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Negative ion mass spectra of some phenalenone derivatives

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ABSTRACT

Temperature dependence of the negative ion mass spectra (NIMS) of six phenalenone derivatives has been investigated using a mass spectrometer with the static magnetic field mass analyzer. The dissociative attachment cross-section and the mean lifetime of the molecular NI's decreases approximately exponentially with the temperature rising, and the dissociative attachment cross-section of fragment ions generally increases with temperature. The mean lifetime of the molecular anions is at least tens of microseconds for all the investigated compounds.

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1. Introduction

Some organic compounds, e.g. nitrobenzene [1] and anthraquinone derivatives [2], may produce long-lived molecular negative ions (MNI) having a dissociation decay channel at low electron energies. Their NIMS have peaks at the molecular mass what proves that the dissociation proceeds on a time scale comparable with the time of flight through a mass spectrometer—tens of microseconds. The mechanism of this phenomenon is not yet fully understood what motivated our search for compounds producing metastable MNIs. Phenalenone derivatives are widely distributed in nature [3,4]. Some of them exhibit antibiotic activity [5]. They are studied as environmental contaminants, as coal hydrogenation byproducts, as precursors to fullerenes [6], and as monomers for the synthesis of electroconductive polymers. Halogen-substituted phenalenone derivatives are used as laser dyes.

When a molecule captures an electron the resulting anion has an excess energy which is equal to the electron affinity plus the impinging electron energy plus the initial vibrational energy of the molecule [7,8]. Statistically, this last value is proportional to the gas temperature [9]. If the anion initially survives a time of order a molecular vibration period, the excess energy may be redistributed among internal degrees of freedom of the ion. For large molecules, the number of degrees of freedom allows thermodynamical description, and the resulting ion state may be characterized by an effective temperature [9,10].

The further evolution of the ion may proceed through the autodetachment of the electron and/or the dissociation:

$$M^{-*} \xrightarrow{k_a} M + e^-,$$

 $M^{-*} \xrightarrow{k_d} [M-R] + R^-,$

here M stands for the molecule, and R for an appropriate fragment. Under the above conditions, one can expect that the ion's life time is long enough, and the rate constants, k_a and k_d , have an Arrhenius-type behavior with the ion temperature. It should be noted, however, that the calculation of this temperature is, generally, a very complicated problem [9,10]. Nevertheless, within this framework many useful conclusions may be made even on a qualitative level.

A negative ion mass spectrometer has an observation window of tens of microseconds. For sufficiently long-lived ions, a data gathered in a single experiment contains enough information to estimate different rate constants even when competing reaction channels are present. Analysis of dependence of these values on the target gas temperature makes possible to conclude on the validity of the above model and assess a possible contribution of repulsive electronic terms to the ion dynamics.

Phenalenone derivatives are large aromatic molecules with a positive electron affinity which makes them promising objects for this kind of study. To our best knowledge, these compounds have not yet been investigated by means of the NIMS.

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Table 1NI mass spectra of phenalenone derivatives

