Reaction data for 70 elements using O_2, NH_3 and H_2 gases with the Agilent 8800 Triple Quadrupole ICP-MS

Technical note

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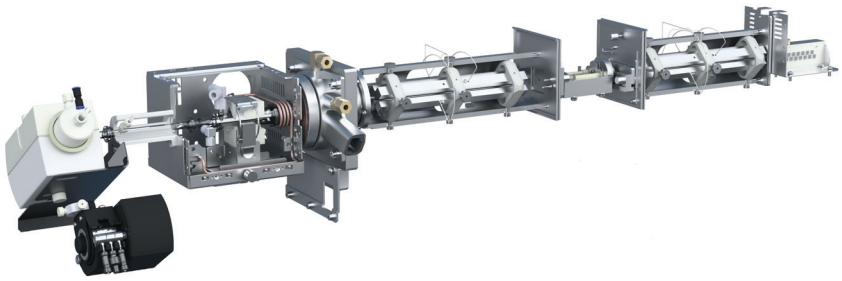

Introduction

Currently, methods based on Collision/Reaction Cell (CRC) technology are the most commonly used approach to resolve spectral interferences in ICP-MS. Collision mode uses a chemically inert gas, usually helium (He), to discriminate an analyte ion from any interfering polyatomic ions on the basis of Kinetic Energy Discrimination (KED). KED is effective for all polyatomic ion interferences and rarely requires optimization or customization for particular interferences or sample types, so collision mode using He is the most widely applicable approach for resolving interferences in elemental analysis by ICP-MS. The alternative approach is reaction mode, which relies on a chemical reaction taking place between the interfering ion (or the analyte) and the reactive cell gas in the CRC to resolve a specific interference.

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Various reactive gases are used in reaction cell mode including hydrogen (H_2), oxygen (O_2), ammonia (NH_3), methane (CH_4), nitrous oxide (N_2O), carbon dioxide (CO_2) etc, with the choice of gas depending on the individual interference that needs to be addressed. As reactions occur very quickly in the cell (often proceeding with the first collision between the ion and reaction gas molecule), a reaction gas may be more effective than a collision gas for the removal of a given interference. As a result, reaction mode is often used to remove the most intense plasma-based interferences, such as $^{40}Ar^{+}$on $^{40}Ca^{+}$, $^{40}Ar^{16}O^{+}$ on $^{56}Fe^{+}$, and $^{40}Ar_2^{+}$ on $^{80}Se^{+}$, when ultra-trace level analysis is required, for example in high purity semiconductor reagents. However, conventional quadrupole ICP-MS (ICP-QMS) has been unable to utilize the full potential of reaction mode for more complex or variable samples, because the reaction gas will also react with matrix elements, other analytes, and polyatomic species, resulting in the formation of new and unwanted interferences, which often leads to inaccurate and inconsistent results. For this reason, the application of reactive gases with ICP-QMS has been limited to the determination of a small number of analytes with predictable and consistent interferences in simple, well characterized matrices.

To meet the growing demand from industry for more reliable determination of a wider range of elements at lower concentrations and in a greater variety of matrices, a new type of ICP-MS, a triple quadruple ICP-MS (ICP-QQQ) has been developed. The Agilent 8800 ICP-QQQ realizes the full potential of reaction chemistry in ICP-MS, by using MS/MS mode to control the reaction chemistry, eliminating the errors and variability of reaction cell operation in ICP-QMS. This enables the Agilent 8800 ICP-QQQ to remove interferences far more effectively, offering significantly improved detection limits and much more consistent reaction mode performance than conventional quadrupole ICP-MS. In MS/MS mode, both quadrupoles are operated as mass filters (unit mass resolution), with the first quadruple (Q1, positioned in front of the cell) controlling which ions enter the CRC and take part in the reactions. This ensures that the chemical reactions in the cell are consistent and predictable even when the sample composition is variable, allowing the operator to use reaction chemistry to achieve much more reliable results and lower detection limits than is possible when the same reaction chemistry is used with ICP-QMS.

The MS/MS configuration of ICP-QQQ also simplifies reaction mode method development by eliminating the interference- or analyte/isotope-specific customization of cell conditions that is often required when using reactive cell gases with ICP-QMS.

Information available in the literature relating to reaction cell technology [1, 2, 3] and thermochemical reaction data [4, 5] can be used as a reference to aid development of reaction cell methods. In this technical note, specific guidance on the important tuning parameters and some fundamental reaction data is provided to guide method development when using an 8800 ICP-QQQ in reaction mode.

Reaction cell methods

On-mass mode and mass-shift mode

There are two distinct reaction cell modes of operation for the 8800 ICP-QQQ: on-mass mode and mass-shift mode.

On-mass mode detects the analyte ion at its true isotope mass e.g., $^{51}V^{+}$ would be detected at *m/z* 51. This method is used when the analyte ion is relatively unreactive with the chosen cell gas, while the interfering ion reacts efficiently with the cell gas. The interfering ion is therefore removed from the mass of the analyte ion, either by being converted to a neutral species, or by forming a reaction product ion at a new mass away from the analyte ion.

By contrast, mass-shift mode detects the analyte ion as a reaction product ion at the product ion mass. For example, using O_2 as the cell gas, $^{51}V^{+}$ would be detected as VO^{+} at *m/z* 67. This method is used when the analyte ion reacts efficiently with the cell gas to form a new reaction product ion, while the interfering ion reacts slowly or not at all with the cell gas, so does not contribute significantly to the signal at the

new mass of the analyte product ion. Both methods are illustrated schematically in Figure 1 using the determination of vanadium in a chlorine matrix as an example.

Evaluation of different reaction gases

The three reaction gases that are most commonly used with the Agilent 8800 ICP-QQQ are O_2, NH_3 (used as a mixture of 10% NH_3 in He), and H_2. As the characteristics of the three gases differ, the reaction of 70 elements with these gases was investigated.

