Collision-Induced and Infrared Multiphoton Dissociation Studies on $M(\text{acetone})_2^+$ ($M = \text{Al}, \text{Fe}, \text{Co}, \text{Cu}, \text{ScO}$) in the Gas Phase

Paul I. Surjasmita and Ben S. Freiser

H. C. Brown Laboratory of Chemistry, Purdue University, West Lafayette, Indiana, USA

In this paper we report an extension of our earlier study on the structure of $\text{Al}(\text{acetone})_2^+$. Collision-induced dissociation (CID) on $M(\text{acetone})(\text{acetone-d}_6)^+$ for $M = \text{Al}, \text{Fe}, \text{Co}$, and Cu yields primarily, if not exclusively, nearly equal amounts of acetone and acetone-d₆. Likewise, infrared multiphoton dissociation (IRMPD) at 10.6 μm yields, exclusively, nearly equal losses of the labeled and unlabeled acetones. These results suggest that the two acetone ligands bind in an equivalent fashion. Sc^+ was also studied, which proved to be the most interesting. Sc^+ reacts with acetone to form primarily ScO^+ , which undergoes higher order reactions leading to several products including $\text{ScO}(\text{acetone})_2^+$. IRMPD on this ion produces $\text{ScO}(\text{acetone})(\text{CH}_2\text{CO})^+$, while its perdeuterated analog also produces $\text{ScO}(\text{acetone-d}_6)^+$ in addition to $\text{ScO}(\text{acetone-d}_6)(\text{CD}_2\text{CO})^+$. The IRMPD results are supplemented by studying the primary and higher order reactions of Sc^+ with acetone, as well as the CID of $\text{ScO}(\text{acetone})_2^+$. Finally, a qualitative assessment of the infrared photodissociation cross sections is given. It is found that the relative photodissociation cross sections follow the orders $\text{Co}(\text{acetone-d}_6)_2^+ > \text{Co}(\text{acetone})(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})_2^+$ and $\text{Co}(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})^+$. (*J Am Soc Mass Spectrom* 1993, 4, 135–144)

The nature of the bonding between metal ions and ligands has been an area of intense research. In particular, a variety of techniques have been employed to probe these ionic structures in the gas phase, including selected ion–molecule reactions [1–5], collision-induced dissociation (CID) [6–10], and photodissociation [11–15]. In the area of photodissociation, UV and visible light has been used extensively to obtain spectroscopic, thermodynamic, and kinetic information about ions and their reactions [16–20]. Infrared multiphoton dissociation (IRMPD) [21, 22] has also been used widely to investigate ionic structure. However, while this method has been applied successfully to many organic structures [23–30], surprisingly few papers have appeared dealing with metal containing ions [21, 31–32]. This paper extends the use of the infrared multiphoton experiment to examine the ionic structures of a series of $M(\text{acetone})_2^+$ complexes with $M = \text{Al}, \text{Fe}, \text{Co}, \text{Cu}$, and ScO . An attempt to produce

$\text{Sc}(\text{acetone})_2^+$ was not successful because Sc^+ reacts with acetone to produce primarily ScO^+ from which $\text{ScO}(\text{acetone})_2^+$ is eventually formed. CID was also performed on these ions to obtain additional structural information and for comparison to the IRMPD results.

This work was originally prompted by an earlier study of McMahon and co-workers [33] in which they proposed that the binding between Al^+ with two acetone ligands yields the unsymmetrical Structure 1 rather than the expected Structure 2. Subsequent experimental studies, however, indicated that the two acetone molecules bind to Al^+ in a symmetrical way. This result was supported by theory, which revealed, however, that the O–Al–O angle is not 180°, but rather about 90° (Structure 3) [34, 35]. A key result from the experimental study was that when $\text{Al}(\text{acetone})(\text{acetone-d}_6)^+$ was irradiated with light from a CO_2 infrared laser at 10.6 μm , equal loss of acetone and acetone-d₆ was observed. This then led us to investigate a series of $M(\text{acetone})(\text{acetone-d}_6)^+$ species to test their infrared absorption and fragmentation characteristics.

Address reprint requests to Ben S. Freiser, H. C. Brown Laboratory of Chemistry, Purdue University, West Lafayette, IN 47907.