2.e.B.e.phankane. Import emperature into it. Import 20.4 1.399 (1.4. 2000)7.0000 (1.0. 2000)M.73124.5.46511007.2000.00 (1.0. 1000)M.74123.0.510013.27M.M.7410.30.30.1113.27M.M.750.4.11051005.76-5600(0.0.4 20)M.760.4.61006.77-5600(0.0.4 20)M.M.760.4.61006.77-5600(0.0.4 20)M.M.760.4.61006.76-576-5600(0.0.4 20)M.780.4.61006.76-76-7600M.M.780.1113.54.44.61-550(0.0.1 1000)M.M.780.1113.54.412.5M.M.M.790.271.40.0724200(0.0.4 20)M.M.740.111005.453.24-200(0.0.1 1000)M.M.790.231.40.41.241.24M.M.M.740.131005.453.24-200(0.0.1 1000)M.M.M.740.131005.4512.44-200(0.0.1 1000)M.M.M.M.740.131005.4512.44-200(0.0.1 1000)M.M.M.M.M.M.M.M.M.M.M.M.M. <td< th=""><th>m/z</th><th>E_{\max} (eV)</th><th>Relative intensity</th><th>Intensity (%)</th><th>Integral intensity</th><th>Lifetime (µs)</th><th>Structure</th></td<>	m/z	E_{\max} (eV)	Relative intensity	Intensity (%)	Integral intensity	Lifetime (µs)	Structure
138 0.4 262 100 9125 -1000 (n) 720 (0.14) Mr 79 0.5 120 4.6 654 720 (0.14) Mr 70 0.3 0.3 0.11 13.7 Mr 71 1.4 163 Mr Mr Mr 2.6. Repetuatement to returne turine tur	2,6-Br ₂ -phena	alenone. Ion source ten	nperature 110 °C. EA _a = 1.539 eV				
78 0.5 120 45.8 0514 Latter of the second secon	338	0.14	262	100	9125	\sim 1000 (0.0) 720 (0.14 eV)	M-
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M ⁶ -0.33 3.7 1.4 163 M ⁻ = 138 0.14 165 100 5376 -360 (0.0) M ⁻ 138 0.14 101 657 6376 580 (0.34 eV) M ⁻ 79 -46 100 657 6376 580 (0.34 eV) M ⁻ m ⁻ = 18.46 -3 8 2.58 78 637 78 78 78 78 78 78 78 78 78 78 78 78 79 1.3 79 637 1.3 79 79 73 1.3 79 79 73 1.3 70 72 73 1.3 70 72 73 74 74 74 74 74 74 74 74 74 74 74 74 74 74 74 <th74< th=""> 74 74 <th7< td=""><td>$m^* = 18.46$</td><td>~0.3</td><td>0.3</td><td>0.11</td><td>13.27</td><td></td><td>$M^- \to Br^-$</td></th7<></th74<>	$m^* = 18.46$	~0.3	0.3	0.11	13.27		$M^- \to Br^-$
2.1.8.3 - nother temperature 10 - C	M ⁰	~0.33	3.7	1.4	163		$M^- \to M^0 + e^-$
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13 -3.1 12 0.73 0.74	70	0.46	110	66.7	6202	500 (0.14 eV)	Br ⁻
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$\begin{array}{c c c c c c c c c c c c c c c c c c c $		~3	8	4.8			
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2.8 by -phenale none. Ion source temperature 170°C 94.4 4061 $50(0.0)$ $30'''$ $30''''$ $30''''''$ $30''''''''''''''''''''''''''''''''''''$	M ⁰	~0.3	3.4	2.1	127		$M^- ightarrow M^0$ + e^-
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r_3 r_3 r_4 r_4 r_5 r_4 <t< td=""><td>70</td><td>0.27</td><td>142</td><td>100</td><td>7820</td><td>390 (0.14 eV)</td><td>Dr-</td></t<>	70	0.27	142	100	7820	390 (0.14 eV)	Dr-
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	15	0.37	145	8.4	7825		DI
