The Reaction Fragility Spectrum

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Electronic Supplementary Information

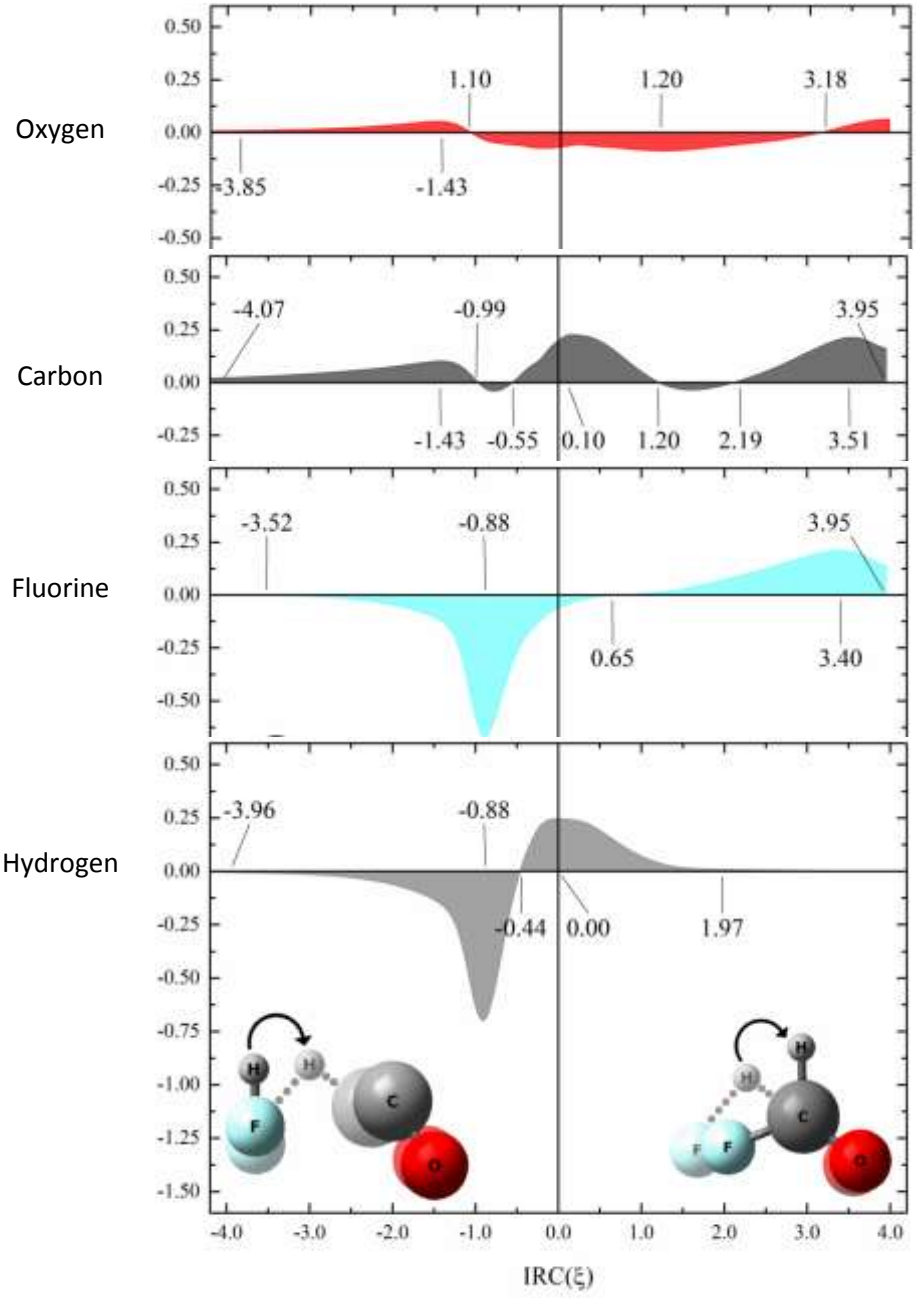


Figure 4
Reaction fragility spectra for individual atoms; reaction HF/CO. The peak positions and the limits for the peak integration have been marked.

