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Mass Spectra of Beryllium Dioxoacetates

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Beryllium dioxoacetates described earlier, $Be_7O_2(OOCCH_3)_8(OH)_2$, $Be_6O_2(OOCCH_3)_8$, and $Be_5O_2(OOCCH_3)_6$ [1], were subjected to the mass spectrometric study using a CH-6 (Varian) instrument equipped with a direct inlet system. The conditions were: sample compartment temperature 150–250 °C, ion source temperature 180 °C, ionizing energy 70 eV. The spectra and tentative assignments of the ions are represented in Tables I–III (ions with m/e above 200 only are included). The intensities are given in percent relative to the ions $(M-CH_3COO)^+$, which are the most intense ions in the spectra of $Be_7O_2(OOCCH_3)_8(OH)_2$ and $Be_6O_2(OOCCH_3)_8$.

TABLE I. Mass Spectrum of $Be_7O_2(OOCCH_3)_8(OH)_2$.

m/e	%	Ion
542	100.0	$Be_7O_7(OOCCH_3)_7(OH)_2^+$
524	15.0	$Be_7O_2(OOCCH_3)_7(O)^+$
482	65.1	$Be_7O_2(OOCCH_3)_6(O)(OH)^+$
467	0.7	
440	2.5	$Be_7O_2(OOCCH_3)_5(O)(OH)_2^+$
422	25.0	$Be_7O_2(OOCCH_3)_5(O)_2^+$
397	1.2	$Be_6O_2(OOCCH_3)_5(O)^+$
380	20.0	$Be_7O_2(OOCCH_3)_4(O)_2(OH)^+$
372	0.6	$Be_5O_2(OOCCH_3)_5^+$
355	4.6	$Be_6O_2(OOCCH_3)_4(O)(OH)^+$
347	1.8	$Be_4O(OOCCH_3)_5^+$
338	7.0	$Be_7O_2(OOCCH_3)_3(O)_2(OH)_2^+$
330	2.4	$Be_5O_2(OOCCH_3)_4(OH)^+$
320	4.6	$Be_7O_2(OOCCH_3)_3(O)_3^+$
313	0.6	$Be_6O_2(OOCCH_3)_3(O)(OH)_2^+$
305	1.5	$Be_4O(OOCCH_3)_4(OH)^+$
295	4.6	$Be_6O_2(OOCCH_3)_3(O)_2^+$
278	3.6	$Be_7O_2(OOCCH_3)_2(O)_3(OH)^+$
263	4.6	$Be_4O(OOCCH_3)_3(OH)_2^+$
253	2.4	$Be_6O_2(OOCCH_3)_2(O)_2(OH)^+$
245	1.2	$Be_4O(OOCCH_3)_3(O)^+$
236	0.9	$Be_7O_2(OOCCH_3)(O)_3(OH)_2^+$
228	0.6	$Be_5O_2(OOCCH_3)_2(O)(OH)^+$
220	10.0	$Be_3O(OOCCH_3)_3^+$
211	5.3	$Be_6O_2(OOCCH_3)(O_2)(OH)_2^+$
203	1.5	$Be_4O(OOCCH_3)_2(O)(OH)^+$

TABLE II. Mass Spectrum of $Be_6O_2(OOCCH_3)_8$.

m/e	%	Ion
499	100.0	$Be_6O_2(OOCCH_3)_7^+$
456	1.0	$Be_6O_2(OOCCH_3)_6(O)^+$
397	3.8	$Be_6O_2(OOCCH_3)_5(O)^+$
372	17.5	$Be_5O_2(OOCCH_3)_5^+$
355	5.6	$Be_6O_2(OOCCH_3)_4(O)(OH)^+$
347	51.0	$Be_4O(OOCCH_3)_5^+$
330	5.3	$Be_5O_2(OOCCH_3)_4)OH)^+$
313	0.6	$Be_6O_2(OOCCH_3)_3(O)(OH)_2^+$
305	9.5	$Be_4O(OOCCH_3)_4(OH)^+$
295	6.0	$Be_6O_2(OOCCH_3)_3(O)_2^+$
270	1.6	$Be_5O_2(OOCCH_3)_3(O)^+$
253	2.4	$Be_6O_2(OOCCH_3)_2(O)_2(OH)^+$
245	8.3	$Be_4O(OOCCH_3)_3(O)^+$
220	51.0	$Be_3O(OOCCH_3)_3^+$
211	0.6	$Be_6O_2(OOCCH_3)(O)_2(OH)_2^+$
203	8.7	$Be_4O(OOCCH_3)_2(O)(OH)^+$