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29 0.28 183 100 973 B^{-} -2.1 12 6.6 -3 8 4.4 M^{-} M^{0} -0.15 3.2 1.7 115 M^{-} M^{0} -0.15 3.2 1.7 115 M^{-} $2.8r$ -phenalenone. Ion source temperature 90° C. EA, $s = 1307$ eV 220 211 49 2431 255 (0.0) M^{-} $2.8r$ -phenalenone. Ion source temperature 90° C. EA, $s = 1307$ eV 220 M^{-} 355 (0.0) M^{-} $2.8r$ -phenalenone. Ion source temperature 110° C 220 (0.22 eV) M^{-} 232 (0.22 eV) M^{-} 79 0.48 119 100 6791 232 (0.22 eV) M^{-} $2.8r$ -phenalenone. Ion source temperature 170° C 22 966 230 (0.0) M^{-} $2.8r$ -phenalenone. Ion source temperature 170° C 22 966 230 (0.0) M^{-} $2.8r$ -phenalenone. Ion source temperature 170° C 22 966 230 (0.0) M^{-} 79 0.33 167	70	0.00	100	100	0770	290 (0.14 eV)	P
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III - 10-40 IIII - 10-40 IIIII - 10-40 IIIIII - 10-40 IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	$m^* - 10.4C$	~3	8	4.4	12.10		M D=-
m results 2.2 1.7 1.1 1.1 m m m m m m m m m m m m m m m m	$M^{0} = 16.40$	- 0.15	2.2	17	12.19		$M^- \rightarrow M^0 + \alpha^-$
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	111	~0.15	5.2	1./	115		$IVI \rightarrow IVI + C$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	mlz	Emax (eV)	Relative intensity	Intensity (%)	Integral intensity	Lifetime (u.s)	Structure
2-Br-phenalenone. Ion source temperature 90 °C. E.A., = 1.307 eV 258 0.22 71 49 (431) 255 (0.0) M ⁻ 220 (0.22 eV) M ⁻ 79 0.32 145 100 7965 M ⁻ m [*] =24.19 ~0.35 0.4 0.28 14.61 M ⁻ → M ⁰ ~0.34 2.57 1.8 89.89 M ⁻ → 2-Br-phenalenone. Ion source temperature 110 °C 2-Br-phenalenone. Ion source temperature 100 °C 2-Br-phenalenone. Ion source temperature 170 °C 2-Br-phenalenone. Ion source temperature 270 °C 2-Br-phenalenone. Ion source temperature 200 °C 2-Br-phenalenone. Ion source temperature 100 °C, 3446 °C 3-C 3-C 3-C 3-C 3-C 3-C 3-C 3-			Relative intensity	intensity (70)	megrarmensity	Electrine (µ3)	Structure
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2-Br-phenaler	none. Ion source tempe	rature 90 °C. EA _a = 1.307 eV				
79 0.52 145 100 7965 Br m*=24.19 -0.35 0.4 0.28 14.61 M M ⁰ -0.34 2.57 1.8 89.89 M 2-8r-phenalenone. lon source temperature 110 °C 258 0.19 51 42.9 1717 320 (0.0) M- 79 0.48 119 100 6791 Br M 79 -3 17 14.3 M M M m*=24.19 -0.35 0.23 0.19 8.33 M M 2-8r-phenalenone. lon source temperature 170 °C 226 10.6 64.17 M 258 0.16 32 19.2 966 230 (0.0) M 79 0.38 167 100 9333 Br M m*=24.19 -0.36 0.22 0.13 10.97 M 2-8r-phenalenone. lon source temperature 200 °C 23 1.35 0.81 44.67 M 2-8r-phenalenone. lon source temperature 200 °C 25 0.19 0.08	258	0.22	71	49	2431	355 (0.0)	M-
