

ESI of the paper "A quasi-classical trajectory study of the OH + SO reaction: the role of ro-vibrational energy"

W. A. D. Pires, J. D Garrido, M. A. C. Nascimento, and M. Y. Ballester

Table 1: Results of trajectory calculations

v_{OH}, v_{SO}	$E_{tr}/$ kcal mol ⁻¹	$b_{max}/$ Å	QCT				VEQMT _C			
			N_T	N_{com}	N_{rec}	N_r	N_T	N_{com}	N_{rec}	N_r
1,0	0.199	8.7	2000	1662	992	670	1681	1357	694	663
	0.396	7.7	2000	1587	980	607	1680	1284	687	597
	0.596	7.1	2000	1542	911	631	1696	1254	636	618
	0.993	6.4	2000	1401	860	541	1704	1125	592	533
	1.987	5.4	2000	1308	871	437	1695	1026	598	428
	5.962	4.0	2000	1247	939	308	1727	1008	705	303
	9.936	3.9	2000	1119	933	186	1760	912	729	183
2,0	0.199	8.7	2000	1589	1001	588	1895	1496	909	587
	0.396	7.7	2000	1496	900	596	1894	1405	810	595
	0.596	7.1	2000	1488	940	548	1897	1393	847	546
	0.993	6.4	2000	1354	841	513	1894	1259	746	513
	1.987	5.4	2000	1298	812	486	1901	1218	733	485
	5.962	4.0	2000	1242	895	347	1892	1158	815	343
	9.936	4.1	2000	1034	814	220	1903	963	746	217
3,0	0.199	8.7	2000	1544	762	782	1968	1522	740	782
	0.396	7.7	2000	1475	757	718	1951	1432	714	718
	0.596	7.1	2000	1446	731	715	1948	1410	695	715
	0.993	6.4	2000	1314	652	662	1964	1291	629	662
	1.987	5.4	2000	1269	694	575	1952	1235	660	575
	5.962	4.0	2000	1243	731	512	1945	1208	696	512
	9.936	4.1	2000	1036	641	395	1934	996	602	394
4,0	0.199	8.7	2000	1510	396	1114	1984	1498	384	1114
	0.396	7.7	2000	1456	366	1090	1983	1443	353	1090
	0.596	7.1	2000	1408	369	1039	1975	1391	352	1039
	0.993	6.4	2000	1298	325	973	1980	1290	317	973
	1.987	5.4	2000	1221	346	875	1979	1210	335	875
	5.962	4.0	2000	1223	417	806	1975	1208	402	806
	9.936	4.4	2000	873	338	535	1974	862	327	535

Continued on next page

Table 1 – continued from previous page

$v_{\text{OH}}, v_{\text{SO}}$	$E_{tr}/$ kcal mol ⁻¹	$b_{max}/$ Å	QCT				VEQMT _C			
			N_T	N_{com}	N_{rec}	N_r	N_T	N_{com}	N_{rec}	N_r
5, 0	0.199	8.7	2000	1522	177	1345	1987	1515	170	1345
	0.396	7.7	2000	1445	180	1265	1990	1440	175	1265
	0.596	7.1	2000	1385	194	1191	1992	1384	193	1191
	0.993	6.4	2000	1264	182	1082	1995	1260	179	1081
	1.987	5.4	2000	1186	146	1040	1993	1180	140	1040
	5.962	4.0	2000	1198	186	1012	1975	1196	184	1012
	9.936	4.7	2000	734	154	580	1984	728	148	580
0, 1	0.199	9.0	2000	1602	767	835	1327	994	182	812
	0.396	7.8	1999	1611	798	813	1312	985	201	784
	0.596	7.2	2000	1545	763	782	1336	948	199	749
	0.993	6.6	1999	1369	723	646	1357	800	183	617
	1.987	5.6	1999	1234	745	489	1362	667	202	465
	5.962	4.2	2000	1148	884	264	1396	616	365	251
	9.936	3.7	2000	1174	1011	163	1468	699	543	156
0, 2	0.199	8.8	2000	1634	1047	587	1407	1062	481	581
	0.396	7.8	2000	1553	990	563	1458	1041	489	552
	0.596	7.2	2000	1527	978	549	1464	1014	479	535
	0.993	6.5	2000	1416	936	480	1510	946	476	470
	1.987	5.6	2000	1220	880	340	1508	748	419	329
	5.962	4.1	2000	1177	944	233	1585	778	549	229
	9.936	3.9	2000	1103	983	120	1612	727	612	115
0, 3	0.199	8.8	2000	1617	1128	489	1563	1192	714	478
	0.396	7.9	2000	1560	1132	428	1563	1127	703	424
	0.596	7.2	2000	1506	1067	439	1574	1084	652	432
	0.993	6.4	2000	1424	1043	381	1578	1015	639	376
	1.987	5.6	2000	1200	893	307	1650	861	556	305
	5.962	4.2	2000	1112	926	186	1709	829	649	180
	9.936	3.9	2000	1081	976	105	1741	825	722	103
0, 4	0.199	8.7	2000	1611	1218	393	1680	1298	907	391
	0.396	7.7	2000	1556	1175	381	1688	1247	868	379
	0.596	7.2	2000	1460	1093	367	1692	1156	794	362
	0.993	6.4	2000	1418	1097	321	1694	1117	801	316
	1.987	5.6	2000	1175	919	256	1727	905	651	254
	5.962	4.4	2000	1020	883	137	1803	824	688	136
	9.936	4.0	2000	1018	930	88	1830	850	763	87

