

**Supplementary information**

**Quantum Mechanical study on the oxidation of ethyl vinyl ketone initiated by OH radical**

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**Table S1:** Total energy with zero point correction and Relative Energy (R.E.) of all species at 298 K calculated at M06-2X/6-311++G(d,p) levels of theory .

Species	$E_0$	RE (in kcal mol <sup>-1</sup> )
CH <sub>2</sub> CH(O)CH <sub>2</sub> CH <sub>3</sub> +OH	-346.013089	0
IM1	-346.0225852	-5.96
IM2	-346.0151642	-1.30
IM3	-346.0234857	-6.52
IM4	-346.0225215	-5.92
TS1a	-346.0056518	4.67
TS1b	-346.0107114	1.49
TS2	-346.0084696	2.89
TS3	-346.0119996	0.68
TS4a	-346.0092319	2.42
TS4b	-346.0144331	-0.84
TS5	-346.0165714	-2.19
TS6	-346.0169009	-2.39
TS7	-346.0027648	6.48

P1+H <sub>2</sub> O	-346.022031	-5.61
P2+H <sub>2</sub> O	-346.0294454	-10.26
P3+H <sub>2</sub> O	-346.0527014	-24.86
P4+H <sub>2</sub> O	-346.0377515	-15.48
P5	-346.0593327	-29.01
P6	-346.0738874	-38.15
P7	-346.0406261	-17.28

**Table S2:** Harmonic vibrational frequency of all species obtained at M06-2X/6-311++G(d,p) level of theory

SC1	59	108	207	221	332	432	453	641	648	808	824	
	1007	1022	1028	1061	1089	1091	1152	1275	1325	1385	1424	
	1444	1462	1504	1508	1717	1840	3051	3085	3087	3165	3166	
	3169	3191	3266									
OH	3757											
IM1	8	60	83	115	158	233	243	340	416	444	444	527
	644	651	814	837	1010	1026	1035	1068	1091	1098	1157	1281
	1326	1392	1430	1455	1462	1504	1510	1714	1819	3059	3086	3094
	3165	3174	3178	3201	3273	3642						
IM2	34	45	91	123	133	190	216	303	309	337	432	461
	643	656	811	833	1012	1031	1037	1063	1091	1095	1155	1280
	1329	1386	1421	1449	1464	1513	1516	1724	1836	3055	3071	3094
	3153	3160	3186	3210	3284	3771						
IM3	25	66	105	124	165	224	300	344	430	446	529	543
	645	646	813	827	1008	1018	1027	1064	1090	1093	1155	1276
	1324	1387	1423	1444	1459	1506	1527	1719	1818	3053	3077	3089
	3158	3159	3170	3191	3271	3626						