Experimental

The experiments were performed on a prototype Nicolet (Madison, WI) FTMS 1000 Fourier transform mass spectrometer and a Nicolet FTMS 2000 Fourier transform mass spectrometer [36, 37]. The FTMS 1000 is equipped with a 5.2-cm cubic trapping cell situated between the poles of a Varian (Palo Alto, CA) 15-in electromagnet maintained at 0.9 T. The FTMS 2000 features a dual cell arrangement that permits ion transfer from the "source cell" to the "analyzer cell" and is situated in the bore of a 3.0-T superconducting magnet. The metal ions were generated by laser desorption using the fundamental beam of a Quanta Ray (Mountain View, CA) Nd:YAG laser (1.06 μm) focused onto the metal target. All of the chemicals were obtained commercially in high purity and used as supplied except for multiple freeze-pump-thaw cycles to remove noncondensable gases.

To generate $\text{M}(\text{acetone})(\text{acetone-d}_6)^+$, first acetone was leaked into the cell on the order of 1×10^{-7} torr to generate $\text{M}(\text{acetone})^+$ by direct attachment or by reaction of $\text{M}(\text{CO})^+$ with acetone. Next, $\text{M}(\text{acetone})^+$ was isolated and then deuterated acetone was pulsed into the cell yielding the desired product ion by direct attachment. As mentioned above, the scandium complex was not isolated in the form of $\text{Sc}(\text{acetone})_2^+$,

because Sc^+ reacts with acetone to produce mainly ScO^+ , which eventually yields $\text{ScO}(\text{acetone})_2^+$. Unfortunately, we were not able to isolate $\text{ScO}(\text{acetone})(\text{acetone-d}_6)^+$ in good abundance for CID or IRMPD.

CID was performed as previously described [38, 39] using argon as the collision gas at a pressure of $\sim 1 \times 10^{-6}$ torr. The collision energy of the ions can be varied typically between 0 and 100 eV (in this work reported as laboratory collision energy). For slow collisional activation or sustained off-resonance irradiation (SORI), a technique recently developed by Jacobson and co-workers [40], argon was used at a pressure of 6×10^{-6} torr. Double resonance techniques [41] were used to isolate ions of interest and to confirm parent-product relationships.

For the IRMPD experiments, after generating the desired ion in the source cell, it was then transferred to the low-pressure ($\sim 5 \times 10^{-9}$ torr) analyzer cell where it was irradiated with a Synrad (Bothell, WA) 48-2-115 continuous wave CO_2 laser (3-mm beam diameter) at 10.6 μm . Irradiances were typically on the order of 4 to 30 W for 0.5 to 5 sec trapping time. A Uniblitz (Rochester, NY) mechanical shutter model VS25S2W0 was used to gate the infrared laser, and a Coherent (Palo Alto, CA) model 201 power meter was used to monitor the nominal power of the CO_2 laser. Because of some slight variations in the way the ions were generated, and the possibility that for some experiments the focusing of the infrared laser was not optimum, the percentage of dissociation does not directly reflect the ease of dissociation.

Infrared spectra of acetone and acetone- d_6 were taken on a Galaxy 6021 FTIR spectrometer using a 10-cm path length gas cell at a pressure of 3 torr.

Results and Discussion

Collision-induced dissociation of $\text{M}(\text{acetone})(\text{acetone-d}_6)^+$ produces their monomers and M^+ for $\text{M} = \text{Al}$ and Cu :

For $\text{M} = \text{Fe}$ and Co , the CID of the mixed dimer species also produces $\text{M}(\text{CO})^+$ in addition to their monomers and M^+ :

Figure 1 displays the CID profile for $\text{Fe}(\text{acetone})(\text{acetone-d}_6)^+$. In contrast to the CID results, IRMPD of the mixed dimer species for these metals produces only

the monomers (reactions 9 and 10), although these ions can undergo further IRMPD (see Table 1).