79 0.52 145 100 7955 967 -3 17 11.7 11.7 11.7 11.7 $m^* = 24.19$ ~ 0.35 0.4 0.28 14.61 M ⁻ \rightarrow M^0 ~ 0.34 2.57 1.8 89.89 M ⁻ \rightarrow 2.8r-phenalenone. lon source temperature 110 ° C 225 0.19 51 42.9 1717 320 (0.0) M ⁻ 79 0.48 119 100 6791 87 87 M ⁻ $m^* = 24.19$ ~ 0.35 0.23 0.19 8.93 M ⁻ \rightarrow M ⁻ \rightarrow M^0 ~ 0.34 1.92 1.6 64.17 M ⁻ \rightarrow 2.8r-phenalenone. lon source temperature 170 ° C 258 0.16 32 19.2 966 230 (0.0) M ⁻ \rightarrow 79 0.38 167 100 9333 B ⁻ M ⁻ \rightarrow $m^* = 24.19$ ~ 0.36 0.22 0.13 10.97 M ⁻ \rightarrow M^0 ~ 0.33 227 100 12134 M ⁻ \rightarrow 79 0.33	79	0.50	4.45	100	7005	220 (0.22 eV)	D -
$m^* = 24.19$ ~ -3.5 0.4 0.28 14.61 $M^- \rightarrow M^- \rightarrow M^- \rightarrow 0.35$ M^0 ~ 0.34 2.57 1.8 89.89 $M^- \rightarrow M^- \rightarrow 0.35$ $2.8r$ -phenalenone. Ion source temperature 110°C 258 0.19 51 42.9 1717 $320(0.0)$ $M^- \rightarrow 0.35$ 79 0.48 119 100 6791 $235(0.22 eV)$ $B^ n^* = 24.19$ ~ 0.35 0.23 0.19 8.93 $M^- \rightarrow 0.36$ M^0 ~ 0.34 1.92 1.6 64.17 $M^- \rightarrow 0.25$ $2.8r$ -phenalenone. Ion source temperature $170^{\circ C}$ $22.8^{\circ 0.16}$ 32 19.2 966 $230(0.0)$ $M^- \rightarrow 160(0.22 eV)$ 79 0.38 167 100 9333 $B^ 3$ 17 10.2 $M^- \rightarrow 0.23$ 135 0.81 44.67 $M^- \rightarrow 0.23$ $2.8r$ -phenalenone. Ion source temperature $200^{\circ C}$ $22.8^{\circ 0.14}$ $20^{\circ 0.13}$ 10.97 $100(0.0)$ $M^- \rightarrow 0.25$		0.52	145	100	7965		Br-
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	m* - 24 10	~3	17	0.29	14 61		M D=-
n 1.0 0.00 0.00 n n 2.87 n n 0.00 n 2 2.Br-phenalenone. Ion source temperature 110° C 235 0.19 51 42.9 1717 320 (0.0) M ⁻ 235 (0.22 eV) N ⁻ 79 0.48 119 100 6791 14.3 N ⁻ → m*=24.19 ~0.35 0.23 0.19 8.93 M ⁻ → 2.Br-phenalenone. Ion source temperature 170°C 258 0.16 32 1.6 64.17 M ⁻ → 2.Br-phenalenone. Ion source temperature 170°C 258 0.16 32 19.2 966 230 (0.0) M ⁻ → 79 0.38 167 100 9333 Br ⁻ m ⁻ → m*=24.19 ~0.36 0.22 0.13 10.97 M ⁻ → M ⁰ ~0.23 1.35 0.81 44.67 M ⁻ → 79 0.33 227 100 12134 M ⁻ → 79 0.33 227 100 12134 M ⁻ → 79 0.25 0.19	$M^{0} = 24.19$	~0.33	2.57	1.8	80.80		$M^- \rightarrow M^0 + \rho^-$
2-Br-phenalenone. Ion source temperature 110 °C 258 0.19 51 42.9 1717 320 (0.0) M° 79 0.48 119 100 6791 Br° $m^* = 24.19$ ~0.35 0.23 0.19 8.93 M° → M^0 ~0.34 1.92 1.6 6417 M° → 2-Br-phenalenone. Ion source temperature 170 °C 2 230 (0.0) M° → 2-Br.phenalenone. Ion source temperature 170 °C 7 100 9333 Br° → 79 0.38 167 100 9333 Br° → 160 (0.22 eV) M° → 79 0.38 167 100.2 9 M° → M° → M^0 ~0.23 1.35 0.81 44.67 M° → 2-Br.phenalenone. Ion source temperature 200 °C 2 110 (0.22 eV) M° → 258 0.14 20 8.8 579 160 (0.0) M° → 258 0.14 20 8.8 560 110 (0.22 eV) M° → 79 0.33 2.27 100 12134 M° →	111	~0.54	2.57	1.0	05.05		$1VI \rightarrow 1VI + C$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	2-Br-phenaler	none. Ion source tempe	rature 110 °C				
