Experimental Determination of the Gas Phase Proton Affinities of the Periodinane Anions IBX^- and IBA^-

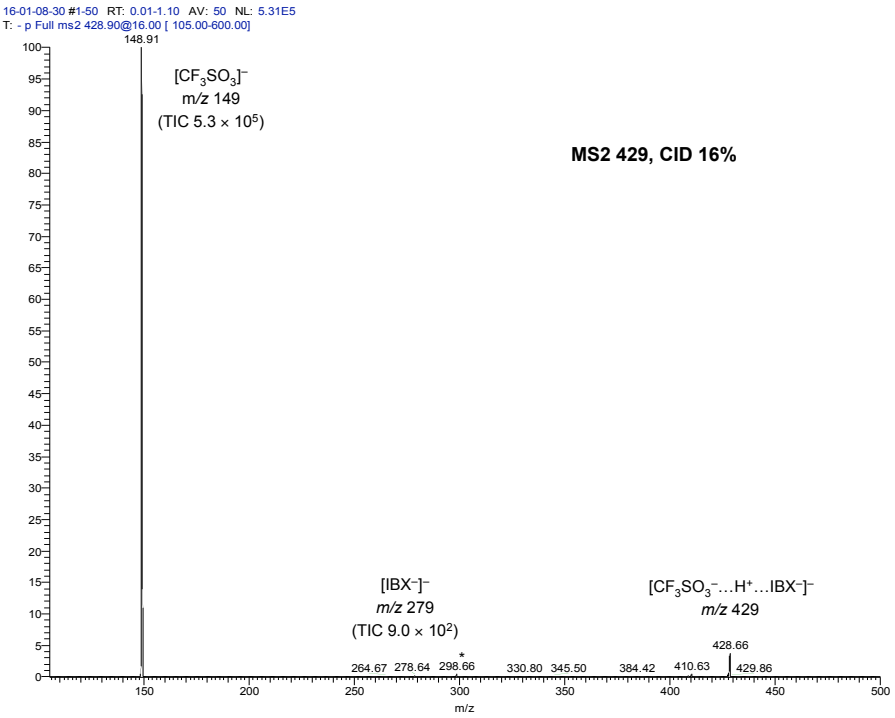
Tom Waters, Jack Boulton, Timothy Clark, Michael J. Gallen, Craig M. Williams, and Richard A. J. O'Hair*

SUPPLEMENTARY INFORMATION

Contents

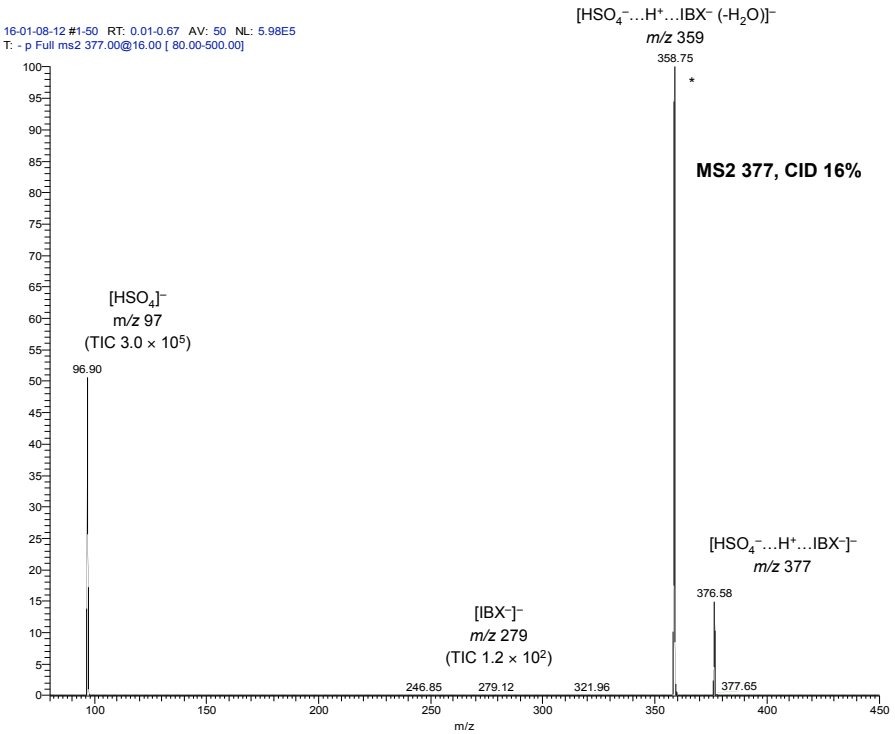
Full Citation for Reference 7: Gaussian 03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

$[CF_3SO_3^-\ldots H^+\ldots IBX^-]^-$



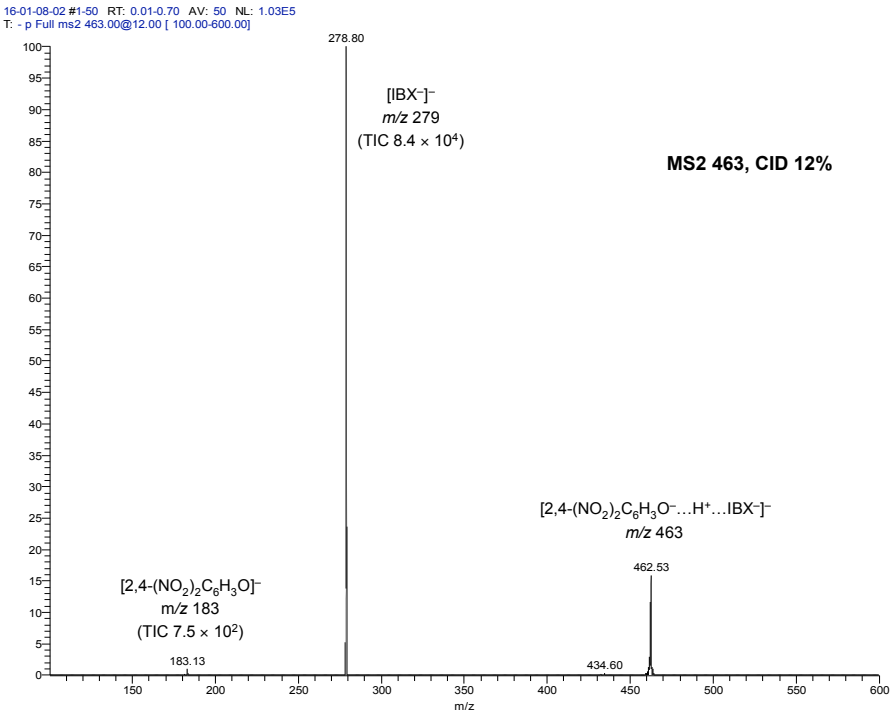
* *m/z* 299 assigned to $[CF_3SO_3^-\ldots H^+\ldots CF_3SO_3^-]^-$ formed from reaction of product *m/z* 149 with some residual CF_3SO_3H present in ion trap

