THE UNIVERSITY OF ALABAMA AT BIRMINGHAM

Development of ^{211}At:

Understanding its chemical behavior

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Department of Chemistry
Department of Radiology

DOE Isotope Program Virtual Seminar Series – At-211,
October 3, 2023
Virtual

^{211}At Background

13	14	15	16	17	18
					2 He Helium 4.003
5 B Boron 10.81	6 C Carbon 12.01	7 N Nitrogen 14.01	8 O Oxygen 16.00	9 F Fluorine 19.00	10 Ne Neon 20.18
13 Al Aluminium 26.98	14 Si Silicon 28.09	15 P Phosphorus 30.97	16 S Sulfur 32.06	17 Cl Chlorine 35.45	18 Ar Argon 39.95
31 Ga Gallium 69.72	32 Ge Germanium 72.64	33 As Arsenic 74.92	34 Se Selenium 78.96	35 Br Bromine 79.90	36 Kr Krypton 83.79
49 In Indium 114.8	50 Sn Tin 118.7	51 Sb Antimony 121.8	52 Te Tellurium 127.6	53 I Iodine 126.9	54 Xe Xenon 131.3
81 Tl Thallium 204.38	82 Pb Lead 207.2	83 Bi Bismuth 209.0	84 Po Polonium (209)	85 At Astatine (210)	86 Rn Radon (222)
113 Nh Nihonium (284)	114 Fl Flerovium (289)	115 Mc Moscovium (288)	116 Lv Livermorium (293)	117 Ts Tennessine (294)	118 Og Oganesson (294)

https://www.acs.org/content/acs/en/education/whatischemistry/periodictable.html (accessed 4/19/22)