IM4	28	63	86	112	162	197	232	344	427	456	513	579
	644	653	814	831	1008	1029	1045	1067	1088	1097	1156	1277
	1329	1389	1425	1457	1459	1497	1505	1716	1826	3050	3079	3085
	3161	3163	3173	3196	3271	3639						
TS1a	<b>1408i</b>	43	60	85	103	171	188	198	288	387	463	563
	640	757	803	829	856	974	997	1037	1060	1086	1140	1245
	1270	1277	1305	1387	1421	1459	1495	1503	1700	1844	3049	3076
	3085	3159	3161	3189	3222	3804						
TS1b	<b>1634i</b>	46	71	158	172	204	223	332	413	435	514	606
	619	667	773	812	880	900	957	1007	1064	1086	1091	1144
	1270	1307	1386	1419	1457	1464	1495	1502	1695	1833	3049	3079
	3084	3149	3161	3165	3217	3713						
TS2	<b>1120i</b>	43	63	80	169	192	205	223	308	423	431	555
	630	695	781	814	849	1002	1008	1030	1078	1090	1127	1237
	1272	1302	1391	1416	1428	1450	1501	1507	1715	1843	3057	3077
	3090	3157	3158	3161	3260	3818						
TS3	<b>817i</b>	45	60	82	133	184	203	210	327	428	455	602
	648	763	810	854	991	1025	1028	1042	1067	1090	1139	1205
	1315	1338	1390	1419	1439	1451	1493	1497	1718	1830	3072	3098
	3148	3168	3176	3204	3274	3778						
TS4a	<b>805i</b>	54	58	70	127	170	193	304	342	421	454	634
	647	719	818	843	978	1025	1034	1059	1080	1086	1135	1254
	1281	1328	1335	1374	1395	1443	1457	1483	1722	1837	3058	3098
	3128	3174	3200	3206	3274	3785						
TS4b	<b>1146i</b>	48	85	143	159	201	322	341	429	454	468	631
	647	752	817	884	949	1025	1026	1032	1075	1087	1095	1162
	1248	1321	1327	1394	1442	1445	1462	1467	1718	1824	3049	3087
	3112	3172	3189	3199	3273	3742						
TS5	<b>419i</b>	57	90	136	186	206	226	294	329	431	494	622
	642	735	806	815	986	1006	1015	1056	1086	1092	1147	1278
	1301	1382	1423	1444	1463	1500	1505	1627	1844	3055	3080	3102
	3162	3163	3186	3217	3297	3781						
TS6	<b>412i</b>	51	60	108	191	201	244	332	423	440	521	634
	690	759	810	829	978	1005	1019	1054	1081	1102	1156	1277



**Table S3:** Cartesian coordinates of all species (in Å) at M06-2X/6-311++G(d,p) level of theory**EVK (SC1)**

At. No.(Z)	X	Y	Z
6	2.556096000	0.015187000	0.000309000
1	3.508722000	-0.504047000	0.000351000
1	2.557831000	1.102012000	0.000724000
6	1.396743000	-0.642404000	-0.000224000
1	1.359480000	-1.729710000	-0.000683000
6	0.093789000	0.096126000	-0.000160000
8	0.048801000	1.309913000	-0.000253000
6	-1.159273000	-0.755807000	0.000018000
6	-2.440820000	0.063722000	0.000198000
1	-1.104776000	-1.419905000	0.873752000
1	-1.104976000	-1.419877000	-0.873749000
1	-3.317399000	-0.588279000	0.000313000
1	-2.484136000	0.709746000	0.880008000
1	-2.484368000	0.709812000	-0.879546000

**TS1a**

At. No.(Z)	X	Y	Z
6	1.723062000	0.554187000	-0.144395000
1	2.847956000	0.099149000	-0.234905000
1	1.647123000	1.638571000	-0.148195000
6	0.707918000	-0.292828000	-0.063630000
1	0.870631000	-1.368936000	-0.062968000
6	-0.711288000	0.207721000	0.000737000
8	-0.966028000	1.390921000	0.068437000
6	-1.786915000	-0.857464000	-0.030292000
6	-3.194245000	-0.285226000	0.043871000
1	-1.587197000	-1.551365000	0.797830000
1	-1.636228000	-1.445815000	-0.946023000
1	-3.937472000	-1.085096000	0.008755000

1	-3.331954000	0.280672000	0.968094000
1	-3.375944000	0.399582000	-0.787523000
1	4.022086000	-0.360695000	0.972678000
8	3.972254000	-0.461471000	0.005877000

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### TS1b

At. No.(Z)	X	Y	Z
6	-1.905810000	1.117808000	0.000115000
1	-2.657908000	1.902248000	0.000299000
1	-2.419062000	-0.019591000	0.000301000
6	-0.591196000	1.292088000	-0.000313000
1	-0.178799000	2.301970000	-0.000581000
6	0.399832000	0.169158000	-0.000260000
8	0.063743000	-1.000581000	-0.000578000
6	1.856418000	0.576771000	0.000350000
6	2.810713000	-0.607542000	0.000155000
1	2.013601000	1.223845000	0.874461000
1	2.014194000	1.224620000	-0.873074000
1	3.847928000	-0.265351000	0.000823000
1	2.647722000	-1.234013000	0.880034000
1	2.648559000	-1.233053000	-0.880567000
1	-1.847640000	-1.578300000	0.000040000
8	-2.749785000	-1.200928000	0.000327000