In each of these cases, for both CID and IRMPD, equal loss of acetone and acetone-d₆ was observed within experimental error, suggesting that the two acetone molecules are equivalent, thus ruling out Structure 1 and suggesting either Structure 2 or 3. Figure 2 shows spectra of $\text{Co}(\text{acetone})(\text{acetone-d}_6)^+$ prior to and after CID, while Figure 3 shows similar results using IRMPD. Interestingly, CID of $\text{Cu}(\text{acetone})(\text{acetone-d}_6)^+$ consistently produces a 1.2:1 ratio of $\text{Cu}(\text{acetone})^+$ to $\text{Cu}(\text{acetone-d}_6)^+$. In contrast, $\text{Ag}(\text{acetone})(\text{acetone-d}_6)^+$ gives equal loss, thus ruling out a simple explanation based on a d^{10} electronic structure. Further studies are under way to try to understand this observation.

Surprisingly, $\text{ScO}(\text{acetone})_2^+$ did not give $\text{ScO}(\text{acetone})^+$ (loss of neutral acetone) when irradiated with the CO₂ laser (Figure 4). Instead, the loss of CH₄ was

the only photodissociation channel observed:

Irradiation of $\text{ScO}(\text{acetone-d}_6)_2^+$, however, yields two

■ $\text{Fe}(\text{acetone})(\text{acetone-d}_6)^+$ ▲ $\text{Fe}(\text{CO})^+$
● $\text{Fe}(\text{acetone-d}_6)^+$ ◆ Fe^+
△ $\text{Fe}(\text{acetone})^+$

Figure 1. CID profile of $\text{Fe}(\text{acetone})(\text{acetone-d}_6)^+$ showing parent peak (m/z 178) and product ion intensities vs kinetic energy.

Figure 2. CID of $\text{Co}(\text{acetone})(\text{acetone-d}_6)^+$ (a) prior to CID, (b) after CID in which there is an additional 50-ms delay after the CID pulse to allow fragmentation to occur. Equal loss of acetone and acetone-d₆ suggests a symmetric structure.

Figure 3. Photodissociation of $\text{Co}(\text{acetone})(\text{acetone-d}_6)^+$ with (a) laser off, (b) laser on (30 W) for 1 s. As in Figure 2, almost equal loss of acetone and acetone- d_6 suggests a symmetric structure.

Figure 4. Photodissociation of $\text{Sc}(\text{acetone})_2^+$ with (a) laser off, (b) laser on (20 W) for 5-s trapping time.

reaction channels:

In order to try to understand this striking difference in the behavior of $\text{ScO}(\text{acetone})_2^+$ and the other $\text{M}(\text{acetone})_2^+$ complexes, the ion-molecule chemistry of these systems was investigated further.

The interactions between transition metal ions and ketones have been the subject of intense investigation [42-47]. In agreement with previous studies [48], we found that Al^+ and Cu^+ react with acetone to produce the direct condensation products:

We also found that these monomers react with ace-

tone- d_6 to produce the mixed dimer, $\text{M}(\text{acetone})(\text{acetone-d}_6)^+$. Also in agreement with previous reports [49, 50], Fe^+ and Co^+ were observed to react with acetone mainly to produce $\text{M}(\text{CO})^+$ as the primary

¹ Halle et al. [50] reported that the reaction of Co^+ with acetone produces 90% of $\text{Co}(\text{CO})^+$ and 10% of $\text{Co}(\text{CH}_3)_2^+$. They also noted the formation of cobalt ion-acetone adduct, which may result either from collisional stabilization of the reaction intermediate or by further reaction of $\text{Co}(\text{CO})^+$ and/or $\text{Co}(\text{CH}_3)_2^+$ with acetone. Our finding was that $\text{Fe}(\text{acetone})^+$ and $\text{Co}(\text{acetone})^+$ did not disappear completely upon continuous ejection of $\text{Fe}(\text{CO})^+$ and $\text{Co}(\text{CO})^+$, respectively. Like $\text{Al}(\text{acetone})^+$ and $\text{Cu}(\text{acetone})^+$, the formation of vibrationally excited $\text{Fe}(\text{acetone})^+$ and $\text{Co}(\text{acetone})^+$ can also be stabilized by infrared radiative processes.

reaction product:

Reacting Fe^+ and Co^+ with perdeuterated acetone confirmed this reaction and indicated that no $M(\text{C}_2\text{H}_4)^+$ is formed. The $M(\text{CO})^+$ ions then react with acetone by displacement to produce $M(\text{acetone})^+$, which in turn reacts with another acetone molecule to produce $M(\text{acetone})_2^+$. The reduced reactivity of Al^+ and Cu^+ toward acetone (absence of cleavage products and slower reaction rate) compared to Fe^+ and Co^+ can be attributed to their closed valence shell systems ($3s^2$ and d^{10} , respectively).