79 0.48 119 100 6791 Br ⁻ $n^* = 24.19$ -0.35 0.23 0.19 8.93 M ⁻ \rightarrow M^0 ~0.34 1.92 1.6 64.17 M ⁻ \rightarrow 2-Br-phenalenone. lon source temperature 170 °C 258 0.16 32 19.2 966 230 (0.0) M ⁻ \rightarrow 79 0.38 167 100 9333 Br ⁻ 160 (0.22 eV) Br ⁻ 79 0.38 167 100.2 100.2 M ⁻ \rightarrow M ⁻ \rightarrow M ⁻ \rightarrow N^0 ~0.23 1.35 0.81 44.67 M ⁻ \rightarrow M ⁻ \rightarrow 2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M ⁻ \rightarrow 258 0.14 20 8.8 579 100 (0.22 eV) Br ⁻ \rightarrow 79 0.33 227 100 12134 M ⁻ \rightarrow	258	0.19	51	42.9	1717	320 (0.0)	M-
79 0.48 19 100 6791 Br- $^{-3}$ 17 14.3 m*=24.19 $^{-0.35}$ 0.23 0.19 8.93 M ⁻ → M^0 $^{-0.34}$ 1.92 1.6 64.17 M ⁻ → 2-Br-phenalenone. Ion source temperature 170 °C 2 2 1.6 64.17 M ⁻ → 2-Br-phenalenone. Ion source temperature 170 °C 2 966 230 (0.0) M ⁻ 79 0.38 167 100 9333 Br ⁻ $^{-3}$ 17 10.2 M ⁻ → M ⁻ → M^0 ~0.36 0.22 0.13 10.97 M ⁻ → M^0 ~0.23 1.35 0.81 44.67 M ⁻ → 2-Br-phenalenone. Ion source temperature 200 °C 2 2 100 12134 Br ⁻ $^{-3}$ 17 7.5 7.6 M ⁻ → M ⁻ → M ⁻ → $2-N_0$ 0.14 20 8.8 579 160 (0.0) M ⁻ → $m^* = 24.19$ ~0.25 0.19 0.08 7.60 M ⁻ →						235 (0.22 eV)	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	79	0.48	119	100	6791		Br-
		~3	17	14.3			
$ M^0 $ ~0.34 1.92 1.6 64.17 M ⁻ → 2-Br-phenalenone. Ion source temperature 170 °C 258 0.16 32 19.2 966 230 (0.0) M ⁻ 160 (0.22 eV) 79 0.38 167 100 9333 Br ⁻ ~3 17 10.2 M ⁻ → M ⁰ ~0.23 1.35 0.81 44.67 M ⁻ → $M^0 $ ~0.23 1.35 0.81 44.67 M ⁻ → 2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M ⁻ 110 (0.22 eV) 79 0.33 227 100 12134 Br ⁻ T^3 17 7.5 M ⁻ → $M^0 $ ~0.18 1.13 0.5 34.46 M ⁻ → $M^- → $ $M^- →$	$m^* = 24.19$	~0.35	0.23	0.19	8.93		$M^- \rightarrow Br^-$
2-Br-phenalenone. Ion source temperature 170 °C 258 0.16 32 19.2 966 230 (0.0) (0.22 eV) (0.22 eV) M ⁻ 79 0.38 167 100 9333 Br ⁻ 160 (0.22 eV) Br ⁻ m [*] = 24.19 ~0.36 0.22 0.13 10.97 M ⁻ → 0 ⁰ ~0.23 1.35 0.81 44.67 M ⁻ → 2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M ⁻ 79 0.33 227 100 12134 Br ⁻ 110 (0.22 eV) Br ⁻ m [*] = 24.19 ~0.25 0.19 0.08 7.60 M ⁻ → 100 (0.20 eV) M ⁻ → m [*] = 24.19 ~0.25 0.19 0.08 7.60 M ⁻ → M ⁻ → M ⁰ ~0.18 1.13 0.5 34.46 M ⁻ → M ⁻ → 2-NO2-phenalenore. Ion source temperature 110 °C. EA _a = 1.818 eV 22 ~50000 (0.0) M M 15700 (0.34 eV) M 255 0.01 1176 100 68802 ~50000 (0.0) <td>M⁰</td> <td>~0.34</td> <td>1.92</td> <td>1.6</td> <td>64.17</td> <td></td> <td>$M^- \rightarrow M^0 + e^-$</td>	M ⁰	~0.34	1.92	1.6	64.17		$M^- \rightarrow M^0 + e^-$
258 0.16 32 19.2 966 230 (0.0) M ⁻ 79 0.38 167 100 9333 Br ⁻ \sim^3 17 10.2 m*=24.19 ~0.36 0.22 0.13 10.97 M ⁻ \rightarrow M ⁰ ~0.23 1.35 0.81 44.67 M ⁻ \rightarrow 2-Br-phenalenone. lon source temperature 200 °C 2 2 100 12134 M ⁻ \rightarrow 79 0.33 227 100 12134 Br ⁻ 110 (0.22 eV) M ⁻ \rightarrow 79 \sim^3 17 7.5 M ⁻ M ⁻ \rightarrow M ⁻ \rightarrow 110 (0.22 eV) Br ⁻ 110 (0.22 eV) Br ⁻ \rightarrow	2-Br-phenaler	none. Ion source tempe	rature 170°C				