H_2 reacts with argide ions (ArM^+) at a relatively fast rate compared to its reaction rate with several interfered elements. It is therefore an effective gas to remove argide-interferences such as $^{40}Ar^+$ on ^{40}Ca, $^{38}ArH^+$ on $^{39}K^+$, $^{40}Ar^{12}C^+$ on $^{52}Cr^+$, $^{40}Ar^{40}Ar^+$ on $^{80}Se^+$, allowing measurement of the analyte ions at their original mass using on-mass mode. In addition, some elements that form MH_n^+ product ions can be measured with H_2 cell gas using mass-shift mode. For example phosphorus (P) can be detected as PH_4^+ to avoid the interference from $^{30}SiH^+$ [6] at *m/z* 31. Likewise, $^{35}Cl^+$ can be measured as $^{35}ClH_2^+$ to avoid interference by $^{16}O^{18}OH^+$ at *m/z* 35 [7].

O_2 is often used in mass-shift methods to "move" the target analyte from its elemental ion mass to its oxide product ion (MO^+) mass, by setting Q2 to 16 amu higher than Q1. For example, sulfur (S) analyte ions react with O_2 cell gas, so O_2 mass shift mode can be used to move $^{32}S^+$ to its product ion $^{32}S^{16}O^+$ at *m/z* 48. Since O_2^+ doesn't react with O_2 cell gas to form O_3^+, this mass shift mode can be used to avoid the intense interference from O_2^+ on ^{32}S at its original elemental ion mass of *m/z* 32.

NH_3 (Agilent 8800 ICP-QQQ uses a mix of NH_3 in He) is highly reactive due to its lone electron pair. It is commonly used as a cell gas in both on-mass mode and mass-shift mode depending on the interference to be resolved. Titanium (Ti) suffers a severe interference from S-based polyatomic ions. To avoid these interferences, NH_3 is used to convert Ti^+ to an ammonium cluster product ion, usually $Ti(NH_3)_6^+$. Using this approach, Ti can be measured at low levels in samples with a matrix containing a large amount of S and Ca [8].

Experimental

An Agilent 8800 Triple Quadrupole ICP-MS (option #100) including an Octopole Reaction System (ORS^3) cell was used. The standard 8800 ICP-QQQ configuration features Ni interface cones, x-lens and a sample introduction system consisting of a MicroMist glass concentric nebulizer, a Peltier-cooled quartz double-pass Scott-type spray chamber, and a quartz torch with 2.5 mm injector.

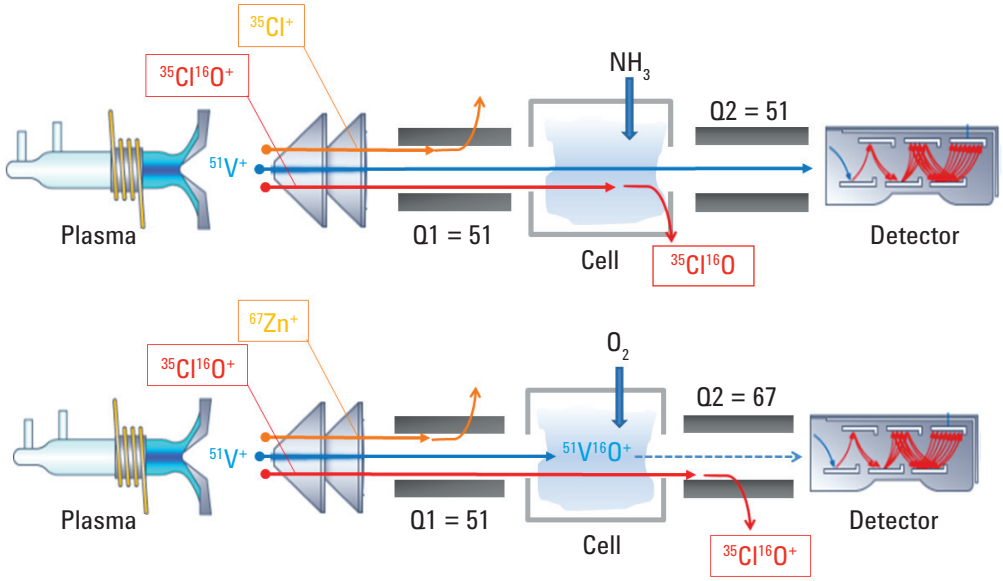

Figure 1. On-mass and mass-shift methods for vanadium measurement in a chlorine matrix: $^{35}Cl^{16}O^+$ interferes with $^{51}V^+$. In on-mass mode (upper), the interfering ion ClO^+ reacts with NH_3 to form neutral ClO (no-charge). ClO is removed while the V^+ analyte ion passes to the detector. In mass-shift mode (lower), the analyte ion V^+ reacts with O_2 to form the product ion VO^+ which is detected at *m/z* 67. The interfering ion ClO^+ remains at *m/z* 51 and is rejected by Q2.

The performance of MS/MS mode was investigated for 3 different reaction gases, O_2,NH_3 and H_2. Soft extraction lens tune (Ex1 = 0 V, Ex2 = -180 V, Omega Bias = -80 V and Omega Lens = +10 V) was applied. The preset plasma condition "low matrix" was used throughout the study, providing robust plasma conditions with a CeO^+/Ce^+ ratio of < 1 %.

Among the various operational settings of the ICP-QQQ, two key tuning parameters affect reaction efficiency: "octopole bias" and "cell gas flow rate". Octopole bias determines an ion's kinetic energy before any reaction occurs in the cell or, if the ion is unreactive with the cell gas, its ion kinetic energy after undergoing a series of collisions in the cell. Cell gas flow rate affects cell gas density, i.e., the probability of an ion experiencing a (reactive) collision with the cell gas, or the number of collisions for an unreactive ion. In this study, these settings were optimized in each cell gas mode as follows: no gas tune was optimized for maximum counts of Co^+; H_2 tune was optimized for maximum counts of PH^+, O_2 tune was optimized for maximum counts of SeO^+, and NH_3 tune was optimized for maximum counts of $Ti(NH_2)^+$.

