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SUPPLEMENTARY DATA

IR study on the electrochemical reduction of nimesulide

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Table S1. Theoretical B3LYP/6-311++G(2df,2dp) frequencies and intensities for nimesulide radical anion **2a**

No	Theoretical data		
	$\nu_{theor.}$[a]	A[b]	Approximate description[c]
1.	3370	93	ν(N-H)
2.	3095	4	ν_{PhA}(C-H)
3.	3091	1	ν_{PhA}(C-H)
4.	3062	4	ν_{PhA}(C-H)
5.	3061	2	ν_{PhB}(C-H)
6.	3058	16	ν_{PhB}(C-H)
7.	3051	31	ν_{PhB}(C-H)
8.	3042	11	ν_{PhB}(C-H)
9.	3038	0	$\nu^{as}(CH_3)$
10.	3035	1	ν_{PhB}(C-H)
11.	3026	0	$\nu^{as}(CH_3)$
12.	2939	0	$\nu^{s}(CH_3)$
13.	1602	49	ν_{PhB}(C=C)
14.	1599	39	ν_{PhB}(C=C)
15.	1584	152	ν_{PhA}(C=C)
16.	1552	67	ν_{PhA}(C=C)
17.	1500	121	δ_{PhB}(C-H)
18.	1489	180	δ_{PhA}(C-H)
19.	1467	5	δ_{PhB}(C-H)

20.	1440	74	ν_{PhA}(C=C); δ_{PhA}(C-H)
21.	1434	48	$\delta^{as}(CH_3)$
22.	1431	18	$\delta^{as}(CH_3)$
23.	1400	43	δ(N-H)
24.	1365	400	$\nu(C\text{-}NO_2)$
25.	1340	1	δ_{PhB}(C-H)
26.	1338	20	$\delta^{s}(CH_3)$
27.	1323	56	ν_{PhA}(C=C); ν_{PhB}(C=C)
28.	1308	15	ν_{PhA}(C=C); ν_{PhB}(C=C)
29.	1289	708	$\nu^{as}(SO_2)$
30.	1271	28	δ_{PhA}(C-H)
31.	1257	102	$\nu^{as}(NO_2)$
32.	1238	717	ν(CO-C), δ_{PhA}(C-H)
33.	1221	123	ν(CO-C), δ_{PhA}(C-H)
34.	1188	54	ν_{PhB}(C=C)
35.	1179	17	ν_{PhA}(C=C); ν_{PhB}(C=C)
36.	1178	5	ν_{PhB}(C=C)
37.	1137	236	$\nu^{s}(SO_2)$
38	1103	17	ν_{PhB}(C=C)
39.[d]	1055	160	$\nu^{s}(NO_2)$

[a] Infrared frequencies [cm^{-1}] scaled by Eqn. (1); [b] Predicted intensities [$km.mol^{-1}$]; [c] Vibrational modes: ν, stretching; δ, in-plane bending; s, symmetrical; as, asymetrical; PhA, phenyl ring A; PhB, phenyl ring B; [d] Followed by 54 lower-frequency vibrations.