79 0.38 167 100 9333 Br \sim^3 17 10.2 0.10 9333 Br \sim^3 17 10.2 M^- \rightarrow M^0 ~ 0.23 1.35 0.81 44.67 M^- \rightarrow \sim^3 $M^- \rightarrow$ 2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M^- 79 0.33 227 100 12134 Br 110 (0.22 eV) 79 0.33 227 100 12134 Br M^- \rightarrow \sim^3 17 7.5 7.60 M^- \rightarrow M^- \rightarrow M^0 ~ 0.18 1.13 0.5 34.46 M^- \rightarrow m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) State 2-NO2-phenalenone. Ion source temperature 110 °C. EAa = 1.818 eV 225 0.01 1176 100 68802 \sim 50000 (0.0) M 195 2.14 16.8 1.4 1599 M 15700 (0.34 eV) M <td>258</td> <td>0.16</td> <td>32</td> <td>19.2</td> <td>966</td> <td>230 (0.0)</td> <td>M-</td>	258	0.16	32	19.2	966	230 (0.0)	M-
79 0.38 167 100 9333 Br \sim^3 17 10.2						160 (0.22 eV)	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	79	0.38	167	100	9333		Br-
m*=24.19 ~0.36 0.22 0.13 10.97 M ⁻ → M ⁰ ~0.23 1.35 0.81 44.67 M ⁻ → 2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M ⁻ 79 0.33 227 100 12134 Br ⁻ m* = 24.19 ~0.25 0.19 0.08 7.60 M ⁻ → M ⁰ ~0.25 0.19 0.08 7.60 M ⁻ → m/z E _{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (µs) St 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 195 2.14 16.8 1.4 1599 (M M 46 2.33 371 31.5 34.5 150 M		~3	17	10.2			
$ M^0 ~ ~0.23 ~ 1.35 ~ 0.81 ~ 44.67 ~ M^- → 2-Br-phenalenone. Ion source temperature 200 °C258 0.14 20 8.8 579 160 (0.0) M^- 110 (0.22 eV) M^- 110 (0.22 eV) M^- 100 (0.22 eV) M^- 100 (0.22 eV) M^- → 100 (0.22 eV) (0.22 eV) (0.22 eV) M^- → 100 (0.22 eV) (0.22 eV$	$m^* = 24.19$	~0.36	0.22	0.13	10.97		$M^- \to Br^-$
2-Br-phenalenone. Ion source temperature 200 °C 258 0.14 20 8.8 579 160 (0.0) M ⁻ 79 0.33 227 100 12134 Br ⁻ -3 17 7.5 M ⁻ M ⁻ M^0 ~0.25 0.19 0.08 7.60 M ⁻ M^0 ~0.18 1.13 0.5 34.46 M ⁻ m/z E _{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (µs) Structure (µs) 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 195 2.14 16.8 1.4 1599 M 15700 (0.34 eV) M	M ⁰	~0.23	1.35	0.81	44.67		$M^- ightarrow M^0 + e^-$
2 is predictioner for source temperature 200 c 8.8 579 160 (0.0) M ⁻ 258 0.14 20 8.8 579 100 (0.22 eV) 79 0.33 227 100 12134 Br ⁻ $n^* = 24.19$ ~ 0.25 0.19 0.08 7.60 M ⁻ \rightarrow M^0 ~ 0.18 1.13 0.5 34.46 M ⁻ \rightarrow m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 \sim 50000 (0.0) M 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 M M	2_Br_phenaler	none. Ion source tempe	rature 200°C				
2.50 0.14 2.0 0.0 0.0 0.0 0.0 0.0 100 (0.0) 111 (0.0.2 eV) 79 0.33 227 100 12134 Br- 3^{*} 17 7.5 7.60 M ⁻ \rightarrow M^{0} ~ 0.25 0.19 0.08 7.60 M ⁻ \rightarrow M^{0} ~ 0.18 1.13 0.5 34.46 M ⁻ \rightarrow m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 $\sim 50000 (0.0)$ M 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 M M	2-bi-pricitater 258	0 14	20	8.8	579	160(0.0)	M-