The 8800 ICP-QQQ includes a deflection lens positioned after the ORS^3. An ion's trajectory within the deflection lens is determined by the kinetic energy of the ion and the voltage applied to the lens. Changes in octopole bias and/or cell gas flow rate alter the kinetic energy of the ion at the deflection lens, so the "deflect" voltage was tuned to maximize ion transmission for each set of cell conditions. Tuning parameters for each of the three gas modes are summarized in Table 1.

Table 1. 8800 ICP-QQQ tuning parameters for each gas mode

	No gas mode	H_2 mode	O_2 mode	NH_3 mode
Cell exit (V)	-90			
Deflect (V)	20	-10	-4	3
Plate bias (V)	-100			
Cell gas	N/A	H_2	O_2	NH_3/He
Cell gas flow rate (mL/min)	N/A	5.0	0.5	1.5
Octopole bias (V)	-8	-25	-18	-8
Octopole RF (V)	180			
KED (V)	5	-8		

Plasma conditions were tuned for robustness. Theoretically, the plasma conditions (which determine the plasma temperature) could affect reaction efficiency since each ionic species may exist in multiple electronic states (ground state and excited states) in the plasma, and ions in different electronic states are known to have different reactivity [9, 10]. However, it is unlikely that small changes in plasma conditions would have a significant effect on reaction efficiency as long as the plasma is operated consistently in "hot plasma conditions" as defined by Ce^+/CeO^+ of < a few %.

Sample preparation

Six multi-element solutions were prepared from multi-element standards purchased from SPEX Certiprep (New Jersey, USA) and single standards bought from Kanto Kagaku (Saitama, Japan) as detailed below.

Solution 1: 1 ppm of each of Li, Be, Na, Mg, Al, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, As, Se, Rb, Sr, Ag, Cd, Cs, Tl, Pb, Bi, Th and U in 1% HNO_3

Solution 2: 1 ppm of each of Sc, Y, La, Ce, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu in 1% HNO_3

Solution 3: 1 ppm of each of B, Si, P, S, Ti, Ge, Zr, Nb, Mo, Ta, W and Re in 0.1% HF

Solution 4: 1 ppm of each of Ru, Rh, Pd, Sn, Sb, Te, Hf, Ir, Pt and Au in 1% HNO_3/0.5% HCl

Solution 5: 1 ppm of each of Cl, Br and I in 1% TMAH

Solution 6: 100 ppb Hg in 1% HNO_3/0.5% HCl

Blank solutions matching the acid content of each standard were also prepared for blank subtraction to determine the net sensitivity in each mode. For each element, several mass-pairs (combinations of Q1 set mass and Q2 set mass) were surveyed in order to determine the net sensitivity of the element and its various product ions. So for each analyte mass-pair, Q1 was set to the mass of the natural isotope (the precursor ion), and Q2 was set to either the same mass

(Q1 = Q2) or the mass-shifted *m/z* of the product ion (Q2 = Q1+Δm). The common mass-shift settings (the mass difference between Q1 and Q2) associated with the most common reaction product ion transitions (e.g., +16 amu for O_2 reaction mode) are predefined in the ICP-MS MassHunter software, to aid method development.

Reaction data

The sensitivity of 70 elements and their respective product ions was studied in no gas, O_2, NH_3 and H_2 modes and the results are summarized in Table 2A (absolute sensitivity) and Table 2B (sensitivity as % relative to no gas mode).

It should be emphasized that the sensitivity data given here has not been optimized for individual elements; all results were obtained using the tuning parameters given in Table 1. Tuning cell parameters for a target analyte ion would lead to an increase in sensitivity of that ion.

The data given in the tables is designed to provide an insight on the reactivity and product ion formation of a wide range of elements with O_2, NH_3 and H_2. For example, we can see from the data that some elements form not only oxides but also dioxides and trioxides. In certain applications, it may be possible to achieve lower detection limits by measuring higher cluster ions.

Conclusions

This note provides fundamental reaction data that was obtained experimentally using an Agilent 8800 Triple Quadrupole ICP-MS (ICP-QQQ) with ORS^3 collision reaction cell. The tandem mass spectrometer layout allows the 8800 ICP-QQQ to use MS/MS mode, where both quadrupoles (Q1 and Q2) are operated as unit mass filters. This allows precise control of reaction chemistry in either on-mass or mass-shift mode, to eliminate problematic spectral interferences that cannot be removed with conventional ICP-QMS. With MS/MS, mass selection is performed by the first quadrupole (Q1), allowing the cell to operate much more efficiently and selectively, and opening up the potential of reaction cell chemistry in ICP-MS to a wide range of elements. The sensitivity data for 70 elements obtained in different reaction gas modes (oxygen, ammonia and hydrogen) has been investigated in order to provide valuable insight into reaction cell methodology and to aid method development when using the 8800 ICP-QQQ in reaction mode. By referring to the data in the tables, you can see at a glance which elements form potentially useful product ions.