$[HSO_4^-\ldots H^+\ldots IBX^-]^-$

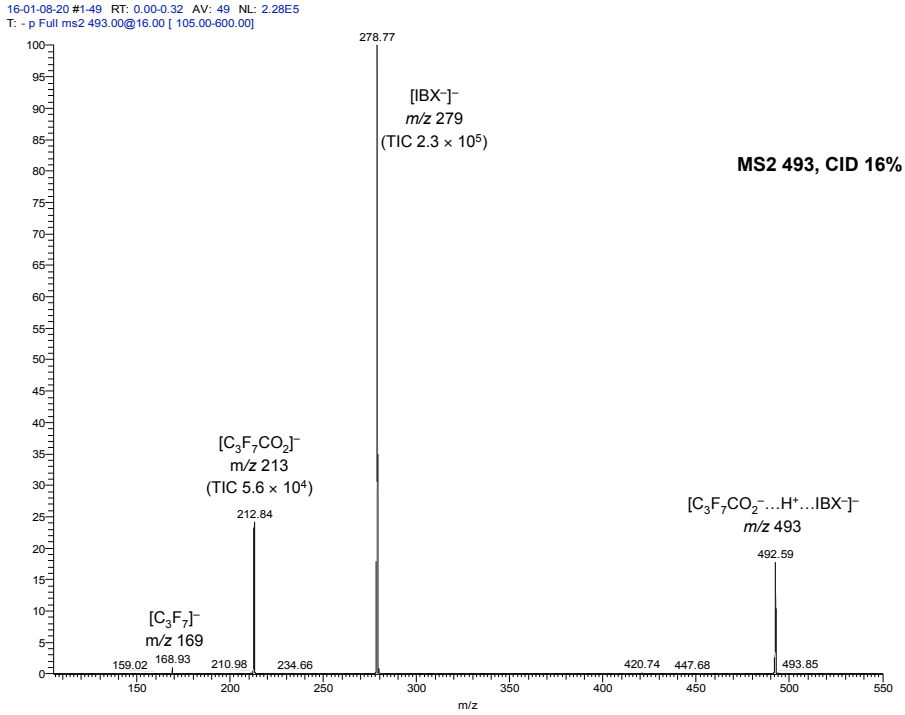


* *m/z* 359 assigned to loss of water from parent $[HSO_4^-\ldots H^+\ldots IBX^-]^-$ (*m/z* 377).

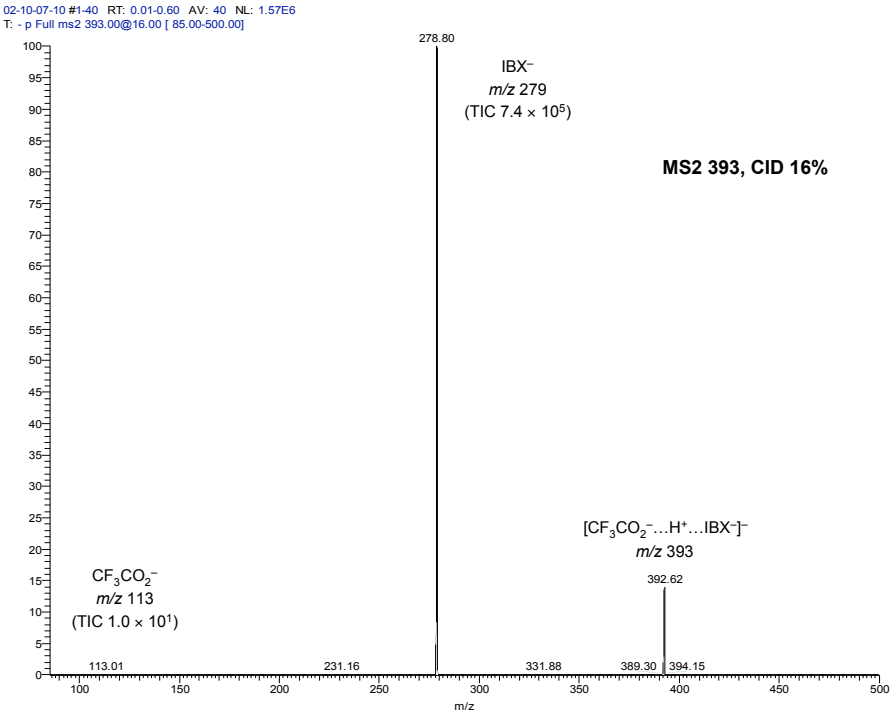
$[2,4\text{-}(NO_2)_2C_6H_3O^-\ldots H^+\ldots IBX^-]^-$



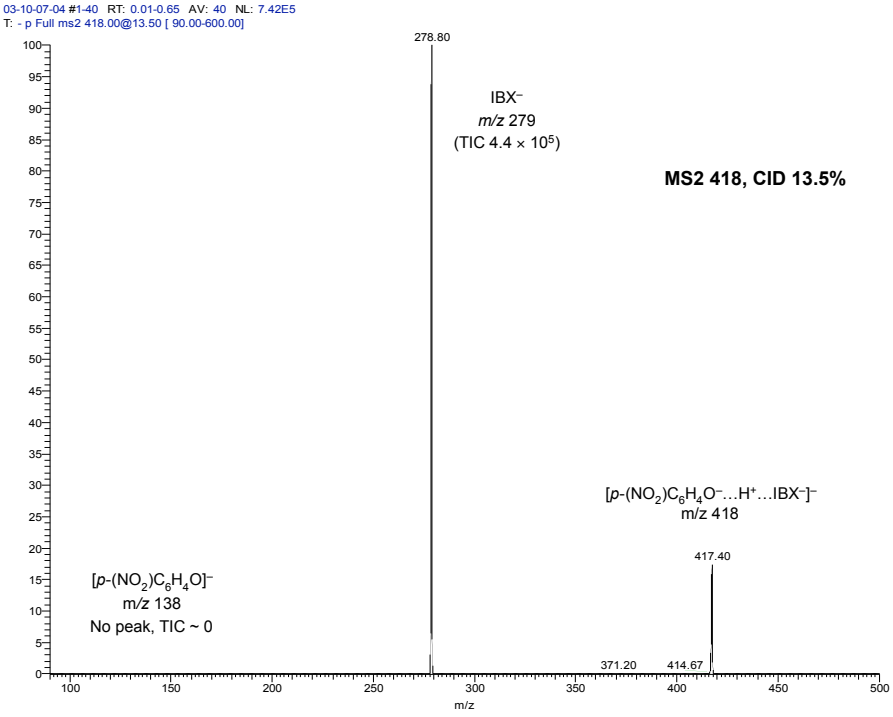
$[C_3F_7CO_2^-\ldots H^+\ldots IBX^-]^-$