Sc^+ , on the other hand, shows a rich chemistry with acetone. Like other early transition metals, Sc^+ forms a

strong bond with oxygen; thus ScO^+ is the major product formed together with some $\text{ScO}(\text{C}_3\text{H}_4)^+$:

ScO^+ then reacts with acetone to produce $\text{ScO}(\text{H}_2\text{O})^+$, reaction 20. Tertiary products and so forth are shown below:

Collision-induced dissociation of $\text{ScO}(\text{acetone})_2^+$ gives $\text{ScO}(\text{acetone})(\text{CH}_2\text{CO})^+$ as one of its products:

Figure 5 is a CID breakdown plot of $\text{ScO}(\text{acetone})_2^+$, which shows ion intensities as a function of kinetic

energy. CID of the other product ions yields reactions 32-48, which are in accord with the assigned structures:

The modes of ion excitation for CID and IRMPD are different. In CID, the ion of interest is first kinetically excited. Upon multiple collisions with argon, a variable amount of internal energy is transferred to the ion, which then dissociates, usually producing a number of different fragment ions. In IRMPD, however, as the ion is irradiated, it absorbs in a sequential fashion multiple photons at ~ 2.7 kcal/photon. It is assumed that the ion maintains complete randomization of energy throughout all of the normal modes, ultimately leading to dissociation via the lowest activation energy pathway [51]. Thus, multiphoton dissociation of $\text{ScO}(\text{acetone})_2^+$ to generate $\text{ScO}(\text{acetone})(\text{CH}_2\text{CO})^+$ via

process 11 indicates that loss of CH_4 is the lowest activation process.

The appearance of two photoproducts, as shown in reactions 12 and 13, is interesting. In general, the observance of more than one IRMPD product can arise because of one or more of these factors:

1. The ions consist of more than one isomer before they are irradiated with the laser. An example of this situation is FeC_4H_8^+ [52] produced by the reaction of Fe^+ with *n*-butane.
2. The ions, which consist of one isomer when "cold," undergo isomerization in the transition state and

Figure 5. CID profile of $\text{ScO}(\text{acetone})_2^+$ showing parent peak and product ion intensities vs kinetic energy.

this releases sufficient energy to make accessible more than one reaction channel. An example of this is the proton-bound *n*-propyl alcohol dimer, $(n\text{-C}_3\text{H}_7\text{OH})_2\text{H}^+$, which isomerizes to $(n\text{-C}_3\text{H}_7\text{OH})(i\text{-C}_3\text{H}_7\text{OH})\text{H}^+$ [53].

3. The activation energies for the formation of both products are similar, so that dissociation through a slightly higher activation energy competes with photon absorption in the quasi-continuum state, as suggested by Brauman and co-workers [54]. This is probably the situation encountered in $\text{ScO}(\text{acetone-d}_6)_2^+$.

In 1991 Jacobson and co-workers [40] introduced an alternative to IRMPD by the application of a sustained (≥ 500 ms) "off-resonance" radiofrequency field. As a result of applying the rf field near the natural cyclotron frequency of the ion, the ion experiences acceleration and deceleration cycles during which time the ion undergoes multiple "soft" collisions. Thus, internal energy is added in smaller increments than conventional CID and in a stepwise fashion analogous to multiphoton infrared absorption. The photoproducts of $\text{ScO}(\text{acetone})_2^+$ and its perdeuterated analog were checked against slow collisional activation or SORI and were found in good agreement.

Although there are known exceptions, Bomse and Beauchamp [53] noted that the infrared photodissociation spectra of ions are similar to the absorption profile for the neutral molecule [21, 55]. Thus it is not surprising that the acetone systems in general required higher irradiation levels than is typically reported, considering that the liquid-phase spectra (Standard Infrared

Figure 6. Gas phase spectra of neutral (a) acetone and (b) acetone- d_6 showing almost no absorption at $10.6\ \mu\text{m}$ ($943\ \text{cm}^{-1}$). The spectra were recorded at a pressure of 3 torr and with a 10-cm path length.