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Table 2A. Sensitivity of elemental ions and their reaction product ions in no gas mode and three reaction cell modes. The green circle represents sensitivity > 1000 cps/ppb and the yellow circle represents sensitivity > 100 cps/ppb

Element	Atomic Num	Mass Num	No gas (cps/ppb)	H_2 (cps/ppb)				O_2 (cps/ppb)			
				M^+	MH^+	MH_2^+	MH_3^+	M^+	MO^+	MO_2^+	MO_3^+
			ΔM	0	1	2	3	0	16	32	48
Li	3	7	41759	4521	0	0	0	232	0	0	0
Be	4	9	10193	3898	526	1	1	136	18	6	0
B	5	11	5266	2193	5	39	0	317	6	1	0
Na	11	23	57839	39584	0	0	0	16182	0	0	0
Mg	12	24	39815	24945	9	0	0	13593	1031	8	2
Al	13	27	56763	34045	1	0	0	22139	1398	3	22
Si	14	28	16421	10884	5137	22	1	3386	2482	187	7
P	15	31	2486	1285	485	95	6	21	902	3	0
S	16	32	6181	4137	631	97	4	131	2038	2	0
Cl	17	35	226	2	6	102	0	0	6	0	0
K	19	39	43539	33850	0	0	0	20183	0	0	0
Ca	20	44	2142	1249	0	0	0	987	80	22	0
Sc	21	45	95839	48343	807	0	0	1186	45969	524	16
Ti	22	47	5107	2940	21	0	0	77	2502	49	17
V	23	51	74095	43074	132	0	0	2118	46960	1605	170
Cr	24	52	64552	34482	7	0	0	28691	11279	254	52
Mn	25	55	81996	33599	40	0	0	37512	13080	22	24
Fe	26	56	66340	32190	143	0	0	29356	15154	66	14
Co	27	59	69707	45629	57	1	0	29359	16187	59	31
Ni	28	60	14472	12522	2	0	0	7848	1877	22	2
Cu	29	63	34480	27423	0	0	0	20842	294	35	0
Zn	30	66	11313	3930	0	0	0	6120	303	2	1
Ga	31	71	38632	14743	0	0	0	22568	0	0	0
Ge	32	72	17998	7688	92	0	0	7062	1719	161	1
As	33	75	10603	6438	131	1	0	334	6013	6	0
Se	34	82*	732	282	9	0	0	212	204	0	0
Br	35	81	1847	799	260	8	0	116	173	1	0
Rb	37	85	76018	32869	0	0	0	43163	0	0	0
Sr	38	88	95671	40573	15	0	0	52149	5582	1471	0
Y	39	89	150007	81923	98	0	0	978	77354	1877	11
Zr	40	90	58386	31671	35	0	0	188	26699	5106	1432
Nb	41	93	102753	76003	57	0	0	557	4744	48482	14
Mo	42	95	17028	10677	3	0	0	752	956	6125	6
Ru	44	101	16832	10171	1	0	0	4789	3427	121	46
Rh	45	103	85372	47902	5	0	0	32214	7102	40	6
Pd	46	105	15176	11137	1	0	0	8697	161	7	0
Ag	47	107	42300	24631	0	0	0	29437	1	1	0
Cd	48	111	10075	3724	0	0	0	6238	55	0	0
Sn	50	118	28708	8585	2	0	0	10789	1496	88	0
Sb	51	121	34183	12507	4	0	0	8256	8954	31	0
Te	52	125	1413	554	0	0	0	394	324	0	0
I	53	127	20843	10059	5	0	0	9338	2819	2	0

[82]Se was used in order to allow measurement of the no gas mode sensitivity

Table 2A. continued showing H_2 and O_2

Element	Atomic Num	Mass Num	No gas (cps/ppb)	H_2 (cps/ppb)				O_2 (cps/ppb)			
				M^+	MH^+	MH_2^+	MH_3^+	M^+	MO^+	MO_2^+	MO_3^+
			ΔM	0	1	2	3	0	16	32	48
Cs	55	133	100507	45313	0	0	0	72832	0	0	0
La	57	139	132424	98130	24	0	0	320	87357	2007	0
Ce	58	140	130831	53284	18	0	0	115	80926	1311	72
Pr	59	141	181014	47241	18	0	0	139	88626	767	0
Nd	60	146	26895	9859	3	0	0	30	16631	175	0
Sm	62	147	21771	8404	2	0	0	315	14053	305	0
Eu	63	153	85415	28133	7	0	0	24774	19372	1969	0
Gd	64	157	28661	9333	4	0	0	1282	14006	362	1
Tb	65	159	164457	56971	17	0	0	511	95468	1918	5
Dy	66	163	36080	14809	6	0	0	175	28535	420	1
Ho	67	165	181582	56523	27	0	0	680	99092	2435	11
Er	68	166	50501	18679	9	0	0	296	34575	982	7
Tm	69	169	172859	51606	73	0	0	8973	100996	2411	17
Yb	70	172	34696	11596	30	0	0	10624	9081	415	1
Lu	71	175	153754	55401	11	0	0	1994	104484	3932	32
Hf	72	178	36060	13109	6	0	0	15	13849	7833	0
Ta	73	181	150282	63258	48	0	0	63	5121	75315	235
W	74	182	36381	17171	20	0	0	60	2035	17187	266
Re	75	185	48114	19353	36	0	0	3173	4413	10111	5323
Ir	77	193	50400	41464	57	3	0	17592	12528	664	105
Pt	78	195	18826	17165	12	3	0	10722	1409	11	1
Au	79	197	32902	31730	4	3	0	18775	114	4	0
Hg	80	202	8205	3859	0	0	0	4710	4	0	0
Tl	81	205	67878	25667	0	0	0	42998	0	0	0
Pb	82	208	46191	18386	0	0	0	26069	589	0	0
Bi	83	209	77596	29212	1	0	0	41364	3776	0	0
Th	90	232	87948	31544	22	2	0	2	16035	NA	NA
U	92	238	90868	32366	14	0	0	2	559	NA	NA