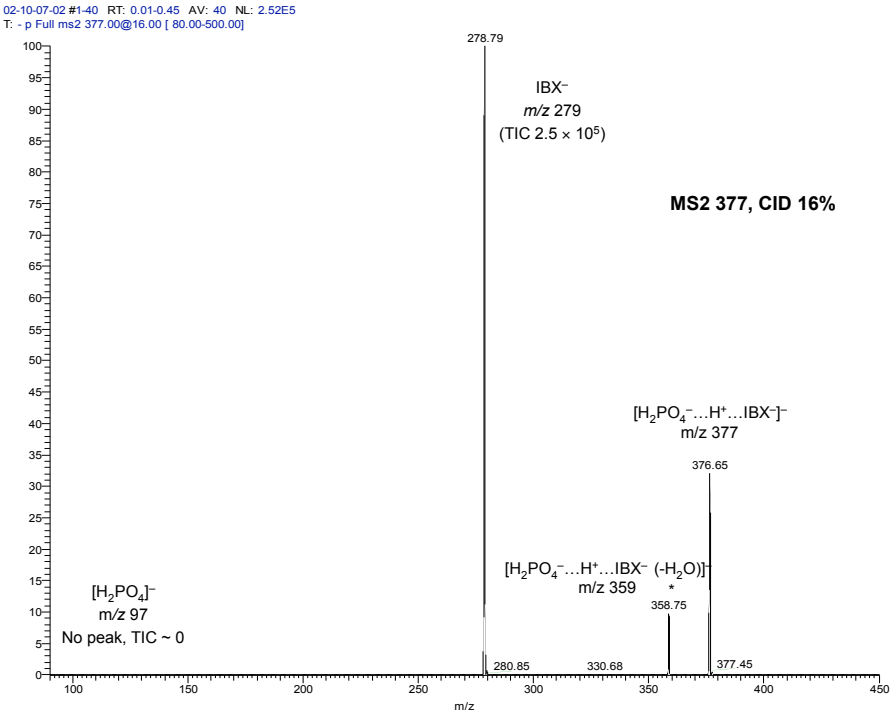
$[CF_3CO_2^-\ldots H^+\ldots IBX^-]^-$



$[p\text{-}(NO_2)C_6H_4O^-\ldots H^+\ldots IBX^-]^-$

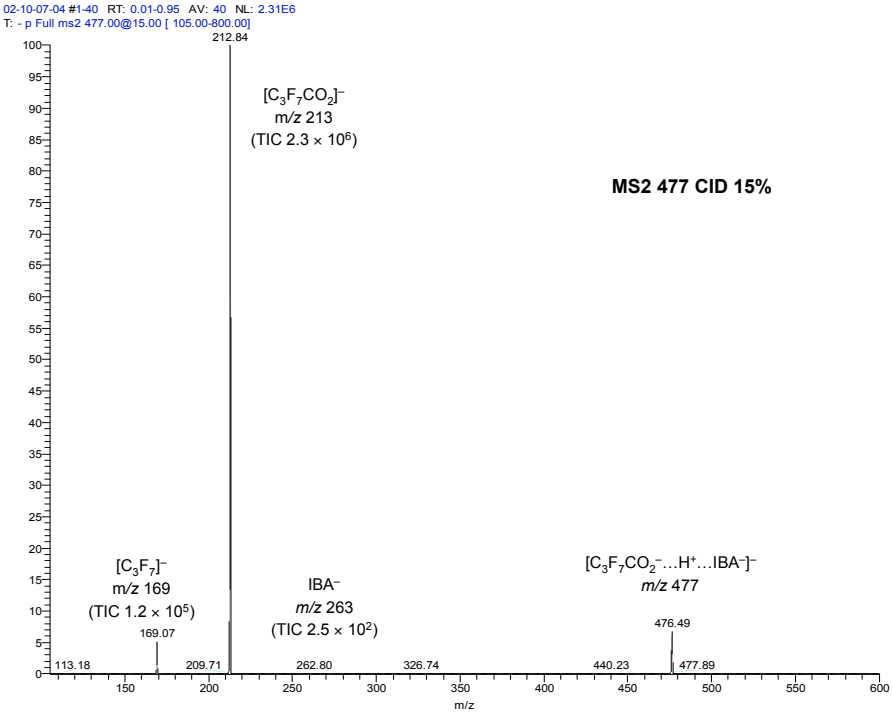


$[H_2PO_4^-\ldots H^+\ldots IBX^-]^-$

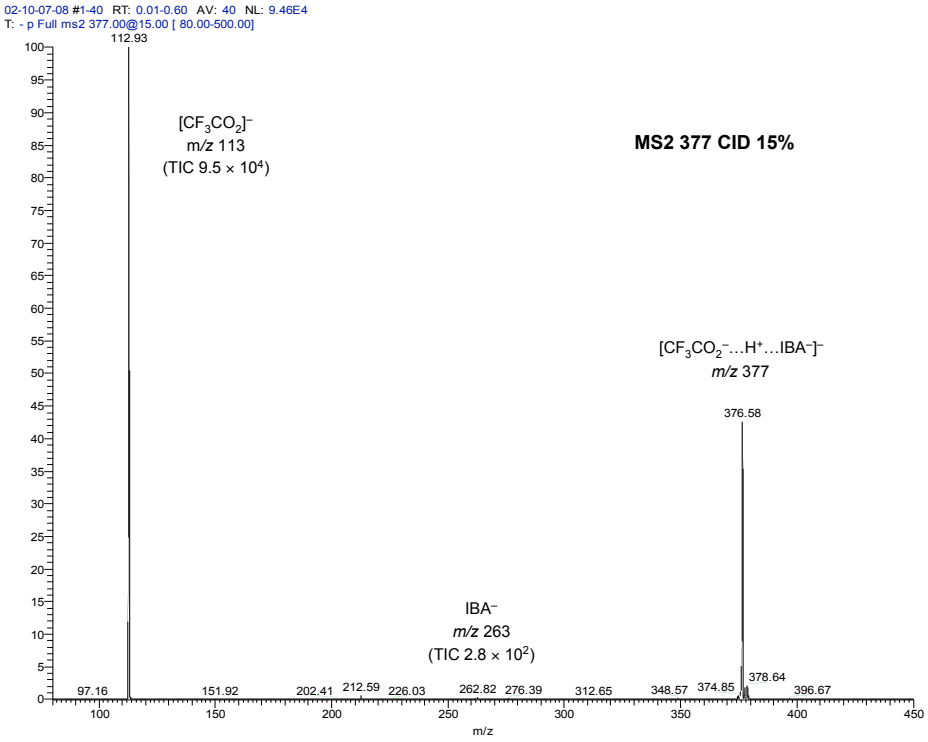


* *m/z* 359 assigned to loss of water from parent $[H_2PO_4^-\ldots H^+\ldots IBX^-]^-$ (*m/z* 377).