Prism Spectra, Nos. 233 and 43117, Sadtler Research Laboratories Inc., Philadelphia, PA) and particularly the gas-phase spectra (Figure 6), show no absorption for acetone and very little for acetone- d_6 in the CO_2 laser region ($10.6\ \mu\text{m}$ or $943\ \text{cm}^{-1}$).

Finally, experiments were performed to qualitatively order the relative photodissociation cross sections for the $\text{Co}(\text{acetone})_2^+$ system. In order to compare the relative photodissociation cross sections, it is important that the ions are produced under identical conditions. To do this, $\text{Co}(\text{acetone-d}_6)_2^+$, $\text{Co}(\text{acetone})(\text{acetone-d}_6)^+$, and $\text{Co}(\text{acetone})_2^+$ were irradiated simultaneously. By comparing the absolute ion intensities before and after irradiation, it was found that the relative photodissociation cross sections follow the order $\text{Co}(\text{acetone-d}_6)_2^+ > \text{Co}(\text{acetone})(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})_2^+$ (Figure 7). It was also found that $\text{Co}(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})^+$. A somewhat similar observation was made by Bomse and Beauchamp [56] in which $(\text{CD}_3)_2\text{Cl}^+$ was observed to undergo IRMPD,

Figure 7. Photodissociation of $\text{Co}(\text{acetone-d}_6)_2^+$, $\text{Co}(\text{acetone})(\text{acetone-d}_6)^+$, and $\text{Co}(\text{acetone})_2^+$ simultaneously with (a) laser off, (b) laser on (2 s, 30 W). From the absolute ion abundances before and after radiation, it was found that the order of photodissociation cross sections is $\text{Co}(\text{acetone-d}_6)_2^+ > \text{Co}(\text{acetone})(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})_2^+$. $\text{Co}(\text{CO})^+$ is produced mainly from the subsequent photodissociation of $\text{Co}(\text{acetone-d}_6)^+$ with some small contribution from $\text{Co}(\text{acetone})^+$.

while $(\text{CH}_3)_2\text{Cl}^+$ and $(\text{CH}_3)(\text{CD}_3)\text{Cl}^+$ were not. In the present studies, it is also evident that the absorption in this region can be shifted significantly by the attached metal. Finally, photodissociation of $\text{M}(\text{acetone})(\text{acetone-d}_6)^+$ to produce both $\text{M}(\text{acetone})^+$ and $\text{M}(\text{acetone-d}_6)^+$ would indicate that energy is randomized even in the event that only the acetone-d₆ ligand is absorbing. However, both ligands probably absorb in the mixed dimer.

Conclusions

The use of infrared CO_2 laser radiation to photodissociate transition metal-containing species has been extended to a series of metal acetone compounds. While CID often gives several products, IRMPD usually gives only one product having the lowest activation barrier. CID and IRMPD suggest that the two acetone ligands bind in an equivalent fashion in $\text{M}(\text{acetone})(\text{acetone-d}_6)^+$ where $\text{M} = \text{Al}, \text{Fe},$ and Co . Interestingly, photodissociation of $\text{ScO}(\text{acetone})_2^+$ yielded $\text{ScO}(\text{acetone})(\text{CH}_2\text{CO})^+$ and its perdeuterated analog yielded $\text{ScO}(\text{acetone-d}_6)(\text{acetone-d}_6)^+$ in addition to $\text{ScO}(\text{acetone})(\text{CD}_2\text{CO})^+$. The relative ease of IRMPD was found as follows: $\text{Co}(\text{acetone-d}_6)_2^+ > \text{Co}(\text{acetone})(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})_2^+$ and $\text{Co}(\text{acetone-d}_6)^+ > \text{Co}(\text{acetone})^+$. In general the deuterated acetone complexes absorbed more strongly than the undeuterated complexes.

Acknowledgments

Acknowledgment is made to the Division of Chemical Sciences in the Office of Basic Energy Sciences in the U.S. Department of Energy (DE-FG02-87ER13766) for supporting this research and to the National Science Foundation (CHE-8920085) for supporting FTICRMS instrumentation. The authors also thank Drs. Denley Jacobson and Yongqing Huang for helpful discussions, as well as Mr. Bruce McNamara for help in obtaining the gas-phase infrared spectra of acetone and acetone-d₆.