Continued on next page

Table 1 – continued from previous page

$v_{\text{OH}}, v_{\text{SO}}$	$E_{tr}/$ kcal mol ⁻¹	$b_{max}/$ Å	QCT				VEQMT _C			
			N_T	N_{com}	N_{rec}	N_r	N_T	N_{com}	N_{rec}	N_r
0, 5	0.199	8.7	2000	1597	1216	381	1744	1345	967	378
	0.396	7.8	2000	1483	1163	320	1775	1260	940	320
	0.596	7.2	2000	1418	1138	280	1766	1185	905	280
	0.993	6.5	2000	1329	1057	272	1777	1106	834	272
	1.987	5.6	2000	1164	922	242	1806	973	732	241
	5.962	4.4	2000	1012	875	137	1860	873	738	135
	9.936	4.0	2000	1000	877	123	1874	874	753	121
0, 6	0.199	8.6	2000	1576	1299	277	1803	1380	1103	277
	0.396	7.8	2000	1461	1192	269	1829	1291	1023	268
	0.596	7.2	2000	1403	1136	267	1832	1237	971	266
	0.993	6.5	2000	1292	1053	239	1826	1120	881	239
	1.987	5.6	2000	1146	946	200	1868	1016	816	200
	5.962	4.4	2000	1018	883	135	1911	929	794	135
	9.936	4.0	2000	997	898	99	1901	900	803	97
0, 7	0.199	8.6	2000	1563	1311	252	1882	1446	1194	252
	0.396	7.8	2000	1424	1201	223	1864	1288	1065	223
	0.596	7.2	2000	1386	1153	233	1859	1246	1013	233
	0.993	6.5	2000	1281	1056	225	1887	1168	943	225
	1.987	5.6	2000	1083	909	174	1905	988	814	174
	5.962	4.5	2000	938	797	141	1925	863	723	140
	9.936	4.0	2000	959	845	114	1938	897	784	113
0, 8	0.199	8.5	2000	1513	1302	211	1907	1420	1209	211
	0.396	7.8	2000	1405	1164	241	1894	1300	1060	240
	0.596	7.2	2000	1352	1134	218	1909	1262	1044	218
	0.993	6.6	2000	1179	983	196	1929	1108	912	196
	1.987	5.6	2000	1090	957	133	1903	993	860	133
	5.962	4.5	2000	931	826	105	1956	887	782	105
	9.936	4.0	2000	944	842	102	1958	902	800	102
0, 9	0.199	8.5	2000	1468	1260	208	1925	1393	1185	208
	0.396	7.8	2000	1381	1174	207	1942	1323	1118	205
	0.596	7.2	2000	1332	1126	206	1930	1262	1057	205
	0.993	6.6	2000	1165	983	182	1954	1119	937	182
	1.987	5.6	2000	1079	939	140	1956	1035	896	139
	5.962	4.6	2000	888	785	103	1961	849	746	103
	9.936	4.0	2000	923	834	89	1977	900	812	88