79 0.33 227 100 12134 Br n^3 17 7.5 m* = 24.19 ~ 0.25 0.19 0.08 7.60 M ⁻ \rightarrow M^0 ~ 0.18 1.13 0.5 34.46 M ⁻ \rightarrow m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 \sim 50000 (0.0) M 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 M M	230	0.14	20	0.0	575	110(0.22 eV)	141
~ 3 17 7.5 $m^* = 24.19$ ~ 0.25 0.19 0.08 7.60 $M^- \rightarrow 0.18$ M^0 ~ 0.18 1.13 0.5 34.46 $M^- \rightarrow 0.18$ m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St 2-NO2-phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 $\sim 50000 (0.0)$ M 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 M M	79	0.33	227	100	12134	110 (0.22 cv)	Br-
$m^* = 24.19$ ~ 0.25 0.19 0.08 7.60 $M^- \rightarrow M^ M^0$ ~ 0.18 1.13 0.5 34.46 $M^- \rightarrow M^ m/z$ E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St $2-NO_2$ -phenalenone. Ion source temperature 110° C. $EA_a = 1.818 \text{ eV}$ Z_2 0.01 1176 100 68802 $\sim 50000 (0.0)$ M 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 $M^- \rightarrow M^-$		~3	17	7.5			
M^0 ~0.18 1.13 0.5 34.46 M^- → <i>m/z E</i> _{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μs) St 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 0.34 1157 98.4 15700 (0.34 eV) 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 M	m* = 24.19	~0.25	0.19	0.08	7.60		$M^- \to B r^-$
m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) St 2-NO2-phenalenone. Ion source temperature 110 °C. EA_a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 2.14 1157 98.4 15700 (0.34 eV) 15700 (0.34 eV) 146 233 371 31.5 100	M ⁰	~0.18	1.13	0.5	34.46		$M^- \to M^0 + e^-$
m/z E_{max} (eV) Relative intensity Intensity (%) Integral intensity Lifetime (μ s) Si 2-NO ₂ -phenalenone. Ion source temperature 110 °C. EA_a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 2.5 0.34 1157 98.4 15700 (0.34 eV) 15700 (0.34 eV) M 195 2.14 16.8 1.4 1599 M M							
2-NO2-phenalenone. Ion source temperature 110 °C. EA _a = 1.818 eV 225 0.01 1176 100 68802 ~50000 (0.0) M 0.34 1157 98.4 15700 (0.34 eV) 15700 (0.34 eV) 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 (M	m/z	$E_{\rm max}~({\rm eV})$	Relative intensity	Intensity (%)	Integral intensity	Lifetime (µs)	Structure
225 0.01 1176 100 68802 ~50000 (0.0) M 0.34 1157 98.4 15700 (0.34 eV) 15700 (0.34 eV) 195 2.14 16.8 1.4 1599 (M 46 2.33 371 31.5 (M	2-NO ₂ -phenal	lenone. Ion source tem	perature 110 °C. EA _a = 1.818 eV				
0.34 1157 98.4 15700 (0.34 eV) 195 2.14 16.8 1.4 1599 (N 46 2.33 371 31.5 (N	225	0.01	1176	100	68802	${\sim}50000(0.0)$	M^{-}
195 2.14 16.8 1.4 1599 (N		0.34	1157	98.4		15700 (0.34 eV)	
46 2.33 371 31.5 N	195	2.14	16.8	1.4	1599		(M-NO) ⁻
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