Table 2A. continued showing NH_3

Element	Atomic Num	Mass Num	NH_3 (cps/ppb)									
			M+	$M(NH)^+$	$M(NH_2)^+$	$M(NH_3)^+$	$MNH(NH_3)^+$	$MNH_2(NH_3)^+$	$M(NH_3)_2^+$	$MNH(NH_3)_2^+$	$MNH_2(NH_3)_2^+$	$M(NH_3)_3^+$
			0	15	16	17	32	33	34	49	50	51
Li	3	7	1543	0	0	2	0	0	1	0	0	1
Be	4	9	366	0	38	3	0	116	16	0	190	249
B	5	11	131	0	12	2	51	1	0	258	3	0
Na	11	23	40985	0	0	80	0	0	15	0	0	0
Mg	12	24	28157	0	0	178	0	0	55	1	0	36
Al	13	27	35328	0	0	80	0	2	3	1	0	0
Si	14	28	1511	0	438	3	1	0	0	1	0	0
P	15	31	9	1	2	0	0	0	0	0	0	0
S	16	32	0	0	0	0	0	0	0	0	0	0
Cl	17	35	16	0	0	0	0	0	0	0	0	0
K	19	39	36532	0	0	21	0	0	1	0	0	0
Ca	20	44	1562	0	1	5	1	0	1	0	0	0
Sc	21	45	18843	7197	2139	64	2167	372	47	1256	406	115
Ti	22	47	1148	469	78	1	100	13	0	84	17	2
V	23	51	39430	831	4927	185	301	362	124	338	668	130
Cr	24	52	48910	8	9	182	3	1	405	4	3	14
Mn	25	55	64783	0	4	278	0	1	187	0	1	26
Fe	26	56	50691	2	27	280	1	8	2474	2	7	254
Co	27	59	48441	3	20	493	2	5	3499	2	4	800
Ni	28	60	10516	0	1	96	0	0	317	0	0	566
Cu	29	63	25533	0	1	210	0	0	1856	0	0	17
Zn	30	66	9000	0	0	119	0	0	61	0	0	12
Ga	31	71	30730	0	0	68	0	0	11	0	0	0
Ge	32	72	6211	0	2571	25	0	1418	73	0	185	588
As	33	75	2569	8	1599	59	1	230	32	1	16	4
Se	34	82*	347	0	0	0	0	0	0	0	0	0
Br	35	81	1	0	0	0	0	0	0	0	0	0
Rb	37	85	54979	1	0	0	0	0	0	0	0	0
Sr	38	88	79654	0	48	147	15	2	16	3	1	11
Y	39	89	47349	22301	5740	587	5828	974	154	1903	672	187
Zr	40	90	11579	10060	790	14	2172	155	6	1433	255	29
Nb	41	93	19857	6968	206	5	28	1	0	22	1	0
Mo	42	95	10344	23	12	31	0	0	143	0	0	1
Ru	44	101	11426	1	2	47	0	0	137	0	0	10
Rh	45	103	55102	0	3	226	0	1	548	0	0	27
Pd	46	105	11381	0	0	49	0	0	127	0	0	130
Ag	47	107	37325	0	0	81	0	0	247	0	0	3
Cd	48	111	8290	0	0	21	0	0	6	0	0	1
Sn	50	118	16684	0	5	76	0	1	69	0	0	3
Sb	51	121	24016	3	13	1147	1	3	179	1	1	4
Te	52	125	1096	0	0	0	0	0	0	0	0	0
I	53	127	5	0	0	0	0	0	0	0	0	0

[82]Se was used in order to allow measurement of the no gas mode sensitivity

Table 2A. continued showing NH_3

Element	Atomic Num	Mass Num	NH_3 (cps/ppb)									
			M+	$M(NH)^+$	$M(NH_2)^+$	$M(NH_3)^+$	$MNH(NH_3)^+$	$MNH_2(NH_3)^+$	$M(NH_3)_2^+$	$MNH(NH_3)_2^+$	$MNH_2(NH_3)_2^+$	$M(NH_3)_3^+$
			0	15	16	17	32	33	34	49	50	51
Cs	55	133	80994	0	0	3	0	0	0	0	0	0
La	57	139	51900	31021	12190	868	1145	284	96	245	123	76
Ce	58	140	47439	22882	8447	521	915	328	68	238	130	71
Pr	59	141	96491	3154	7649	505	107	158	47	26	47	39
Nd	60	146	18452	190	1053	62	10	22	8	2	8	7
Sm	62	147	14593	1	513	32	1	16	7	0	7	7
Eu	63	153	59006	0	150	79	4	3	8	1	0	7
Gd	64	157	11875	4066	840	56	589	77	13	160	44	12
Tb	65	159	78912	13589	4297	160	3202	498	67	941	318	77
Dy	66	163	28299	121	635	33	11	42	8	3	18	7
Ho	67	165	112235	826	2120	133	93	262	35	20	98	31
Er	68	166	32776	367	730	38	45	89	10	9	32	10
Tm	69	169	113722	27	749	103	4	64	20	1	16	17
Yb	70	172	22193	0	24	22	0	1	3	0	0	3
Lu	71	175	115121	1507	3205	259	359	449	56	85	153	47
Hf	72	178	6021	13915	703	15	2018	99	2	470	54	4
Ta	73	181	23148	29292	2691	32	230	16	1	117	5	0
W	74	182	9277	6208	315	3	13	1	0	1	0	0
Re	75	185	39126	289	19	2	1	0	0	0	0	0
Ir	77	193	25337	1931	20	143	89	22	31	4	5	1
Pt	78	195	15021	7	4	82	2	2	200	1	2	121
Au	79	197	23788	5	1	112	2	0	595	1	0	7
Hg	80	202	2	0	0	0	0	0	0	0	0	0
Tl	81	205	52670	0	0	2	0	0	0	0	0	0
Pb	82	208	35788	0	1	5	0	0	1	0	0	0
Bi	83	209	60593	2	4	11	0	0	1	0	0	0
Th	90	232	15603	32219	6181	229	NA	NA	NA	NA	NA	NA
U	92	238	29649	24271	4917	248	NA	NA	NA	NA	NA	NA

Table 2B. Sensitivity (relative to no gas mode sensitivity) of elemental ions and their respective product ions in three reaction cell modes. The green circle represents sensitivity > 2 % and the yellow circle represents sensitivity > 0.5%.