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### TS2

At. No.(Z)	X	Y	Z
6	1.954015000	1.427229000	-0.066485000
1	3.028793000	1.292262000	-0.136006000
1	1.559656000	2.439066000	0.010715000
6	1.114936000	0.400364000	-0.084171000
1	1.538382000	-0.718348000	-0.202371000
6	-0.380651000	0.503595000	0.003856000
8	-0.902888000	1.590252000	0.136177000

6	-1.155337000	-0.786940000	-0.088308000
6	-2.660287000	-0.586041000	-0.000541000
1	-0.779847000	-1.451282000	0.701540000
1	-0.858685000	-1.278163000	-1.025199000
1	-3.179300000	-1.544663000	-0.068851000
1	-2.932648000	-0.106927000	0.942886000
1	-3.012484000	0.060218000	-0.807974000
1	2.431924000	-1.794335000	0.878734000
8	2.023907000	-1.921135000	0.003875000

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**TS3**

<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	2.753167000	0.249266000	0.055271000
1	3.566534000	0.896251000	0.366231000
1	2.981695000	-0.593952000	-0.591117000
6	1.496799000	0.464910000	0.445418000
1	1.230987000	1.299662000	1.089555000
6	0.394766000	-0.443731000	0.006910000
8	0.568588000	-1.328623000	-0.809245000
6	-0.962987000	-0.192855000	0.616702000
6	-2.042662000	-1.165039000	0.197303000
1	-1.242102000	0.888892000	0.284539000
1	-0.875465000	-0.072302000	1.703772000
1	-3.011056000	-0.867839000	0.605048000
1	-2.114379000	-1.220116000	-0.891444000
1	-1.805646000	-2.171608000	0.555464000
1	-1.416631000	1.822754000	-1.325667000
8	-1.462142000	2.146492000	-0.406505000

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**TS4a**

<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	-3.251477000	-0.428694000	-0.037642000
1	-4.066220000	-1.145026000	-0.040133000



1	-3.492751000	0.630558000	-0.068252000
6	-1.976556000	-0.815301000	0.002090000
1	-1.700542000	-1.866974000	0.034050000
6	-0.869860000	0.191741000	0.005160000
8	-1.086965000	1.385792000	-0.036693000
6	0.539537000	-0.369859000	0.062704000
6	1.602445000	0.704325000	0.073268000
1	0.667672000	-1.044265000	-0.794551000
1	0.610892000	-1.008335000	0.953102000
1	2.629768000	0.140540000	0.102293000
1	1.591024000	1.322958000	-0.825525000
1	1.573505000	1.333126000	0.964753000
1	4.353521000	0.017827000	-0.455599000
8	3.783040000	-0.645002000	-0.026259000

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**TS4b**

<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	2.892081000	-0.481056000	-0.066727000
1	3.920637000	-0.301183000	-0.360932000
1	2.652340000	-1.416050000	0.432472000
6	1.929248000	0.410886000	-0.300694000
1	2.135580000	1.356381000	-0.796814000
6	0.520400000	0.141970000	0.114367000
8	0.203365000	-0.899373000	0.660462000
6	-0.488699000	1.231781000	-0.187108000
6	-1.863294000	0.963845000	0.379011000
1	-0.524240000	1.348855000	-1.279115000
1	-0.078437000	2.177248000	0.197274000
1	-2.596888000	1.723360000	0.103563000
1	-2.285821000	-0.044919000	-0.103792000
1	-1.859316000	0.785195000	1.455471000
1	-1.646049000	-1.659261000	-0.072211000
8	-2.410392000	-1.297399000	-0.561588000

