.65	48.36	53.07	57.77	62.46
IM3	-86.86	-81.63	-76.63	-71.14	-65.89	-60.64	-55.41	-50.19
TSRC2-4	18.03	23.24	28.22	33.70	38.93	44.16	49.40	54.62
IM4	-91.09	-85.75	-80.63	-75.01	-69.63	-64.26	-58.90	-53.55

Table S3. Zero-point energies (ZPE, hartree), *T1* diagnostic values, total energies (*E*, hartree), and ZPE corrected relative energies (ΔE , kJ/mol) of all stationary points involved in the IM1+O₂ reaction

Species	ZPE, BHandHLYP/ 6-311++G(d,p)	<i>T1</i> Diag	<i>E</i> [CCSD(T)/6-311+G(d,p)]	<i>E</i> [CCSD(T)+ 0.9335×ZPE]	ΔE
(Z)-PO21+OH+O ₂	0.159866	0.010, 0.010, 0.017	-496.746296	-496.597061	0.00
IM1+O ₂	0.165781	0.012, 0.017	-496.797055	-496.642299	-118.77
IM5	0.173676	0.019	-496.853101	-496.690974	-246.57
TS5-P7	0.166514	0.023	-496.796435	-496.640994	-115.35
P7+HO ₂	0.167869	0.012, 0.028	-496.825448	-496.668742	-188.20
TS5-P8-new	0.165627	0.025	-496.7906813	-496.636068	-102.41
P8-new+HO ₂	0.167793	0.012, 0.028	-496.826338	-496.669703	-190.72
TS5-7	0.166236	0.030	-496.8065878	-496.651406	-142.68
IM7	0.171598	0.016	-496.8196761	-496.659489	-163.91
TS7-P9	0.168623	0.020	-496.8010814	-496.643672	-122.38
P9-new+OH+HCHO	0.158332	0.013, 0.010, 0.016	-496.863683	-496.715880	-311.96
TS5-7A	0.166585	0.039	-496.8090307	-496.653524	-148.24
IM7A	0.171981	0.017	-496.8213067	-496.660762	-167.25
TS7A-P10	0.169141	0.021	-496.8049393	-496.647046	-131.24
P10+OH+HOCH ₂ CHO	0.159162	0.014, 0.010, 0.015	-496.869045	-496.720468	-324.00
TS5-7B	0.168000	0.022	-496.8041087	-496.647281	-131.85
IM7B	0.171726	0.014	-496.8414829	-496.681177	-220.85
TS7B-P7	0.170066	0.024	-496.8168153	-496.658059	-160.15
P7+HO ₂	0.167869	0.012, 0.028	-496.825448	-496.668742	-188.20
TS7B-P11	0.169047	0.037	-496.8318618	-496.674056	-202.15
P11+ OH	0.167355	0.012, 0.010	-496.870084	-496.713858	-306.65
TS5-7C	0.167211	0.021	-496.8012734	-496.645182	-126.34
IM7C	0.171109	0.014	-496.8353016	-496.675571	-206.13
TS7C-P8	0.169826	0.023	-496.8131026	-496.654570	-150.99
P8-new+HO ₂	0.167793	0.012, 0.028	-496.826338	-496.669703	-190.72
TS7C-P12-new	0.168200	0.035	-496.8207243	-496.663710	-174.99
P12-new+OH	0.166109	0.012, 0.010	-496.867266	-496.712203	-302.31
TS5-7D	0.165196	0.018	-496.7986804	-496.644470	-124.47
IM7D	0.170010	0.013	-496.8265928	-496.667888	-185.96
TS7D-P13	0.166746	0.033	-496.7963039	-496.640647	-114.43
P13+OH	0.166225	0.012, 0.010	-496.861016	-496.705845	-285.61
TS5-7E	0.165474	0.017	-496.7982329	-496.643763	-122.62
IM7E	0.168984	0.013	-496.8143697	-496.656623	-156.38
TS7E-P14	0.168191	0.033	-496.8058658	-496.648860	-136.00
P14+OH	0.169006	0.011, 0.010	-496.888134	-496.730367	-350.00