Element	Atomic Num	Mass Num	No gas (cps/ppb)	H_2 (%)				O_2 (%)			
				M^+	MH^+	MH_2^+	MH_3^+	M^+	MO^+	MO_2^+	MO_3^+
			ΔM	0	1	2	3	0	16	32	48
Li	3	7	41759	10.8%	0.0%	0.0%	0.0%	0.6%	0.0%	0.0%	0.0%
Be	4	9	10193	38.2%	5.2%	0.0%	0.0%	1.3%	0.2%	0.1%	0.0%
B	5	11	5266	41.6%	0.1%	0.7%	0.0%	6.0%	0.1%	0.0%	0.0%
Na	11	23	57839	68.4%	0.0%	0.0%	0.0%	28.0%	0.0%	0.0%	0.0%
Mg	12	24	39815	62.7%	0.0%	0.0%	0.0%	34.1%	2.6%	0.0%	0.0%
Al	13	27	56763	60.0%	0.0%	0.0%	0.0%	39.0%	2.5%	0.0%	0.0%
Si	14	28	16421	66.3%	31.3%	0.1%	0.0%	20.6%	15.1%	1.1%	0.0%
P	15	31	2486	51.7%	19.5%	3.8%	0.2%	0.8%	36.3%	0.1%	0.0%
S	16	32	6181	66.9%	10.2%	1.6%	0.1%	2.1%	33.0%	0.0%	0.0%
Cl	17	35	226	1.0%	2.8%	45.3%	0.0%	0.1%	2.6%	0.0%	0.0%
K	19	39	43539	77.7%	0.0%	0.0%	0.0%	46.4%	0.0%	0.0%	0.0%
Ca	20	44	2142	58.3%	0.0%	0.0%	0.0%	46.1%	3.7%	1.0%	0.0%
Sc	21	45	95839	50.4%	0.8%	0.0%	0.0%	1.2%	48.0%	0.5%	0.0%
Ti	22	47	5107	57.6%	0.4%	0.0%	0.0%	1.5%	49.0%	1.0%	0.3%
V	23	51	74095	58.1%	0.2%	0.0%	0.0%	2.9%	63.4%	2.2%	0.2%
Cr	24	52	64552	53.4%	0.0%	0.0%	0.0%	44.4%	17.5%	0.4%	0.1%
Mn	25	55	81996	41.0%	0.0%	0.0%	0.0%	45.7%	16.0%	0.0%	0.0%
Fe	26	56	66340	48.5%	0.2%	0.0%	0.0%	44.3%	22.8%	0.1%	0.0%
Co	27	59	69707	65.5%	0.1%	0.0%	0.0%	42.1%	23.2%	0.1%	0.0%
Ni	28	60	14472	86.5%	0.0%	0.0%	0.0%	54.2%	13.0%	0.1%	0.0%
Cu	29	63	34480	79.5%	0.0%	0.0%	0.0%	60.4%	0.9%	0.1%	0.0%
Zn	30	66	11313	34.7%	0.0%	0.0%	0.0%	54.1%	2.7%	0.0%	0.0%
Ga	31	71	38632	38.2%	0.0%	0.0%	0.0%	58.4%	0.0%	0.0%	0.0%
Ge	32	72	17998	42.7%	0.5%	0.0%	0.0%	39.2%	9.5%	0.9%	0.0%
As	33	75	10603	60.7%	1.2%	0.0%	0.0%	3.2%	56.7%	0.1%	0.0%
Se	34	82*	732	38.5%	1.3%	0.0%	0.0%	29.0%	27.9%	0.1%	0.0%
Br	35	81	1847	43.3%	14.1%	0.4%	0.0%	6.3%	9.4%	0.1%	0.0%
Rb	37	85	76018	43.2%	0.0%	0.0%	0.0%	56.8%	0.0%	0.0%	0.0%
Sr	38	88	95671	42.4%	0.0%	0.0%	0.0%	54.5%	5.8%	1.5%	0.0%
Y	39	89	150007	54.6%	0.1%	0.0%	0.0%	0.7%	51.6%	1.3%	0.0%
Zr	40	90	58386	54.2%	0.1%	0.0%	0.0%	0.3%	45.7%	8.7%	2.5%
Nb	41	93	102753	74.0%	0.1%	0.0%	0.0%	0.5%	4.6%	47.2%	0.0%
Mo	42	95	17028	62.7%	0.0%	0.0%	0.0%	4.4%	5.6%	36.0%	0.0%
Ru	44	101	16832	60.4%	0.0%	0.0%	0.0%	28.4%	20.4%	0.7%	0.3%
Rh	45	103	85372	56.1%	0.0%	0.0%	0.0%	37.7%	8.3%	0.0%	0.0%
Pd	46	105	15176	73.4%	0.0%	0.0%	0.0%	57.3%	1.1%	0.0%	0.0%
Ag	47	107	42300	58.2%	0.0%	0.0%	0.0%	69.6%	0.0%	0.0%	0.0%
Cd	48	111	10075	37.0%	0.0%	0.0%	0.0%	61.9%	0.5%	0.0%	0.0%
Sn	50	118	28708	29.9%	0.0%	0.0%	0.0%	37.6%	5.2%	0.3%	0.0%
Sb	51	121	34183	36.6%	0.0%	0.0%	0.0%	24.2%	26.2%	0.1%	0.0%
Te	52	125	1413	39.2%	0.0%	0.0%	0.0%	27.9%	22.9%	0.0%	0.0%
I	53	127	20843	48.3%	0.0%	0.0%	0.0%	44.8%	13.5%	0.0%	0.0%