Table 1. Comparison of the dissociation pathways for the $\text{M}(\text{acetone})_2^+$ system by CID and IRMPD

Ion	Energy (eV)	CID		Trap time (s), power (W)	IRMPD	
		Product	%		Product	Percentage dissociation ^a
$\text{Al}(\text{acetone})(\text{acetone-d}_6)^+$	17	$\text{Al}(\text{acetone})^+$	49	3 s, 4.5 W	$\text{Al}(\text{acetone})^+$	26
		$\text{Al}(\text{acetone-d}_6)^+$	49		$\text{Al}(\text{acetone-d}_6)^+$	28
		Al^+	2			
$\text{Al}(\text{acetone})_2^+$	17	$\text{Al}(\text{acetone})^+$	90	0.4 s, 30 W	$\text{Al}(\text{acetone})^+$	55
		Al^+	10			
$\text{Al}(\text{acetone-d}_6)_2^+$	20	$\text{Al}(\text{acetone-d}_6)^+$	86	0.4 s, 30 W	$\text{Al}(\text{acetone-d}_6)^+$	77
		Al^+	14			
$\text{Al}(\text{acetone})^+$	18	Al^+	100	8 s, 30 W	Not observed	0
$\text{Al}(\text{acetone-d}_6)^+$	33	Al^+	100	0.3 s, 30 W	Al^+	52

Table 1—Continued

Ion	CID			IRMPD		
	Energy (eV)	Product	%	Trap time (s), power (W)	Product	Percentage dissociation ^a
Fe(acetone)(acetone-d ₆) ⁺	14	Fe(acetone) ⁺	42	4 s, 20 W	Fe(acetone) ⁺	9
		Fe(acetone-d ₆) ⁺	42		Fe(acetone-d ₆) ⁺	11
		Fe(CO) ⁺	5			
		Fe ⁺	11			
Fe(acetone) ₂ ⁺	22	Fe(acetone) ⁺	71	2 s, 30 W	Fe(acetone) ⁺	50
		Fe(CO) ⁺	12			
		Fe ⁺	17			
Fe(acetone-d ₆) ₂ ⁺	17	Fe(acetone-d ₆) ⁺	79	0.7 s, 20 W	Fe(acetone-d ₆) ⁺	76
		Fe(CO) ⁺	5			
		Fe ⁺	16			
Fe(acetone) ⁺	18	Fe(CO) ⁺	24	2 s, 30 W	Fe(CO) ⁺	63
		Fe ⁺	76			
Fe(acetone-d ₆) ⁺	17	Fe(CO) ⁺	28	0.7 s, 20 W	Fe(CO) ⁺	40
		Fe ⁺	72			
Co(acetone)(acetone-d ₆) ⁺	26	Co(acetone) ⁺	35	1 s, 30 W	Co(acetone) ⁺	14
		Co(acetone-d ₆) ⁺	33		Co(acetone-d ₆) ⁺	16
		Co(CO) ⁺	12			
		Co ⁺	20			
Co(acetone) ₂ ⁺	35	Co(acetone) ⁺	89	2 s, 30 W	Co(acetone) ⁺	22
		Co(CO) ⁺	4			
		Co ⁺	7			
Co(acetone-d ₆) ₂ ⁺	33	Co(acetone-d ₆) ⁺	43	1 s, 22 W	Co(acetone-d ₆) ⁺	72
Co(acetone) ⁺	33	Co(CO) ⁺	42	5 s, 30 W	Co(CO) ⁺	49
		Co ⁺	58			
Co(acetone-d ₆) ⁺	31	Co(CO) ⁺	14	1 s, 30 W	Co(CO) ⁺	28
		Co ⁺	86			
Cu(acetone)(acetone-d ₆) ⁺	17	Cu(acetone) ⁺	40	3 s, 23.5 W	Cu(acetone) ⁺	18
		Cu(acetone-d ₆) ⁺	35		Cu(acetone-d ₆) ⁺	13
		Cu ⁺	25			
ScO(acetone) ₂ ⁺	22	ScO(acetone)(CH ₂ CO) ⁺	13	5 s, 20 W	ScO(acetone)(CH ₂ CO) ⁺	18
		ScO(acetone) ⁺	57			
		ScO(H ₂ O) ⁺	16			
		ScO ⁺	14			
ScO(acetone-d ₆) ₂ ⁺	20	ScO(acetone-d ₆)(CD ₂ CO) ⁺	16	3 s, 15 W	ScO(acetone-d ₆)(CD ₂ CO) ⁺	53
		ScO(acetone-d ₆) ⁺	63		ScO(acetone-d ₆) ⁺	11
		ScO(D ₂ O) ⁺	9			
		ScO	12			

^a Calculated as the intensity of the dissociation product, divided by the total ion intensity, multiplied by 100.