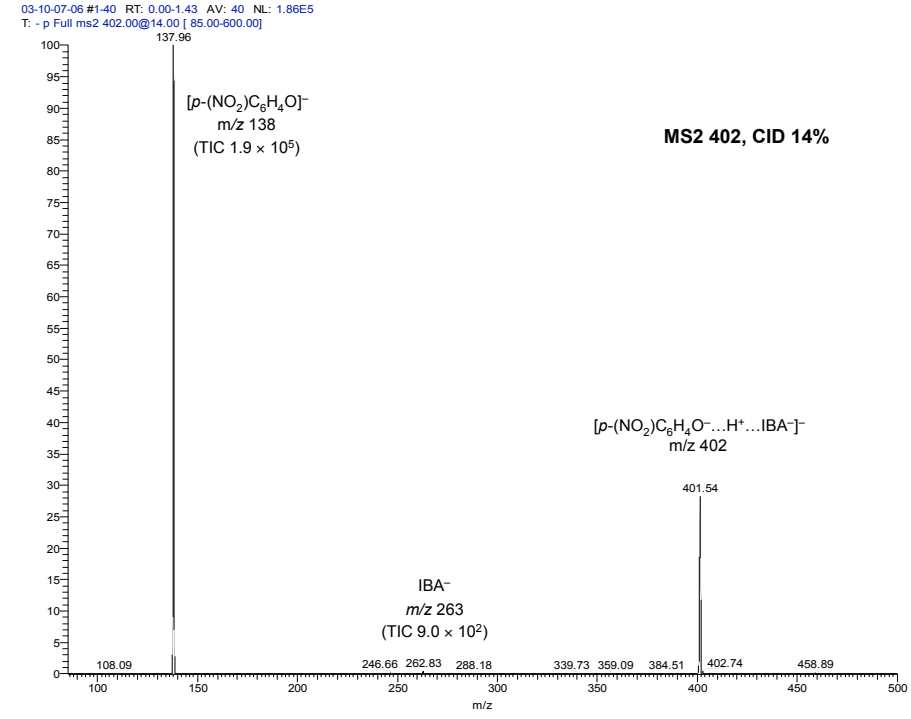
$[C_3F_7CO_2^-\ldots H^+\ldots IBA^-]^-$