[82]Se was used in order to allow measurement of the no gas mode sensitivity

Table 2B. continued showing H_2 and O_2

Element	Atomic Num	Mass Num	No gas (cps/ppb)	H_2 (%)				O_2 (%)			
				M^+	MH^+	MH_2^+	MH_3^+	M^+	MO^+	MO_2^+	MO_3^+
			ΔM	0	1	2	3	0	16	32	48
Cs	55	133	100507	45.1%	0.0%	0.0%	0.0%	72.5%	0.0%	0.0%	0.0%
La	57	139	132424	74.1%	0.0%	0.0%	0.0%	0.2%	66.0%	1.5%	0.0%
Ce	58	140	130831	40.7%	0.0%	0.0%	0.0%	0.1%	61.9%	1.0%	0.1%
Pr	59	141	181014	26.1%	0.0%	0.0%	0.0%	0.1%	49.0%	0.4%	0.0%
Nd	60	146	26895	36.7%	0.0%	0.0%	0.0%	0.1%	61.8%	0.6%	0.0%
Sm	62	147	21771	38.6%	0.0%	0.0%	0.0%	1.4%	64.5%	1.4%	0.0%
Eu	63	153	85415	32.9%	0.0%	0.0%	0.0%	29.0%	22.7%	2.3%	0.0%
Gd	64	157	28661	32.6%	0.0%	0.0%	0.0%	4.5%	48.9%	1.3%	0.0%
Tb	65	159	164457	34.6%	0.0%	0.0%	0.0%	0.3%	58.1%	1.2%	0.0%
Dy	66	163	36080	41.0%	0.0%	0.0%	0.0%	0.5%	79.1%	1.2%	0.0%
Ho	67	165	181582	31.1%	0.0%	0.0%	0.0%	0.4%	54.6%	1.3%	0.0%
Er	68	166	50501	37.0%	0.0%	0.0%	0.0%	0.6%	68.5%	1.9%	0.0%
Tm	69	169	172859	29.9%	0.0%	0.0%	0.0%	5.2%	58.4%	1.4%	0.0%
Yb	70	172	34696	33.4%	0.1%	0.0%	0.0%	30.6%	26.2%	1.2%	0.0%
Lu	71	175	153754	36.0%	0.0%	0.0%	0.0%	1.3%	68.0%	2.6%	0.0%
Hf	72	178	36060	36.4%	0.0%	0.0%	0.0%	0.0%	38.4%	21.7%	0.0%
Ta	73	181	150282	42.1%	0.0%	0.0%	0.0%	0.0%	3.4%	50.1%	0.2%
W	74	182	36381	47.2%	0.1%	0.0%	0.0%	0.2%	5.6%	47.2%	0.7%
Re	75	185	48114	40.2%	0.1%	0.0%	0.0%	6.6%	9.2%	21.0%	11.1%
Ir	77	193	50400	82.3%	0.1%	0.0%	0.0%	34.9%	24.9%	1.3%	0.2%
Pt	78	195	18826	91.2%	0.1%	0.0%	0.0%	57.0%	7.5%	0.1%	0.0%
Au	79	197	32902	96.4%	0.0%	0.0%	0.0%	57.1%	0.3%	0.0%	0.0%
Hg	80	202	8205	47.0%	0.0%	0.0%	0.0%	57.4%	0.0%	0.0%	0.0%
Tl	81	205	67878	37.8%	0.0%	0.0%	0.0%	63.3%	0.0%	0.0%	0.0%
Pb	82	208	46191	39.8%	0.0%	0.0%	0.0%	56.4%	1.3%	0.0%	0.0%
Bi	83	209	77596	37.6%	0.0%	0.0%	0.0%	53.3%	4.9%	0.0%	0.0%
Th	90	232	87948	35.9%	0.0%	0.0%	0.0%	0.0%	18.2%	NA	NA
U	92	238	90868	35.6%	0.0%	0.0%	0.0%	0.0%	0.6%	NA	NA