Table S4. Zero-point energies (ZPE, hartree), *T1* diagnostic values, total energies (*E*, hartree), and ZPE corrected relative energies (ΔE , kJ/mol) of all stationary points involved in the IM2+O₂ reaction

Species	ZPE, BHandHLYP/ 6-311++G(d,p)	T1 Diag	<i>E</i> [CCSD(T)/ 6-311+G(d,p)]	<i>E</i> [CCSD(T)+ 0.9335×ZPE]	ΔE
(Z)-PO21+OH+O ₂	0.159866	0.010, 0.010, 0.017	-496.746296	-496.597061	0.00
IM2+O ₂	0.165394	0.012, 0.017	-496.799250	-496.644855	-125.48
IM6	0.173457	0.020	-496.856384	-496.694461	-255.72
TS6-P15	0.165488	0.023	-496.7907135	-496.636230	-102.84
P15+HO ₂	0.166836	0.011, 0.028	-496.819322	-496.663580	-174.65
TS6-P16	0.166130	0.023	-496.7967994	-496.641717	-117.24
P16+HO ₂	0.166957	0.011, 0.028	-496.817720	-496.661866	-170.15
TS6-8	0.165888	0.034	-496.8109344	-496.656078	-154.95
IM8-new	0.172127	0.017	-496.8231111	-496.662431	-171.63
TS8-P10-new	0.169904	0.021	-496.8118112	-496.653206	-147.41
P10+OH+HOCH ₂ CHO	0.159162	0.014, 0.010, 0.015	-496.869045	-496.720468	-324.00
TS6-8A	0.166483	0.028	-496.8052811	-496.649869	-138.65
IM8A	0.171678	0.016	-496.8238221	-496.663561	-174.59
TS8A-HCHO	0.169459	0.020	-496.8073988	-496.649209	-136.91
HCHO+CH ₃ CH ₂ CH(OOH)CHOH	0.164224	0.016, 0.015	-496.803141	-496.649838	-138.57
TS6-8B	0.167328	0.020	-496.8003323	-496.644132	-123.58
IM8B	0.172611	0.014	-496.8411466	-496.680014	-217.79
TS8B-P15	0.169657	0.025	-496.8129813	-496.654606	-151.09
P15+HO ₂	0.166836	0.011, 0.028	-496.819322	-496.663580	-174.65
TS8B-P17	0.167155	0.036	-496.8183104	-496.662271	-171.21
P17+OH	0.165740	0.012, 0.010	-496.867250	-496.712532	-303.17
TS6-8C	0.168044	0.018	-496.8117587	-496.654890	-151.83
IM8C	0.171741	0.014	-496.837971	-496.677651	-211.59
TS8C-P18	0.168772	0.037	-496.8108984	-496.653350	-147.79
P18+OH	0.167227	0.012, 0.010	-496.875421	-496.719315	-320.98
TS6-8D	0.167074	0.020	-496.7951479	-496.639184	-110.59
IM8D	0.170459	0.013	-496.8304529	-496.671329	-194.99
TS8D-P16	0.168931	0.023	-496.8028587	-496.645162	-126.29
P16+HO ₂	0.166957	0.011, 0.028	-496.817720	-496.661866	-170.15
TS8D-P19	0.167801	0.033	-496.814005	-496.657363	-158.32
P19+OH	0.166935	0.012, 0.010	-496.859499	-496.703665	-279.89
TS6-8E	0.167473	0.018	-496.8081721	-496.651836	-143.81
IM8E	0.170726	0.013	-496.8244098	-496.665037	-178.47
TS8E-P20	0.168395	0.033	-496.7974811	-496.640284	-113.48
P20+OH	0.168600	0.012, 0.010	-496.863467	-496.706079	-286.23