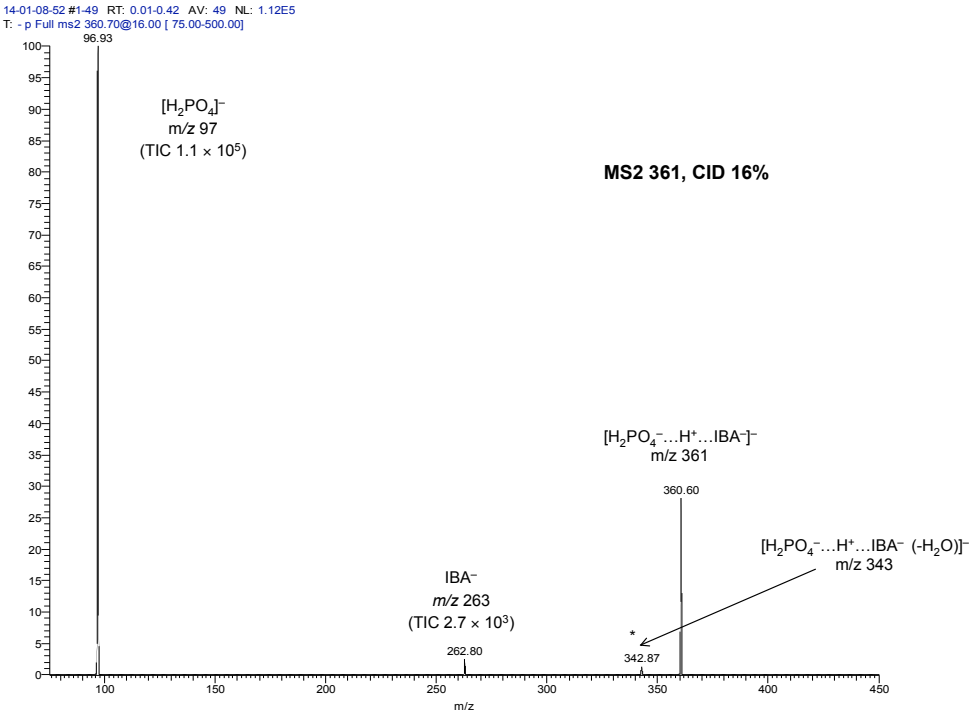
$[CF_3CO_2^-\ldots H^+\ldots IBA^-]^-$



$[p\text{-}(NO_2)C_6H_4O^-\ldots H^+\ldots IBA^-]^-$

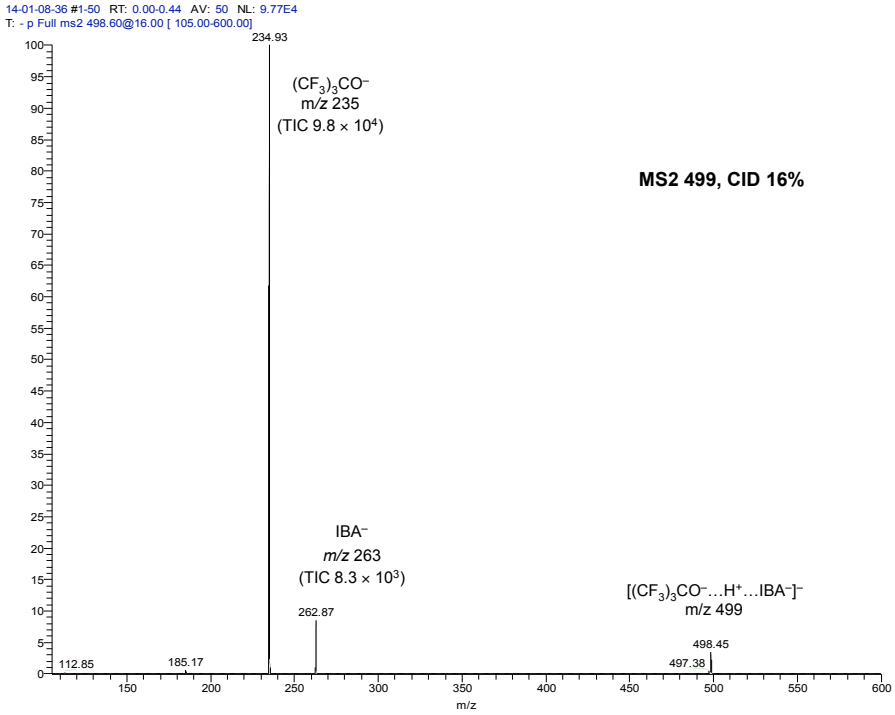


$[H_2PO_4^-\ldots H^+\ldots IBA^-]^-$

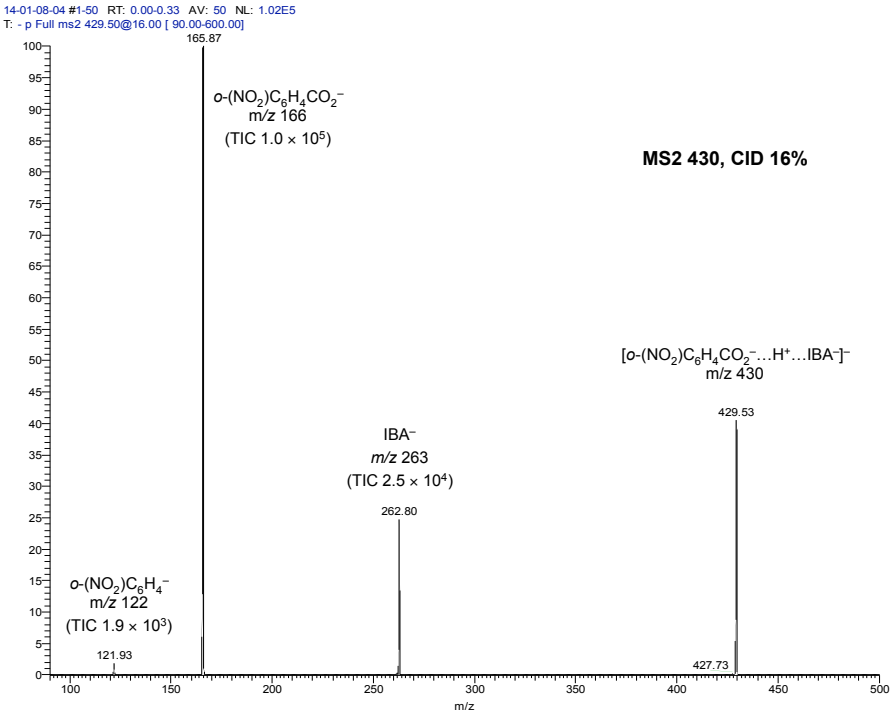


* *m/z* 343 assigned to loss of water from parent $[H_2PO_4^-\ldots H^+\ldots IBA^-]^-$ (*m/z* 361).

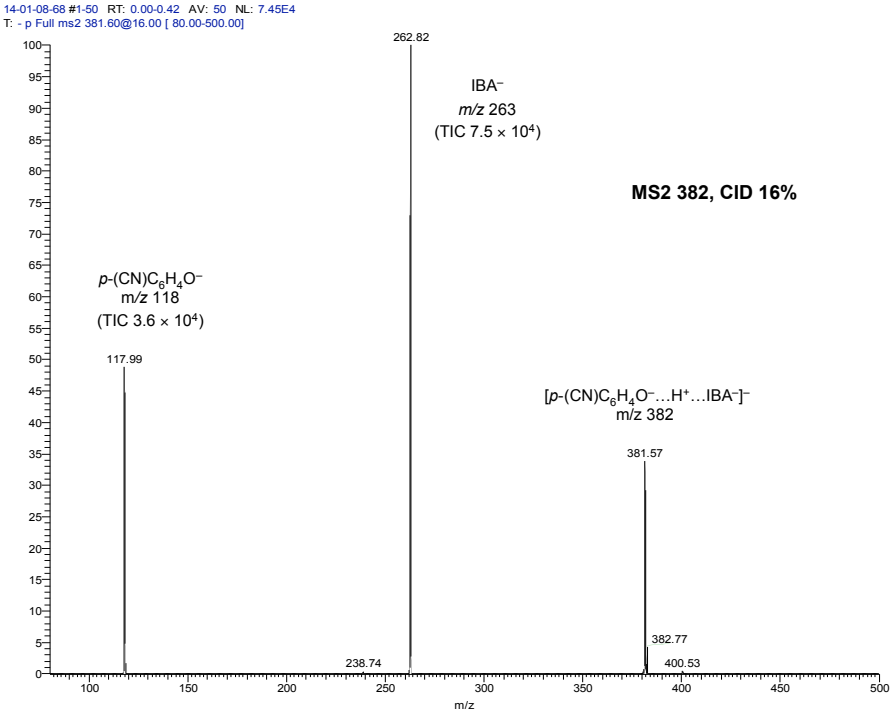
$[(CF_3)_3CO^-\ldots H^+\ldots IBA^-]^-$



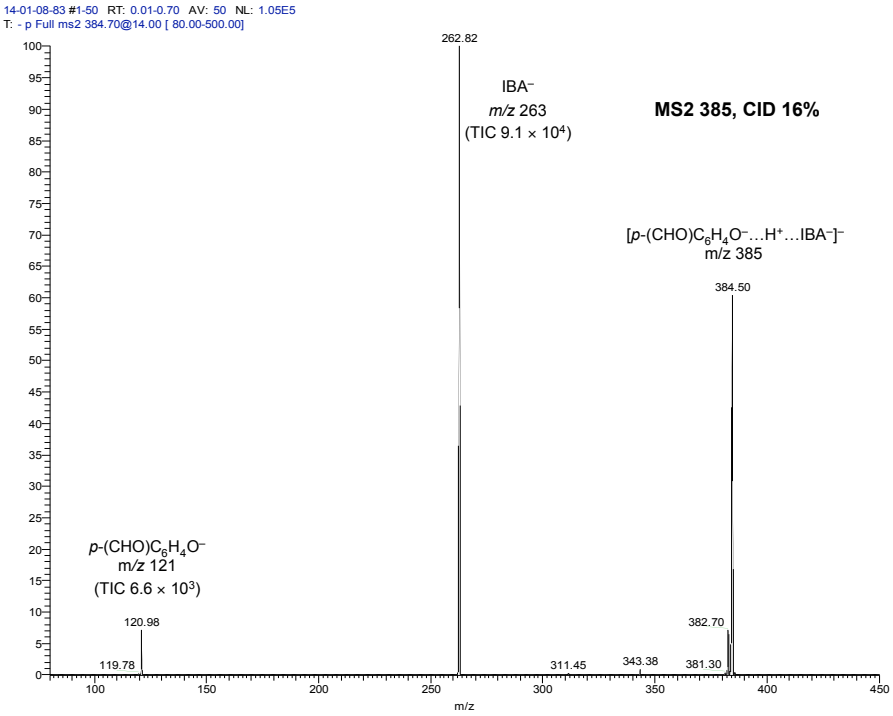
[*o*-$(NO_2)C_6H_4CO_2^-$…H^+…IBA$^-$]$^-$