Table 2B. continued showing NH_3

Element	Atomic Num	Mass Num	NH_3 (%)									
			M+	$M(NH)^+$	$M(NH_2)^+$	$M(NH_3)^+$	$MNH(NH_3)^+$	$MNH_2(NH_3)^+$	$M(NH_3)_2^+$	$MNH(NH_3)_2^+$	$MNH_2(NH_3)_2^+$	$M(NH_3)_3^+$
			0	15	16	17	32	33	34	49	50	51
Li	3	7	3.7%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Be	4	9	3.6%	0.0%	0.4%	0.0%	0.0%	1.1%	0.2%	0.0%	1.9%	2.4%
B	5	11	2.5%	0.0%	0.2%	0.0%	1.0%	0.0%	0.0%	4.9%	0.1%	0.0%
Na	11	23	70.9%	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Mg	12	24	70.7%	0.0%	0.0%	0.4%	0.0%	0.0%	0.1%	0.0%	0.0%	0.1%
Al	13	27	62.2%	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Si	14	28	9.2%	0.0%	2.7%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
P	15	31	0.3%	0.1%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
S	16	32	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Cl	17	35	7.3%	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
K	19	39	83.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Ca	20	44	72.9%	0.0%	0.1%	0.2%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Sc	21	45	19.7%	7.5%	2.2%	0.1%	2.3%	0.4%	0.0%	1.3%	0.4%	0.1%
Ti	22	47	22.5%	9.2%	1.5%	0.0%	2.0%	0.2%	0.0%	1.7%	0.3%	0.0%
V	23	51	53.2%	1.1%	6.7%	0.3%	0.4%	0.5%	0.2%	0.5%	0.9%	0.2%
Cr	24	52	75.8%	0.0%	0.0%	0.3%	0.0%	0.0%	0.6%	0.0%	0.0%	0.0%
Mn	25	55	79.0%	0.0%	0.0%	0.3%	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%
Fe	26	56	76.4%	0.0%	0.0%	0.4%	0.0%	0.0%	3.7%	0.0%	0.0%	0.4%
Co	27	59	69.5%	0.0%	0.0%	0.7%	0.0%	0.0%	5.0%	0.0%	0.0%	1.1%
Ni	28	60	72.7%	0.0%	0.0%	0.7%	0.0%	0.0%	2.2%	0.0%	0.0%	3.9%
Cu	29	63	74.1%	0.0%	0.0%	0.6%	0.0%	0.0%	5.4%	0.0%	0.0%	0.0%
Zn	30	66	79.6%	0.0%	0.0%	1.1%	0.0%	0.0%	0.5%	0.0%	0.0%	0.1%
Ga	31	71	79.5%	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Ge	32	72	34.5%	0.0%	14.3%	0.1%	0.0%	7.9%	0.4%	0.0%	1.0%	3.3%
As	33	75	24.2%	0.1%	15.1%	0.6%	0.0%	2.2%	0.3%	0.0%	0.2%	0.0%
Se	34	82*	47.4%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Br	35	81	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Rb	37	85	72.3%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Sr	38	88	83.3%	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Y	39	89	31.6%	14.9%	3.8%	0.4%	3.9%	0.6%	0.1%	1.3%	0.4%	0.1%
Zr	40	90	19.8%	17.2%	1.4%	0.0%	3.7%	0.3%	0.0%	2.5%	0.4%	0.0%
Nb	41	93	19.3%	6.8%	0.2%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Mo	42	95	60.7%	0.1%	0.1%	0.2%	0.0%	0.0%	0.8%	0.0%	0.0%	0.0%
Ru	44	101	67.9%	0.0%	0.0%	0.3%	0.0%	0.0%	0.8%	0.0%	0.0%	0.1%
Rh	45	103	64.5%	0.0%	0.0%	0.3%	0.0%	0.0%	0.6%	0.0%	0.0%	0.0%
Pd	46	105	75.0%	0.0%	0.0%	0.3%	0.0%	0.0%	0.8%	0.0%	0.0%	0.9%
Ag	47	107	88.2%	0.0%	0.0%	0.2%	0.0%	0.0%	0.6%	0.0%	0.0%	0.0%
Cd	48	111	82.3%	0.0%	0.0%	0.2%	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Sn	50	118	58.1%	0.0%	0.0%	0.3%	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%
Sb	51	121	70.3%	0.0%	0.0%	3.4%	0.0%	0.0%	0.5%	0.0%	0.0%	0.0%
Te	52	125	77.6%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
I	53	127	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

[82]Se was used in order to allow measurement of the no gas mode sensitivity

Table 2B. continued showing NH_3

Element	Atomic Num	Mass Num	NH_3 (%)									
			M+	$M(NH)^+$	$M(NH_2)^+$	$M(NH_3)^+$	$MNH(NH_3)^+$	$MNH_2(NH_3)^+$	$M(NH_3)_2^+$	$MNH(NH_3)_2^+$	$MNH_2(NH_3)_2^+$	$M(NH_3)_3^+$
			0	15	16	17	32	33	34	49	50	51
Cs	55	133	80.6%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
La	57	139	39.2%	23.4%	9.2%	0.7%	0.9%	0.2%	0.1%	0.2%	0.1%	0.1%
Ce	58	140	36.3%	17.5%	6.5%	0.4%	0.7%	0.3%	0.1%	0.2%	0.1%	0.1%
Pr	59	141	53.3%	1.7%	4.2%	0.3%	0.1%	0.1%	0.0%	0.0%	0.0%	0.0%
Nd	60	146	68.6%	0.7%	3.9%	0.2%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%
Sm	62	147	67.0%	0.0%	2.4%	0.1%	0.0%	0.1%	0.0%	0.0%	0.0%	0.0%
Eu	63	153	69.1%	0.0%	0.2%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Gd	64	157	41.4%	14.2%	2.9%	0.2%	2.1%	0.3%	0.0%	0.6%	0.2%	0.0%
Tb	65	159	48.0%	8.3%	2.6%	0.1%	1.9%	0.3%	0.0%	0.6%	0.2%	0.0%
Dy	66	163	78.4%	0.3%	1.8%	0.1%	0.0%	0.1%	0.0%	0.0%	0.1%	0.0%
Ho	67	165	61.8%	0.5%	1.2%	0.1%	0.1%	0.1%	0.0%	0.0%	0.1%	0.0%
Er	68	166	64.9%	0.7%	1.4%	0.1%	0.1%	0.2%	0.0%	0.0%	0.1%	0.0%
Tm	69	169	65.8%	0.0%	0.4%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Yb	70	172	64.0%	0.0%	0.1%	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Lu	71	175	74.9%	1.0%	2.1%	0.2%	0.2%	0.3%	0.0%	0.1%	0.1%	0.0%
Hf	72	178	16.7%	38.6%	2.0%	0.0%	5.6%	0.3%	0.0%	1.3%	0.2%	0.0%
Ta	73	181	15.4%	19.5%	1.8%	0.0%	0.2%	0.0%	0.0%	0.1%	0.0%	0.0%
W	74	182	25.5%	17.1%	0.9%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Re	75	185	81.3%	0.6%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Ir	77	193	50.3%	3.8%	0.0%	0.3%	0.2%	0.0%	0.1%	0.0%	0.0%	0.0%
Pt	78	195	79.8%	0.0%	0.0%	0.4%	0.0%	0.0%	1.1%	0.0%	0.0%	0.6%
Au	79	197	72.3%	0.0%	0.0%	0.3%	0.0%	0.0%	1.8%	0.0%	0.0%	0.0%
Hg	80	202	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Tl	81	205	77.6%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Pb	82	208	77.5%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Bi	83	209	78.1%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Th	90	232	17.7%	36.6%	7.0%	0.3%	NA	NA	NA	NA	NA	NA
U	92	238	32.6%	26.7%	5.4%	0.3%	NA	NA	NA	NA	NA	NA

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