TABLE III. Mass Spectrum of $Be_5O_2(OOCCH_3)_6$.

m/e	%	Ion
651	700.0	$Be_8O_3(OOCCH_3)_9^+$
549	73.9	$Be_8O_3(OOCCH_3)_7(O)^+$
524	163.5	$Be_7O_2(OOCCH_3)_7(O)^+$
499	2.7	$Be_6O_2(OOCCH_3)_7^+$
447	13.8	$Be_8O_3(OOCCH_3)_5(O)_2^+$
422	48.5	$Be_7O_2(OOCCH_3)_5(O)_2^+$
417	4.0	
403	4.5	
397	23.7	$Be_6O_2(OOCCH_3)_5(O)^+$
380	40.7	$Be_7O_2(OOCCH_3)_4(O)_2(OH)^+$
372	100.0	$Be_5O_2(OOCCH_3)_5^+$
355	44.4	$Be_6O_2(OOCCH_3)_4(O)(OH)^+$
347	6.1	$Be_4O(OOCCH_3)_5^+$
338	13.6	$Be_7O_2(OOCCH_3)_3(O)_2(OH)_2^+$
330	16.8	$Be_5O_2(OOCCH_3)_4(OH)^+$
320	12.2	$Be_7O_2(OOCCH_3)_3(O)_3^+$
313	2.3	$Be_6O_2(OOCCH_3)_3(O)(OH)_2^+$
305	11.5	$Be_4O(OOCCH_3)_4(OH)^+$
295	14.7	$Be_6O_2(OOCCH_3)_3(O)_2^+$
278	6.4	$Be_7O_2(OOCCH_3)_2(O)_3(OH)^+$
270	6.7	$Be_5O_2(OOCCH_3)_3(O)^+$
253	3.6	$Be_6O_2(OOCCH_3)_2(O)_2(OH)^+$
245	9.6	$Be_4O(OOCCH_3)_3(O)^+$
220	59.1	$Be_3O(OOCCH_3)_3^+$
203	15.3	$Be_4O(OOCCH_3)_2(O)(OH)^+$

The molecular ions are absent from all the spectra studied. $Be_7O_2(OOCCH_3)_8(OH)_2$, which seemingly contains two OBe_4 tetrahedra sharing an apex, gives

fragment ions corresponding to all beryllium mono- and dioxoacetates known including the trinuclear ion $Be_3O(OOCCH_3)_3^+$ observed in the mass spectrum of $Be_4O(OOCCH_3)_6$ [2].

The spectrum of $Be_6O_2(OOCCH_3)_8$, in which two OBe_4 tetrahedra share an edge [3], includes the same fragment ions excepting those characteristic of dioxoacetates containing OBe_4 tetrahedra sharing an apex, such as $Be_7O_2(OOCCH_3)_8(OH)_2$.

The presence of ions with m/e above the molecular weight of the parent compound is a remarkable feature of the mass spectrum of $Be_5O_2(OOCCH_3)_6$ (this compound seemingly contains two OBe_4 tetrahedra sharing a face [1]. One of these ions (m/e 651) is exceedingly intense. Further investigation is, however, needed to choose between possible interpretations of this phenomenon. The ion m/e 651 ($Be_8O_3(OOCCH_3)_9^+$) appears to be the simplest fragment ion corresponding to beryllium trioxoacetate $Be_8O_3(OOCCH_3)_{10}$.

References

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