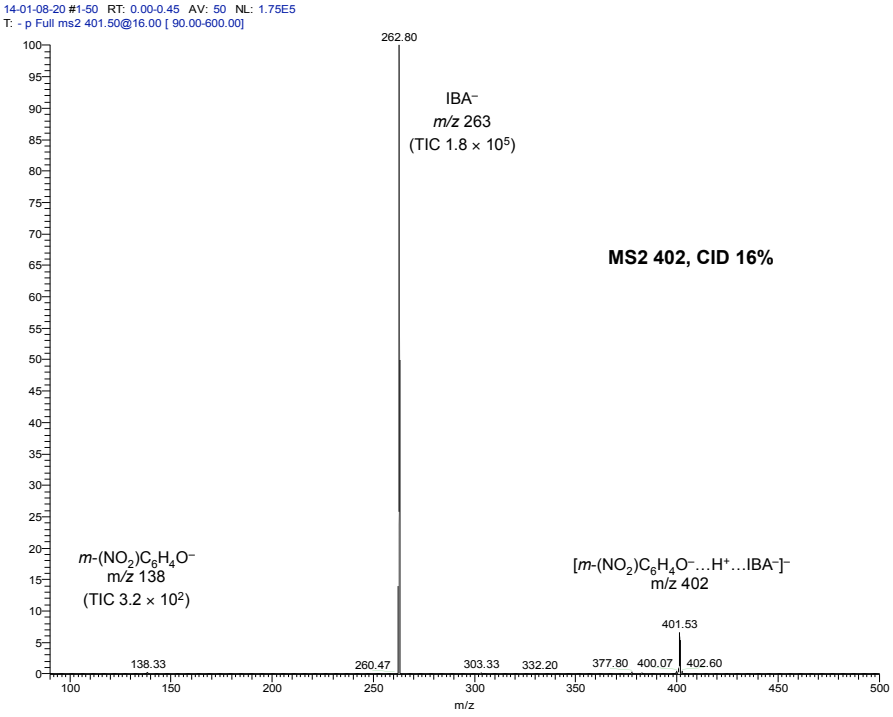
[*p*-$(CN)C_6H_4O^-$…H^+…IBA$^-$]$^-$



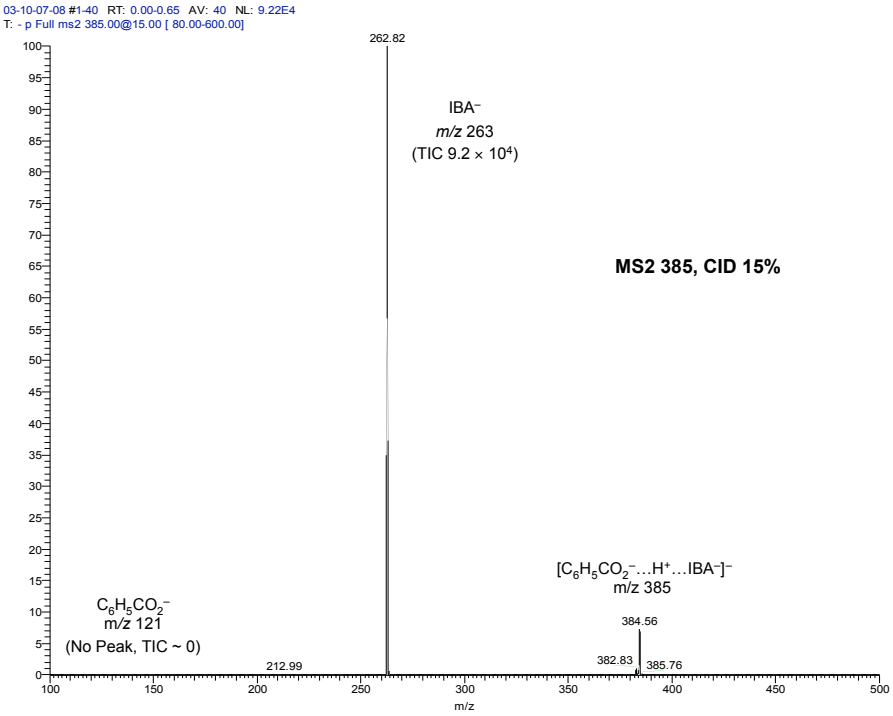
[*p*-(CHO)$C_6H_4O^-$…H^+…IBA$^-$]$^-$



[*m*-(NO_2)$C_6H_4O^-$…H^+…IBA$^-$]$^-$



$[C_6H_5CO_2^-\ldots H^+\ldots IBA^-]^-$



IOH: Summary of Calculations

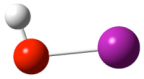
Level of theory: B3LYP//aug-ccPVDZ (H, C, O) and aug-ccPVDZ-pp (I)

IO^-

I	53.0	0.00000000	0.00000000	0.26185301
O	8.0	0.00000000	0.00000000	-1.73477399

Filename: 14_01_08_03
Electronic Energy = -373.025650
Zero-point energy = 0.001305
Sum of electronic and zero-point energies = -373.024345

IOH



I	53.0	0.01510500	-0.29933500	0.00000000
O	8.0	0.01510500	1.73477101	0.00000000
H	1.0	-0.92139798	1.98660696	0.00000000

Filename: 14_01_08_04
Electronic Energy = -373.598608
Zero-point energy = 0.012425
Sum of electronic and zero-point energies = -373.586369

ΔH_{acid} (no ZPVE) = 1504 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1476 kJ mol^{-1}

(Experiment = 1480 ± 8 kJ/mol)