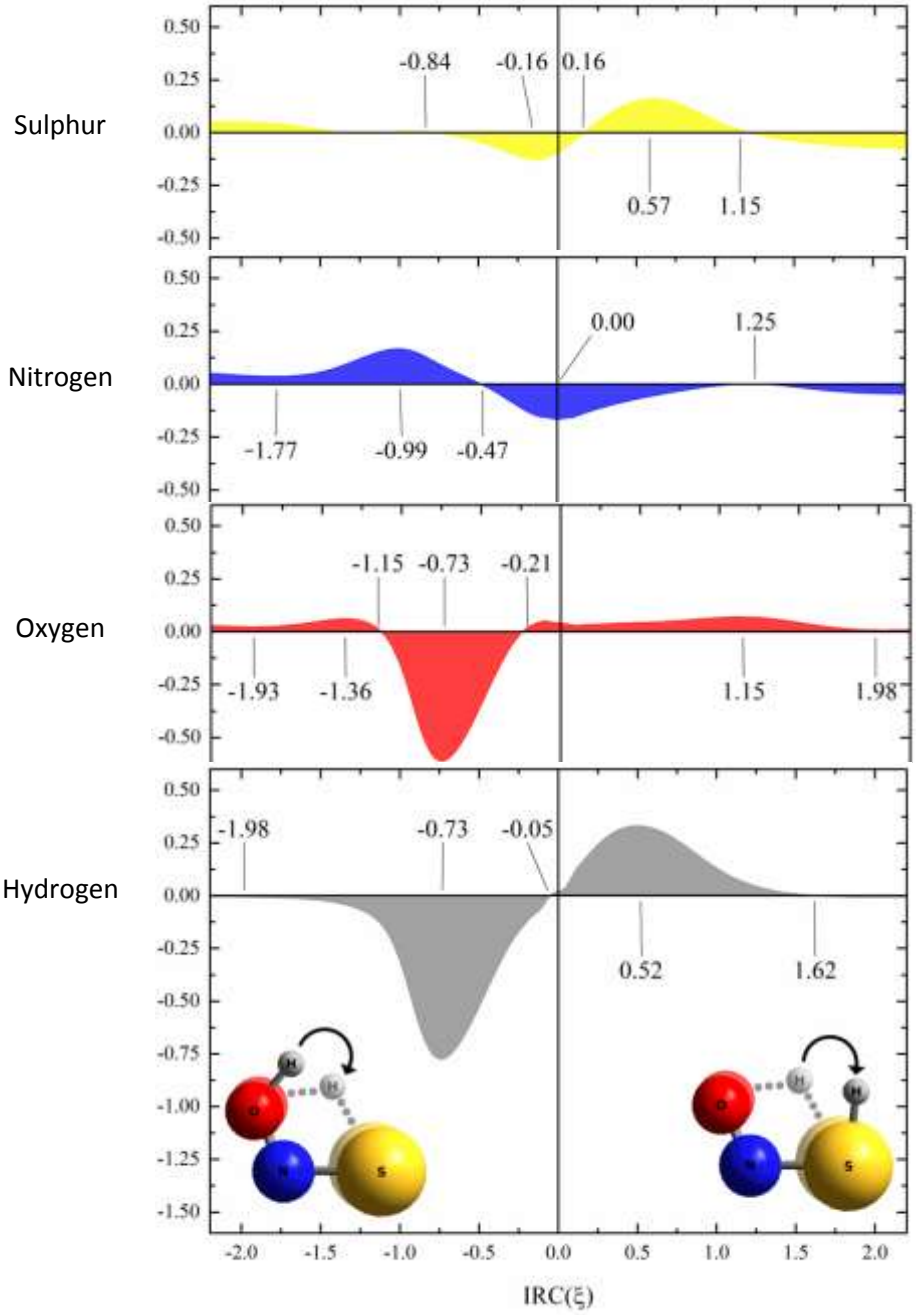
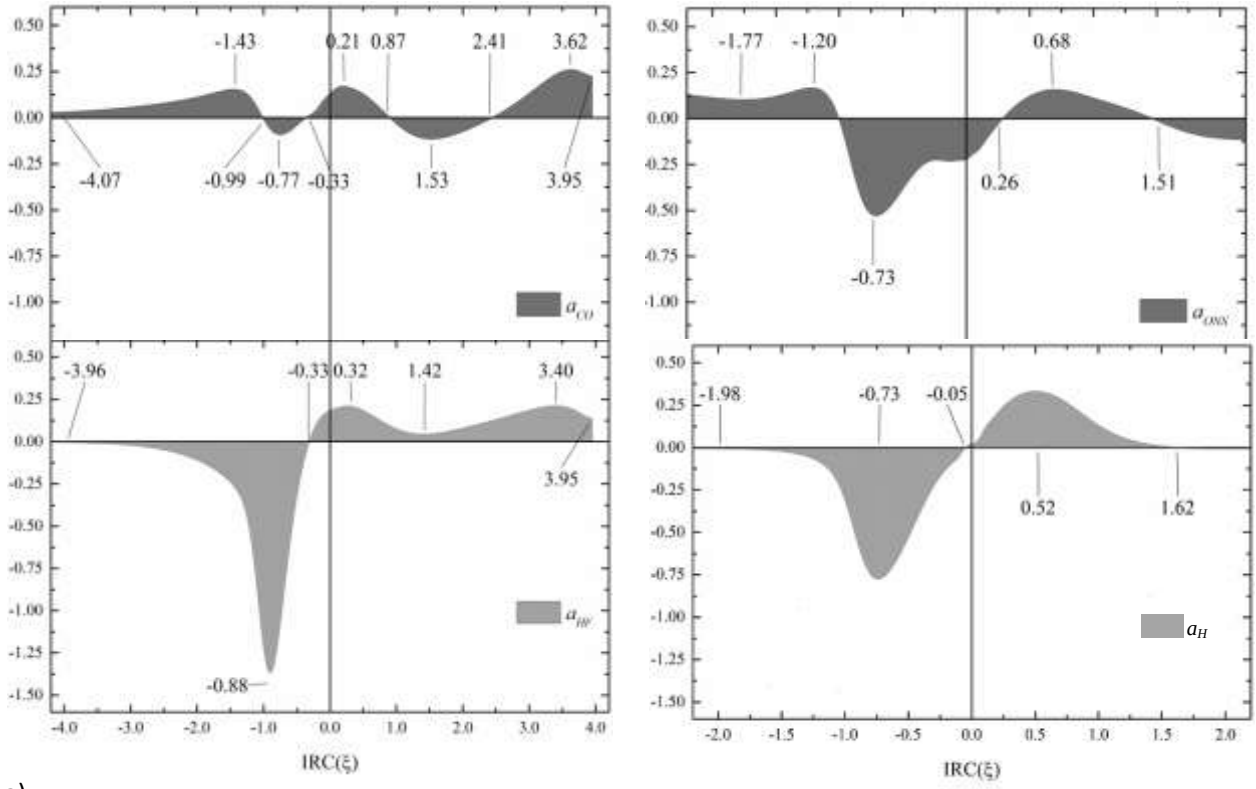