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**TS5**

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<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	2.223062000	-0.801082000	0.343182000
1	3.185007000	-0.642002000	0.816039000
1	2.138545000	-1.550887000	-0.438718000
6	1.137841000	-0.065265000	0.681429000
1	1.170448000	0.628984000	1.515414000
6	-0.202675000	-0.359905000	0.062427000
8	-0.302696000	-1.149038000	-0.854442000
6	-1.379510000	0.388880000	0.638486000
6	-2.685945000	0.093837000	-0.082742000
1	-1.122374000	1.455261000	0.601647000
1	-1.440832000	0.131217000	1.705293000
1	-3.511054000	0.645103000	0.374133000
1	-2.616347000	0.379061000	-1.135078000
1	-2.915868000	-0.973592000	-0.047963000
1	1.593057000	1.068321000	-1.442842000
8	1.423043000	1.564007000	-0.621135000

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**TS6**

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<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	-1.966668000	0.694097000	0.639301000
1	-2.853025000	1.304529000	0.516841000
1	-1.956203000	-0.025486000	1.451523000
6	-0.836254000	0.938151000	-0.065391000
1	-0.795297000	1.727583000	-0.810903000
6	0.363746000	0.081147000	0.129949000
8	0.261363000	-1.021969000	0.641285000
6	1.689307000	0.629967000	-0.348591000
6	2.858402000	-0.304939000	-0.077542000
1	1.834598000	1.609734000	0.125893000
1	1.582224000	0.839267000	-1.421997000
1	3.790684000	0.127607000	-0.447610000

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1	2.961705000	-0.494086000	0.993441000
1	2.701662000	-1.269662000	-0.565075000
8	-2.523732000	-0.807711000	-0.771183000
1	-1.818592000	-1.412579000	-0.469290000

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### TS7

At. No.(Z)	X	Y	Z
6	2.564763000	-0.393727000	0.194674000
1	3.515554000	-0.695062000	-0.231856000
1	2.552804000	-0.015359000	1.212741000
6	1.433697000	-0.475529000	-0.500713000
1	1.409639000	-0.850847000	-1.520740000
6	0.119013000	-0.095335000	0.107989000
8	0.089198000	0.511437000	1.212724000
6	-1.082354000	-0.890618000	-0.365977000
6	-2.409067000	-0.383169000	0.179528000
1	-0.899451000	-1.923604000	-0.037715000
1	-1.074096000	-0.902648000	-1.460509000
1	-3.225747000	-1.041224000	-0.126359000
1	-2.386398000	-0.337126000	1.270413000
1	-2.623112000	0.619268000	-0.200981000
1	-0.607069000	2.097090000	-0.113803000
8	-0.141504000	1.548535000	-0.773249000

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### IM1

At. No.(Z)	X	Y	Z
6	-1.715442000	1.552165000	0.000514000
1	-2.272896000	2.482965000	0.000326000
1	-2.287175000	0.627449000	0.001522000
6	-0.381810000	1.542983000	-0.000415000
1	0.185153000	2.471108000	-0.001314000
6	0.404333000	0.274988000	-0.000086000
8	-0.126614000	-0.823039000	0.000309000

6	1.909191000	0.418454000	-0.000175000
6	2.643082000	-0.913564000	0.000155000
1	2.177540000	1.029149000	0.872885000
1	2.177522000	1.028720000	-0.873536000
1	3.723963000	-0.756825000	0.000271000
1	2.374566000	-1.501898000	0.880460000
1	2.374816000	-1.502206000	-0.880022000
1	-1.860274000	-1.567924000	-0.000145000
8	-2.842054000	-1.622048000	-0.000359000

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### IM2

At. No.(Z)	X	Y	Z
6	3.049113000	0.636134000	-0.225356000
1	3.827318000	1.372276000	-0.053665000
1	3.284288000	-0.234173000	-0.832163000
6	1.826028000	0.774443000	0.285593000
1	1.558866000	1.633413000	0.897211000
6	0.765879000	-0.253190000	0.034661000
8	0.978004000	-1.232206000	-0.653705000
6	-0.577854000	0.000473000	0.682967000
6	-1.594637000	-1.093119000	0.394614000
1	-0.937739000	0.977965000	0.334566000
1	-0.408770000	0.117361000	1.762261000
1	-2.553554000	-0.860551000	0.866735000
1	-1.738243000	-1.205597000	-0.684136000
1	-1.246502000	-2.058792000	0.769417000
1	-3.676686000	0.541438000	-1.152031000
8	-3.343023000	1.148233000	-0.464179000