From http://webbook.nist.gov/chemistry/

IBA: Summary of Calculations

Level of theory: B3LYP//aug-ccPVDZ (H, C,H) and aug-ccPVDZ-pp (I)

$[IBA\text{-}H^+]^-$

C	6.0	-0.22970299	3.13952804	0.00000000
C	6.0	1.16975605	3.23882294	0.00000000
C	6.0	1.95925796	2.08475208	0.00000000
C	6.0	1.36691201	0.81258398	0.00000000
C	6.0	-0.02519300	0.75739902	0.00000000
C	6.0	-0.84461302	1.88206899	0.00000000
H	1.0	-0.84363300	4.04278421	0.00000000
H	1.0	1.64374399	4.22250509	0.00000000
H	1.0	3.04850602	2.13320088	0.00000000
H	1.0	-1.92902696	1.74626303	0.00000000
I	53.0	-0.99183899	-1.15634298	0.00000000
C	6.0	2.19949508	-0.46984300	0.00000000
O	8.0	3.43911004	-0.37247601	0.00000000
O	8.0	1.49956596	-1.54275203	0.00000000
O	8.0	-2.80462503	-0.52607799	0.00000000

Filename: 08_01_08_07
Electronic Energy = -792.682887
Zero-point energy = 0.093828
Sum of electronic and zero-point energies = -792.589058

IBA, Isomer 1

C	6.0	-0.19442700	3.09562993	0.00000000
C	6.0	1.19948101	3.22198009	0.00000000
C	6.0	1.99957895	2.08201504	0.00000000
C	6.0	1.42564595	0.79642802	0.00000000
C	6.0	0.02348000	0.70204002	0.00000000
C	6.0	-0.78973597	1.82992995	0.00000000
H	1.0	-0.82704198	3.98395610	0.00000000
H	1.0	1.66095102	4.20905876	0.00000000
H	1.0	3.08616590	2.15530610	0.00000000
H	1.0	-1.87529695	1.70044994	0.00000000
I	53.0	-1.12887096	-1.13388300	0.00000000
C	6.0	2.35605192	-0.35973200	0.00000000
O	8.0	3.56491303	-0.29343799	0.00000000
O	8.0	1.70507598	-1.56258094	0.00000000
O	8.0	-2.86001611	-0.38238001	0.00000000
H	1.0	2.38516498	-2.25553107	0.00000000

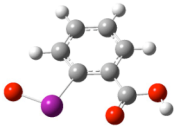
Filename: 08_01_08_11
Electronic Energy = -793.193299
Zero-point energy = 0.106567
Sum of electronic and zero-point energies = -793.086732

Using Isomer 1 for protonated species:

ΔH_{acid} (no ZPVE) = 1340 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1307 kJ mol^{-1}

IBA, Isomer 2



C	6.0	-0.29213101	3.10081792	0.00000000
C	6.0	1.10144401	3.24767900	0.00000000
C	6.0	1.92336404	2.12199593	0.00000000
C	6.0	1.35780299	0.83301198	0.00000000
C	6.0	-0.04089300	0.71677798	0.00000000
C	6.0	-0.87416899	1.82866096	0.00000000
H	1.0	-0.93358999	3.98288894	0.00000000
H	1.0	1.54558396	4.24268818	0.00000000
H	1.0	3.00669289	2.22693992	0.00000000
H	1.0	-1.95680904	1.67934799	0.00000000
I	53.0	-1.06961906	-1.17256403	0.00000000
C	6.0	2.17649698	-0.39281100	0.00000000
O	8.0	3.50913692	-0.17961501	0.00000000
O	8.0	1.70111799	-1.52092898	0.00000000
O	8.0	-2.83786798	-0.50844598	0.00000000
H	1.0	3.93732595	-1.05086696	0.00000000

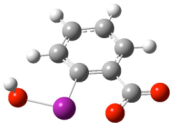
Filename: 08_01_08_12
Electronic Energy = -793.199722
Zero-point energy = 0.107024
Sum of electronic and zero-point energies = -793.092698

Using Isomer 2 for protonated species:

ΔH_{acid} (no ZPVE) = 1357 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1322 kJ mol^{-1}

IBA, Isomer 3



C	6.0	-0.28839201	3.18454194	0.05867200
C	6.0	1.10901499	3.27955198	0.11977000
C	6.0	1.89955795	2.12893295	0.12429200
C	6.0	1.29174197	0.86678302	0.06988600
C	6.0	-0.09493800	0.82001001	0.01833900
C	6.0	-0.92020601	1.93486798	0.00548200
H	1.0	-0.89731801	4.08898783	0.04851100
H	1.0	1.58132195	4.26103592	0.16035099
H	1.0	2.98733401	2.17554593	0.16687800
H	1.0	-2.00207901	1.83587003	-0.05393300
I	53.0	-0.82457298	-1.18665195	-0.06576800
C	6.0	2.08395290	-0.41459599	0.05809400
O	8.0	3.29961801	-0.43121499	0.11163000
O	8.0	1.32956195	-1.50462794	-0.01931000
O	8.0	-2.79198408	-0.52982497	-0.13358700
H	1.0	-3.14886308	-0.54409099	0.76680899

Filename: 08_01_08_08
Electronic Energy = -793.225535
Zero-point energy = 0.106178
Sum of electronic and zero-point energies = -793.119357

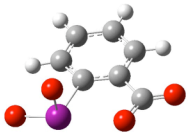
Using Isomer 3 for protonated species:

ΔH_{acid} (no ZPVE) = 1425 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1392 kJ mol^{-1}

IBX: Summary of Calculations

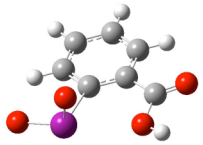
Level of theory: B3LYP//aug-ccPVDZ (H, C,H) and aug-ccPVDZ-pp (I)



$[IBX\text{-}H^+]^-$

C	6.0	-2.65478206	1.88926101	-0.13087900
C	6.0	-1.86825395	3.03697801	0.04681600
C	6.0	-0.47665700	2.93832397	0.13879301
C	6.0	0.15097401	1.68619597	0.06293600
C	6.0	-0.66238397	0.57009399	-0.10445600
C	6.0	-2.04686999	0.63055098	-0.21264100
H	1.0	-3.74046803	1.97478604	-0.20817000
H	1.0	0.15598500	3.81679296	0.26712000
H	1.0	-2.61335897	-0.29037499	-0.36411801
I	53.0	0.28103700	-1.39071596	-0.16159500
C	6.0	1.67464805	1.53860795	0.12774301
O	8.0	2.36018801	2.56388092	0.25686499
O	8.0	2.08199811	0.32882100	0.01613900
O	8.0	0.42489699	-1.80906999	1.63446105
O	8.0	-1.24828994	-2.27731705	-0.75857699
H	1.0	-2.34750700	4.01614189	0.10872100