References

- Campana, J. E.; Eyler, J. R. *Int. J. Mass Spectrom. Ion Phys.* **1983**, *55*, 171.
- Huang, S. K.; Allison, J. *Organometallics* **1983**, *2*, 883.
- Tsarbopoulos, A.; Allison, J. *Organometallics* **1984**, *3*, 86.
- Caldwell, G.; Rozeboom, M. D.; Kiplinger, J. P.; Bartmess, J. E. *J. Am. Chem. Soc.* **1984**, *106*, 809.
- Caldwell, G.; Bartmess, J. E. *Int. J. Mass Spectrom. Ion Phys.* **1983**, *50*, 235.
- Hanley, L.; Ruatta, S. A.; Anderson, S. L. *J. Chem. Phys.* **1987**, *87*, 260.
- Ruatta, S. A.; Hanley, L.; Anderson, S. L. *Chem. Phys. Lett.* **1987**, *37*, 5.
- Cooks, R. G. *Collision Spectroscopy*; Plenum Press: New York, 1978.
- Ervin, K.; Loh, S. K.; Aristov, N.; Armentrout, P. B. *J. Phys. Chem.* **1983**, *87*, 3593.
- Graul, S. T.; Squires, R. R. *Mass Spect. Rev.* **1988**, *7*, 263.
- For a general discussion on photodissociation, see: Dunbar, R. C. In *Gas Phase Ion Chemistry*; Bowers, M. T., Ed.; Academic Press: New York, 1979; Vol. 2, Chapt. 14.
- Faulk, J. D.; Dunbar, R. C. *J. Am. Soc. Mass Spectrom.* **1991**, *2*, 97.
- Morgenthaler, L. N.; Eyler, J. R. *Int. J. Mass Spectrom. Ion Phys.* **1981**, *37*, 153.
- Hughes, R. J.; March, R. E.; Young, A. B. *Int. J. Mass Spectrom. Ion Phys.* **1982**, *42*, 255.