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### IM3

At. No.(Z)	X	Y	Z
6	2.808621000	-0.837872000	0.000050000
1	3.892262000	-0.789261000	0.000779000

1	2.334717000	-1.815850000	-0.001355000
6	2.057480000	0.263560000	0.000810000
1	2.500591000	1.256605000	0.002187000
6	0.567605000	0.175333000	-0.000205000
8	0.000818000	-0.904975000	-0.001435000
6	-0.186553000	1.485057000	0.000207000
6	-1.699718000	1.328983000	-0.000487000
1	0.160318000	2.055711000	-0.872516000
1	0.159604000	2.054937000	0.873706000
1	-2.184975000	2.307512000	-0.000687000
1	-2.038019000	0.780526000	-0.884013000
1	-2.038761000	0.780531000	0.882763000
1	-1.805735000	-1.449660000	0.000094000
8	-2.783895000	-1.553952000	0.001033000

#### IM4

At. No.(Z)	X	Y	Z
6	-1.728063000	1.522686000	0.120778000
1	-2.302774000	2.441257000	0.062668000
1	-2.266062000	0.607857000	0.358719000
6	-0.409551000	1.518247000	-0.082215000
1	0.128176000	2.437698000	-0.302234000
6	0.399683000	0.268237000	0.003767000
8	-0.110949000	-0.831550000	0.140563000
6	1.899769000	0.430757000	-0.085627000
6	2.658447000	-0.882209000	0.030952000
1	2.199096000	1.143653000	0.694944000
1	2.112693000	0.937692000	-1.037188000
1	3.734569000	-0.712355000	-0.047478000
1	2.449874000	-1.365577000	0.988175000
1	2.354962000	-1.574588000	-0.757504000
8	-2.824272000	-1.609558000	-0.125483000
1	-1.850468000	-1.533084000	-0.006671000

**P1**

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<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	-2.625142000	-0.059105000	0.000051000
1	-2.939773000	0.976263000	-0.000066000
6	-1.461472000	-0.673368000	0.000105000
1	-1.398123000	-1.761288000	0.000230000
6	-0.164289000	0.096299000	-0.000006000
8	-0.137054000	1.308178000	-0.000157000
6	1.095726000	-0.746296000	0.000090000
6	2.368316000	0.087286000	-0.000068000
1	1.046833000	-1.409846000	-0.874075000
1	1.046874000	-1.409578000	0.874461000
1	3.250951000	-0.556428000	0.000008000
1	2.405395000	0.733146000	-0.880187000
1	2.405439000	0.733415000	0.879851000

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**P2**

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<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	-2.695520000	-0.383876000	0.000156000
1	-3.247536000	-0.523554000	-0.929688000
1	-3.247231000	-0.523661000	0.930163000
6	-1.439558000	-0.053355000	-0.000016000
6	-0.072115000	0.311606000	-0.000111000
8	0.264411000	1.499922000	-0.000064000
6	0.943552000	-0.823171000	-0.000289000
6	2.375775000	-0.306069000	0.000267000
1	0.748724000	-1.454172000	-0.876175000
1	0.748277000	-1.454944000	0.874931000
1	3.081287000	-1.140436000	-0.000134000
1	2.564324000	0.313840000	-0.879126000
1	2.564062000	0.312734000	0.880499000