Figure 5
Reaction fragility spectra for individual atoms; reaction H/ONS. The peak positions and the limits for the peak integration have been marked.



a)

b)

Figure 6
Reaction fragility spectrum for the group components; a) HF/CO; b) H/ONS.
The peak positions and the limits for the peak integration have been marked.

Table 1

Analysis of the atomic spectral peaks shown in Figure 4 and 5, as well as for the group spectra in Figure 6. Positions of the peak maximum ($\xi_{max/min}$), the peak integral (Δk^A), the change in atomic population over the peak region (ΔN_A, Mulliken) and the average atomic softening index ($\bar{\lambda}^A = \Delta k^A / \Delta N_A$) for the peak region calculated from eq. 9 (atomic units).

Reaction	Atom/Group	$\xi_{max/min}$	Δk^A	ΔN_A	$\bar{\lambda}^A$
HF/CO	O	-1.43	-0.0588	0.1464	-0.4019
		1.20	-0.1124	0.0906	-1.2399
	C	-1.43	0.1743	-0.1326	-1.3145
		0.10	0.2369	-0.3872	-0.6119
		3.51	0.2371	0.0216	10.9977
	F	-0.88	-0.5325	0.2156	-2.4696
		3.40	0.3385	-0.2987	-1.1332
	H	-0.88	-0.4720	0.1159	-4.0717
		0.00	0.2888	0.3530	0.8182
	CO	-1.43	0.2474	-0.0594	-4.1656
		-0.77	-0.0401	-0.2467	0.1626
		0.21	0.1373	-0.2229	-0.6161
		1.53	-0.1145	-0.0092	12.5081
		3.62	0.2447	0.0918	2.6653
	HF	-0.88	-0.9449	0.3072	-3.0757
		0.32	0.2292	0.2402	0.9540
		3.40	0.3446	-0.1000	-3.4474
H/ONS	S	-0.16	-0.0633	-0.0605	1.0459
		0.57	0.0983	-0.0879	-1.1182
	N	-0.99	0.1176	-0.0467	-2.5176
		0.00	-0.1276	-0.0217	5.8764
	O	-1.36	0.0322	-0.0391	-0.8233
		-0.73	-0.2884	-0.0500	5.7643
		1.15	0.0948	-0.1162	-0.8156
	H	-0.73	-0.4739	0.1382	-3.4286
		0.52	0.2613	0.2149	1.2161
	ONS	-1.20	0.0976	-0.0146	-6.6955
		-0.73	-0.3602	-0.1800	2.0019
		0.68	0.1135	-0.1532	-0.7411