

Supplementary Material for “Further Insight into the Reaction $\text{FeO}^+ + \text{H}_2 \rightarrow \text{Fe}^+ + \text{H}_2\text{O}$: Temperature Dependent Kinetics, Isotope Effects, and Statistical Modeling”

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Molecular parameters used in modeling:

FeO⁺ + H₂		Vibrational Frequencies (cm⁻¹)						Rotational Constants (GHz)		
sextet	Int 1	218	235	717	826	976	4080	1703.0	11.6	11.5
	TS 1	-1738	684	754	1048	1588	1765	113.5	13.4	12.0
	Int 2	347	473	529	792	1937	3793	469.9	11.4	11.1
	TS 2	-1199	177	536	730	1392	3731	273.1	11.0	10.6
	Int 3	343	429	559	1680	3750	3833	415.2	7.8	7.7

quartet	Int 1	404	632	984	1040	1483	3496	92.9	16.3	14.1
	TS 1	-974	645	931	960	1735	2263	113.7	15.6	13.7
	Int 2	147	531	689	815	1910	3769	185.9	12.9	12.1
	TS 2	-2176	383	672	946	1628	3786	247.8	11.8	11.4
	Int 3	411	431	674	1695	3775	3850	412.2	8.9	8.7

FeO⁺ + D₂		Vibrational Frequencies (cm⁻¹)						Rotational Constants (GHz)		
sextet	Int 1	173	187	515	691	824	2886	852.1	9.5	9.4
	TS 1	-1251	510	747	749	1129	1266	58.9	13.1	10.7
	Int 2	252	360	404	772	1382	2767	241.8	9.7	9.3
	TS 2	-882	133	417	676	994	2720	140.6	9.8	9.1
	Int 3	328	329	416	1233	2702	2812	207.7	6.8	6.6

quartet	Int 1	309	449	712	1036	1050	2473	49.2	15.6	12.2
	TS 1	-724	459	694	940	1229	1609	58.6	15.3	12.1
	Int 2	109	380	524	796	1364	2746	95.6	11.8	10.5
	TS 2	-1603	281	625	731	1162	2759	130.5	10.6	10.0
	Int 3	315	413	503	1245	2720	2825	206.3	7.8	7.5

FeO⁺ + DH		Vibrational Frequencies (cm⁻¹)						Rotational Constants (GHz)		
sextet	Int 1	197	204	565	823	886	3535	1180.5	10.4	10.3
	TS 1	-1303	620	753	860	1292	1662	87.5	13.1	11.4
	Int 2	328	375	438	773	1937	2767	386.7	10.3	10.0
	TS 2	-1197	134	423	684	1382	2721	271.6	9.8	9.5
	Int 3	334	381	472	1482	2755	3793	284.6	7.3	7.1

quartet	Int 1	334	564	792	1036	1320	3032	63.7	16.0	13.1
	TS 1	-742	542	835	943	1440	2119	83.3	15.3	12.9
	Int 2	126	478	572	796	1910	2746	162.3	11.8	11.0
	TS 2	-2162	297	640	751	1625	2759	213.1	10.7	10.4
	Int 3	366	419	569	1498	2771	3814	282.7	8.3	8.1

FeO⁺ + HD		Vibrational Frequencies (cm⁻¹)						Rotational Constants (GHz)		
sextet	Int 1	197	204	565	823	886	3535	1180.5	10.4	10.3
	TS 1	-1691	535	750	958	1173	1654	69.1	13.4	11.2
	Int 2	257	472	502	791	1382	3793	280.5	10.7	10.3
	TS 2	-883	176	526	718	1013	3731	140.7	10.9	10.1
	Int 3	334	381	472	1482	2755	3793	284.6	7.3	7.1

quartet	Int 1	334	564	792	1036	1320	3032	63.7	16.0	13.1
	TS 1	-937	579	728	946	1461	1905	71.8	15.5	12.8
	Int 2	137	391	683	815	1364	3769	103.7	12.9	11.5
	TS 2	-1620	367	668	912	1170	3786	141.9	11.7	10.9
	Int 3	366	419	569	1498	2771	3814	282.7	8.3	8.1