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**P3**

At. No.(Z)	X	Y	Z
6	-2.180553000	-0.795563000	0.000036000
1	-2.738615000	-1.725749000	0.000010000
1	-2.731409000	0.140855000	0.000114000
6	-0.847392000	-0.778888000	-0.000054000
1	-0.278994000	-1.705173000	-0.000144000
6	-0.099873000	0.516765000	-0.000006000
8	-0.702845000	1.598069000	-0.000007000
6	1.340366000	0.497002000	0.000025000
6	2.181244000	-0.734188000	0.000026000
1	1.808923000	1.476165000	-0.000081000
1	3.243324000	-0.486707000	-0.000205000
1	1.978564000	-1.357279000	0.880367000
1	1.978209000	-1.357423000	-0.880161000

#### P4

At. No.(Z)	X	Y	Z
6	2.496169000	-0.008293000	-0.000034000
1	3.439693000	-0.543707000	-0.000130000
1	2.516451000	1.078290000	0.000104000
6	1.326083000	-0.646928000	-0.000092000
1	1.271117000	-1.733488000	-0.000228000
6	0.037262000	0.112634000	0.000024000
8	0.008044000	1.325635000	0.000050000
6	-1.225939000	-0.730644000	0.000201000
6	-2.481788000	0.058559000	-0.000346000
1	-1.162535000	-1.406833000	0.869893000
1	-1.162361000	-1.407694000	-0.868786000
1	-3.440419000	-0.442666000	-0.000038000
1	-2.437019000	1.139044000	0.000273000

#### P5

At. No.(Z)	X	Y	Z
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6	-2.208865000	0.792518000	-0.312610000
1	-3.254331000	0.508426000	-0.316225000
1	-1.913881000	1.791369000	-0.604523000
6	-1.227989000	-0.102541000	0.353552000
1	-1.351484000	-0.059370000	1.450210000
6	0.219450000	0.364084000	0.111528000
8	0.472897000	1.548535000	0.102810000
6	1.275238000	-0.704560000	-0.050070000
6	2.682782000	-0.130699000	-0.116269000
1	1.027751000	-1.279065000	-0.952036000
1	1.151589000	-1.421450000	0.771293000
1	3.418058000	-0.929435000	-0.237722000
1	2.779873000	0.564090000	-0.953653000
1	2.918958000	0.424545000	0.794740000
1	-1.647483000	-1.531481000	-0.908915000
8	-1.419490000	-1.471090000	0.027195000

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**P6**

<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	-2.167273000	0.484461000	0.213364000
1	-2.882880000	1.205756000	-0.190817000
1	-2.357734000	0.425525000	1.301556000
6	-0.772291000	0.990555000	0.017328000
1	-0.602896000	2.059394000	-0.082479000
6	0.368838000	0.104371000	0.071129000
8	0.217457000	-1.100378000	0.304179000
6	1.749287000	0.695489000	-0.152576000
6	2.858106000	-0.342058000	-0.048488000
1	1.894071000	1.504017000	0.575785000
1	1.750729000	1.179041000	-1.138319000
1	3.833681000	0.121364000	-0.212650000
1	2.855311000	-0.813718000	0.936892000
1	2.716835000	-1.133264000	-0.788154000
8	-2.430280000	-0.747922000	-0.411212000



1	-1.724539000	-1.358622000	-0.150093000
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**P7**

<b>At. No.(Z)</b>	<b>X</b>	<b>Y</b>	<b>Z</b>
6	2.427092000	-0.657093000	0.005779000
1	3.392309000	-0.780930000	-0.473503000
1	2.258880000	-1.164461000	0.951011000
6	1.483789000	0.098611000	-0.544383000
1	1.630042000	0.629500000	-1.481809000
6	0.101144000	0.291697000	0.059791000
8	0.097128000	0.082242000	1.392574000
6	-0.884093000	-0.780066000	-0.528091000
6	-2.323091000	-0.599510000	-0.059728000
1	-0.492260000	-1.765693000	-0.264882000
1	-0.810057000	-0.659333000	-1.613987000
1	-2.967445000	-1.341266000	-0.538929000
1	-2.411020000	-0.723727000	1.022827000
1	-2.701164000	0.389694000	-0.332316000
1	-0.922569000	1.902575000	0.389627000
8	-0.322848000	1.591735000	-0.299855000

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