Filename: 08_01_08_05
Electronic Energy = -867.842006
Zero-point energy = 0.096734
Sum of electronic and zero-point energies = -867.745272



IBX, Isomer 1

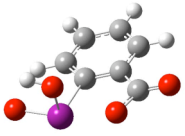
C	6.0	-2.57917309	1.93226504	-0.15795700
C	6.0	-1.80068398	3.07667089	0.03585300
C	6.0	-0.41320401	2.97194505	0.13937201
C	6.0	0.21943200	1.72105205	0.04710200
C	6.0	-0.58775699	0.58684498	-0.14048800
C	6.0	-1.96939695	0.67374903	-0.24526900
H	1.0	-3.66361809	2.01125789	-0.23852500
H	1.0	0.20899700	3.85280299	0.29107600
H	1.0	-2.55441904	-0.23764899	-0.38660499
I	53.0	0.14524899	-1.49296105	-0.17879400
C	6.0	1.70459902	1.70218396	0.15565600
O	8.0	2.39391804	2.64356804	0.47230899
O	8.0	2.23920989	0.48841900	-0.16506401
O	8.0	0.59059399	-1.74943602	1.58501399
O	8.0	-1.48043096	-2.26800108	-0.55380797
H	1.0	-2.27476811	4.05541420	0.10614100
H	1.0	3.19638896	0.54043698	-0.00923600

Filename: 08_01_08_14
Electronic Energy = -868.346873
Zero-point energy = 0.109514
Sum of electronic and zero-point energies = -868.237359

Using Isomer 1 for protonated species:

ΔH_{acid} (no ZPVE) = 1326 kJ mol^{-1}

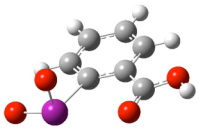
ΔH_{acid} (with ZPVE) = 1292 kJ mol^{-1}



IBX, Isomer 2

C	6.0	-2.67663193	1.92914104	-0.18230300
C	6.0	-1.86698997	3.04961610	0.05773200
C	6.0	-0.48004499	2.92459512	0.19388700
C	6.0	0.11090500	1.66129196	0.08518600
C	6.0	-0.72778600	0.58157903	-0.15575600
C	6.0	-2.10740304	0.65439999	-0.29520300
H	1.0	-3.75576591	2.04643512	-0.28237000
H	1.0	0.15983599	3.78509212	0.38662401
H	1.0	-2.70102096	-0.24251200	-0.47164801
I	53.0	0.28764001	-1.29196596	-0.29233000
C	6.0	1.60060704	1.42194104	0.21897100
O	8.0	2.37514496	2.33981705	0.41928101
O	8.0	1.93902600	0.15582500	0.07199800
O	8.0	0.69880599	-1.67311299	1.63004601
O	8.0	-1.22858799	-2.34565902	-0.33233300
H	1.0	-2.32795596	4.03405523	0.14125900
H	1.0	-0.01105900	-2.29920411	1.87263703

Filename: 08_01_08_06
Electronic Energy = -868.34971
Zero-point energy = 0.108878
Sum of electronic and zero-point energies = -868.240832



IBX, Isomer 3

C	6.0	-2.60179400	1.90826297	-0.16131200
C	6.0	-1.82084596	3.05031610	0.04017300
C	6.0	-0.43175301	2.94625306	0.14510500
C	6.0	0.18846500	1.68970895	0.05027900
C	6.0	-0.61914498	0.55997002	-0.14426400
C	6.0	-1.99794602	0.64611501	-0.25567499
H	1.0	-3.68563294	1.99404705	-0.24450400
H	1.0	0.17933400	3.83407307	0.29595000
H	1.0	-2.58125401	-0.26388699	-0.41137800
I	53.0	0.18378399	-1.48644400	-0.17473499
C	6.0	1.66085398	1.52928197	0.12191300
O	8.0	2.32781792	2.66733694	0.39386699
O	8.0	2.23398304	0.46659601	-0.05937200
O	8.0	0.47677699	-1.75166798	1.61917806
O	8.0	-1.40086901	-2.28690791	-0.66501099
H	1.0	-2.29486799	4.02885103	0.11367900
H	1.0	3.27317190	2.44617796	0.42062500

Filename: 08_01_08_10
Electronic Energy = -868.351584
Zero-point energy = 0.109935
Sum of electronic and zero-point energies = -868.241649

Using Isomer 2 for protonated species:

ΔH_{acid} (no ZPVE) = 1333 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1301 kJ mol^{-1}

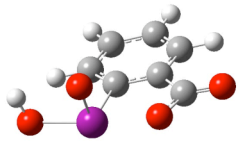
Using Isomer 3 for protonated species:

ΔH_{acid} (no ZPVE) = 1338 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1303 kJ mol^{-1}

IBX: Summary of Calculations (continued)

Level of theory: B3LYP//aug-ccPVDZ (H, C,H) and aug-ccPVDZ-pp (I)



IBX, Isomer 4

C	6.0	-2.69694495	1.90461004	-0.20763101
C	6.0	-1.89887595	3.04132700	-0.01707000
C	6.0	-0.51095998	2.93103290	0.10737800
C	6.0	0.08708900	1.66759300	0.04162800
C	6.0	-0.73814499	0.56451899	-0.14370500
C	6.0	-2.11878610	0.62984401	-0.27514201
H	1.0	-3.77782011	2.00713611	-0.30595899
H	1.0	0.12589900	3.80276108	0.25384700
H	1.0	-2.71418405	-0.26823300	-0.42631999
I	53.0	0.38069701	-1.26880097	-0.16737500
C	6.0	1.57742798	1.46541095	0.15141501
O	8.0	2.35261893	2.38668704	0.30033901
O	8.0	1.94944203	0.18993500	0.04260300
O	8.0	0.52354300	-1.85265195	1.56153297
O	8.0	-1.33694398	-2.32127094	-0.52170599
H	1.0	-2.36750889	4.02425194	0.03262900
H	1.0	-1.55744398	-2.76709294	0.31326500

Filename: 08_01_08_13
Electronic Energy = -868.362658
Zero-point energy = 0.108653
Sum of electronic and zero-point energies = -868.254005

Using Isomer 4 for protonated species:

ΔH_{acid} (no ZPVE) = 1367 kJ mol^{-1}

ΔH_{acid} (with ZPVE) = 1336 kJ mol^{-1}