Continued on next page

Table 1 – continued from previous page

$v_{\text{OH}}, v_{\text{SO}}$	$E_{tr}/$ kcal mol ⁻¹	$b_{max}/$ Å	QCT				VEQMT _C			
			N_T	N_{com}	N_{rec}	N_r	N_T	N_{com}	N_{rec}	N_r
0, 10	0.199	8.5	2000	1479	1284	195	1957	1436	1241	195
	0.396	7.8	2000	1330	1149	181	1953	1283	1102	181
	0.596	7.2	2000	1273	1099	174	1959	1232	1059	173
	0.993	6.6	2000	1108	954	154	1953	1061	909	152
	1.987	5.6	2000	1037	880	157	1961	998	841	157
	5.962	4.6	2000	868	762	106	1979	847	741	106
	9.936	4.0	2000	917	846	71	1986	903	832	71
0, 11	0.199	8.6	2000	1439	1234	205	1967	1406	1201	205
	0.396	7.8	2000	1303	1120	183	1955	1258	1075	183
	0.596	7.4	2000	1199	1026	173	1968	1167	994	173
	0.993	6.5	2000	1118	958	160	1965	1083	924	159
	1.987	5.5	2000	1043	926	117	1979	1022	905	117
	5.962	4.4	2000	923	803	120	1983	906	786	120
	9.936	4.0	2000	899	827	72	1979	878	807	71
0, 12	0.199	8.7	2000	1394	1197	197	1984	1378	1181	197
	0.396	7.8	2000	1260	1105	155	1976	1236	1081	155
	0.596	7.3	2000	1180	1024	156	1981	1161	1005	156
	0.993	6.7	2000	1007	860	147	1986	993	846	147
	1.987	5.7	2000	960	837	123	1986	946	823	123
	5.962	4.3	2000	942	837	105	1984	926	821	105
	9.936	4.0	2000	890	803	87	1991	881	794	87
0, 13	0.199	8.6	2000	1363	1173	190	1983	1346	1156	190
	0.396	7.9	2000	1184	1029	155	1982	1166	1011	155
	0.596	7.3	2000	1148	998	150	1990	1138	988	150
	0.993	6.7	2000	1009	888	121	1994	1003	882	121
	1.987	5.7	2000	943	823	120	1991	934	814	120
	5.962	4.7	2000	786	695	91	1990	776	685	91
	9.936	4.0	2000	875	782	93	1998	873	780	93
1, 1	0.199	9.0	2000	1564	1024	540	1797	1366	829	537
	0.396	8.2	2000	1405	932	473	1816	1230	758	472
	0.596	7.2	2000	1497	993	504	1785	1288	791	497
	0.993	6.6	2000	1318	893	425	1813	1138	721	417
	1.987	5.9	2000	1071	752	319	1817	900	583	317
	5.962	4.4	2000	1078	854	224	1844	927	706	221
	9.936	4.0	2000	1071	923	148	1831	915	767	148

Continued on next page

Table 1 – continued from previous page

$v_{\text{OH}}, v_{\text{SO}}$	$E_{tr}/$ kcal mol ⁻¹	$b_{max}/$ Å	QCT				VEQMT _C			
			N_T	N_{com}	N_{rec}	N_r	N_T	N_{com}	N_{rec}	N_r
2, 1	0.199	8.8	2000	1539	960	579	1938	1483	905	578
	0.396	7.9	2000	1451	971	480	1938	1398	919	479
	0.596	7.3	2000	1384	900	484	1932	1324	842	482
	0.993	6.7	2000	1244	813	431	1947	1191	760	431
	1.987	5.7	2000	1156	782	374	1929	1089	716	373
	5.962	4.4	2000	1089	778	311	1937	1034	723	311
	9.936	4.0	2000	1078	843	235	1932	1018	784	234
3, 1	0.199	8.9	2000	1468	747	721	1971	1447	726	721
	0.396	8.0	2000	1354	705	649	1985	1340	691	649
	0.596	7.3	2000	1363	720	643	1969	1337	695	642
	0.993	6.7	2000	1209	634	575	1977	1190	615	575
	1.987	5.6	2000	1162	631	531	1976	1144	613	531
	5.962	4.5	2000	1032	610	422	1971	1006	584	422
	9.936	4.1	2000	1008	648	360	1968	984	624	360
2, 4	0.199	8.8	2000	1477	1040	437	1979	1456	1019	437
	0.396	8.1	2000	1305	969	336	1981	1286	951	335
	0.596	7.4	2000	1320	949	371	1976	1296	927	369
	0.993	6.6	2000	1230	872	358	1979	1209	851	358
	1.987	5.6	2000	1143	833	310	1981	1124	814	310
	5.962	4.4	2000	1029	786	243	1985	1014	771	243
	9.936	4.0	2000	1038	821	217	1982	1020	803	217