15. von Busch, R.; Dunn, G. H. *Phys. Rev. A* **1972**, 5, 1726.
16. Riggan, M. T.; Dunbar, R. C. *Chem. Phys. Lett.* **1975**, 31, 539.
17. Vestal, M. L.; Mauclaire, G. H.; Futrell, J. H. *23rd Annu. Conf. Mass Spectrom.*; **1975**, Houston, TX.
18. Tabche-Fouhaille, A.; Durup, J.; Moseley, J. T.; Ozenne, J. B.; Pernot, C.; Tadjeddine, M. *Chem. Phys.* **1976**, 17, 81.
19. Cosby, P. C.; Smith, G. P.; Moseley, J. T. *J. Chem. Phys.* **1978**, 69, 2779.
20. Fu, E. W. Ph.D. thesis, Case Western Reserve University, 1976.
21. Hanratty, M. A.; Paulsen, C. M.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1985**, 107, 5074.
22. Meyer, F. K.; Jasinski, J. M.; Rosenfeld, R. N.; Brauman, J. I. *J. Am. Chem. Soc.* **1982**, 104, 663.
23. Thorne, L. R.; Beauchamp, J. L. In *Gas Phase Ion Chemistry*; Bowers, M. T., Ed.; Academic Press: New York, 1984; Vol. 3, Chapt. 18.
24. Bomse, D. S.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1980**, 102, 3967.
25. Bomse, D. S.; Woodin, R. L.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1979**, 101, 5503.
26. Rosenfeld, R. M.; Jansinski, J. M.; Brauman, J. I. *J. Am. Chem. Soc.* **1982**, 104, 658.
27. Jasinski, J. M.; Rosenfeld, R. N.; Meyer, F. K.; Brauman, J. I. *J. Am. Chem. Soc.* **1982**, 104, 652.
28. Baykut, G.; Watson, C. H.; Weller, R. R.; Eyler, J. R. *J. Am. Chem. Soc.* **1985**, 107, 8036.
29. Watson, C. H.; Baykut, G.; Battiste, M. A.; Eyler, J. R. *Anal. Chim. Acta* **1985**, 178, 125.
30. Bensimon, M.; Rapin, J.; Gaumann, T. *Int. J. Mass Spectrom. Ion Proc.* **1986**, 72, 125.
31. Shin, S. K.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1990**, 112, 2057.
32. Shin, S. K.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1990**, 112, 2066.
33. Bouchard, F.; Hepburn, J. W.; McMahon, T. B. *J. Am. Chem. Soc.* **1989**, 111, 8934.
34. Bauschlicher, C. W. Jr.; Bouchard, F.; Hepburn, J. W.; McMahon, T. B.; Surjasmita, I. B.; Roth, L. M.; Gord, J. R.; Freiser, B. S. *Int. J. Mass Spectrom. Ion Proc.* **1991**, 109, 15.
35. Sodupe, M.; Bauschlicher, C. W. Jr. *Chem. Phys. Lett.* **1991**, 181, 321.
36. Cody, R. B.; Freiser, B. S. *Int. J. Mass Spectrom. Ion Phys.* **1982**, 41, 199.
37. Cody, R. B.; Burnier, R. C.; Freiser, B. S. *Anal. Chem.* **1982**, 54, 96.
38. Jacobson, D. B.; Freiser, B. *J. Am. Chem. Soc.* **1983**, 105, 736.
39. Jacobson, D. B.; Freiser, B. *J. Am. Chem. Soc.* **1983**, 105, 7478.
40. Gauthier, J. W.; Trautman, T. R.; Jacobson, D. B. *Anal. Chim. Acta* **1991**, 246, 211.
41. Comisarow, M. B.; Parisod, G.; Grassi, V. *Chem. Phys. Lett.* **1978**, 57, 413.
42. El-Shall, M. S.; Schriver, K. E.; Whetten, R. L.; Mcot-Ner, M. *J. Phys. Chem.* **1989**, 93, 7969.
43. Schroder, D.; Schwarz, H. *Angewandte Chemie (Int. English Ed.)* **1990**, 29, 910.
44. Larsen, B. S.; Ridge, D. P. *J. Am. Chem. Soc.* **1984**, 106, 1912.
45. Uppal, J. S.; Staley, R. H. *J. Am. Chem. Soc.* **1982**, 104, 1235.
46. Ridge, D. P.; Allison, J. *Twenty-Sixth Annual Conference on Mass Spectrometry and Allied Topics*, 1978, p. 224.
47. Kappes, M. M. Ph.D. thesis, Massachusetts Institute of Technology, 1981.
48. Chowdhury, A. K.; Wilkins, C. L. *Int. J. Mass Spectrom. Ion Proc.* **1988**, 82, 163.
49. Burnier, R. C.; Byrd, G. D.; Freiser, B. S. *J. Am. Chem. Soc.* **1981**, 103, 4360.
50. Halle, L. F.; Crowe, W. E.; Armentrout, P. B.; Beauchamp, J. L. *Organometallics* **1984**, 3, 1694.
51. Ambartzumian, R. V.; Letokhov, V. S. In *Chemical and Biochemical Applications of Lasers*; Moore, C. B., Ed.; Academic Press: New York, 1977; Vol. 3, p. 167.
52. Roth, L. M. Ph.D. thesis, Purdue University, 1991.
53. Bomse, D. S.; Beauchamp, J. L. *J. Am. Chem. Soc.* **1981**, 103, 3292.
54. Moylan, C. R.; Jasinski, J. M.; Brauman, J. I. *J. Am. Chem. Soc.* **1985**, 107, 1934.
55. Woodin, R. L.; Bomse, D. S.; Beauchamp, J. L. *Chem. Phys. Lett.* **1979**, 63, 630.
56. Bomse, D. S.; Beauchamp, J. L. *Chem. Phys. Lett.* **1981**, 77, 25.