^{211}At α-particles

LET_{mean} = 99 keV/μm

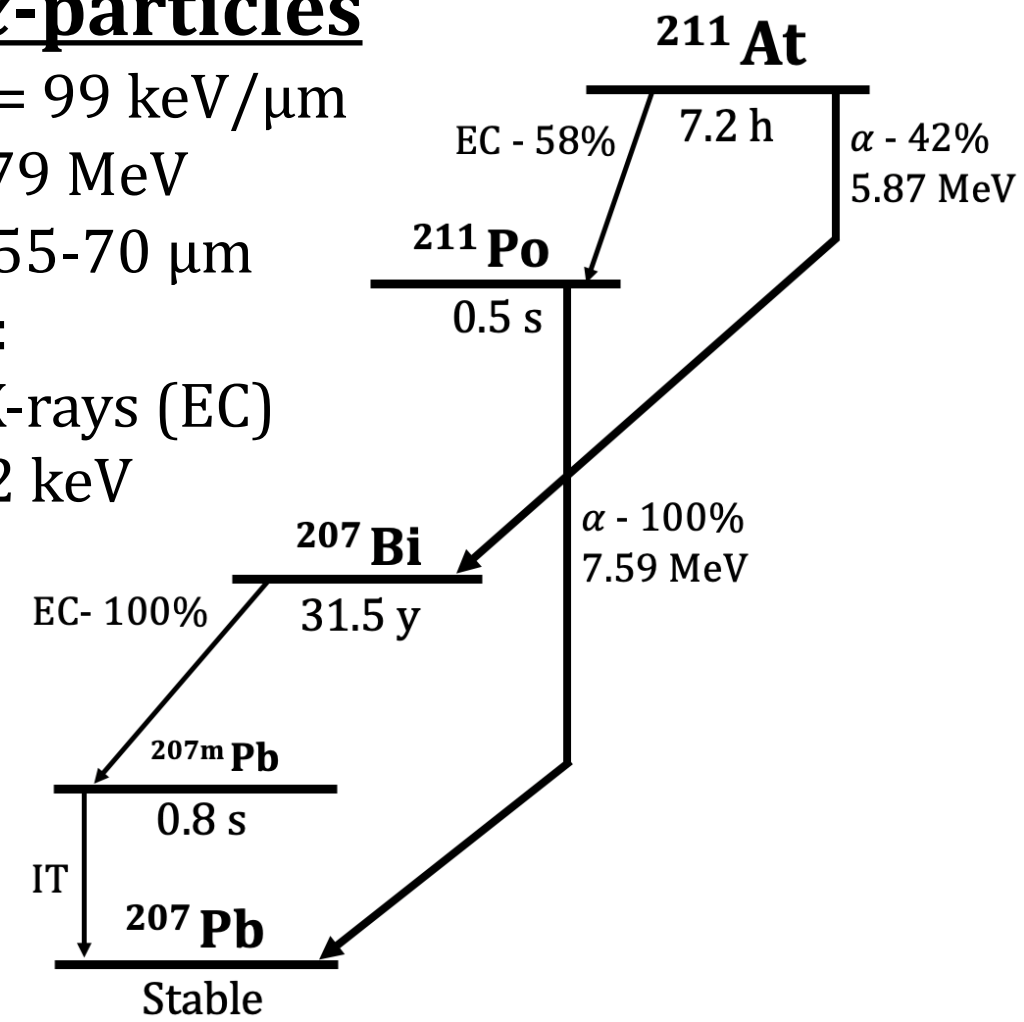
E_{avg} = 6.79 MeV

range = 55-70 μm

Imaging:

^{211}At K X-rays (EC)

77–92 keV



Adapted from Zalutsky, M. and Pruszynski M. *Curr. Radiopharm.* **2008**, *1*, 177–196.

^{211}At Chemistry in HNO_3

Inorganica Chimica Acta 362 (2009) 2654–2661

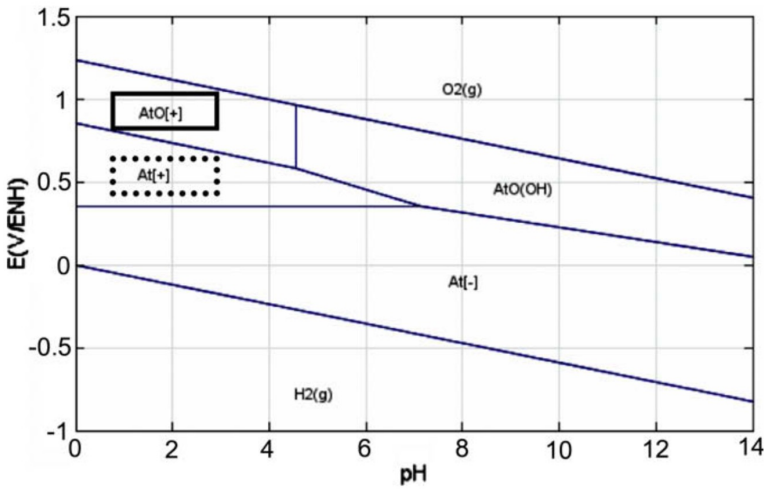
Contents lists available at ScienceDirect

Inorganica Chimica Acta

journal homepage: www.elsevier.com/locate/ica

Determination of stability constants between complexing agents and At(I) and At(III) species present at ultra-trace concentrations

J. Champion [a], C. Alliot [b], S. Huclier [a], D. Deniaud [c], Z. Asfari [d], G. Montavon [a,*]



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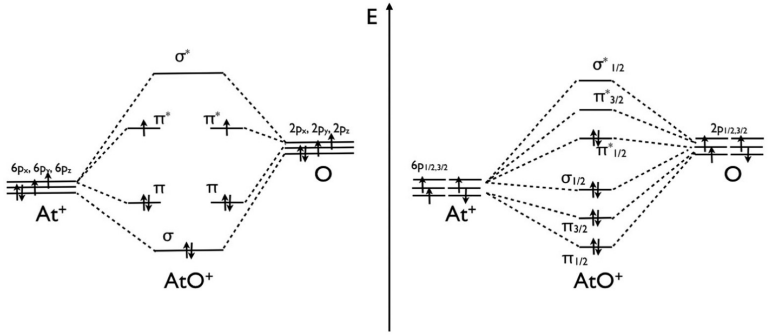
Cite this: *Phys. Chem. Chem. Phys.*, 2014, **16**, 9238

Electronic structure investigation of the evanescent AtO^+ ion†

André Severo Pereira Gomes,*[a] Florent Réal,[a] Nicolas Galland,[b] Celestino Angeli,[c] Renzo Cimiraglia[c] and Valérie Vallet[a]



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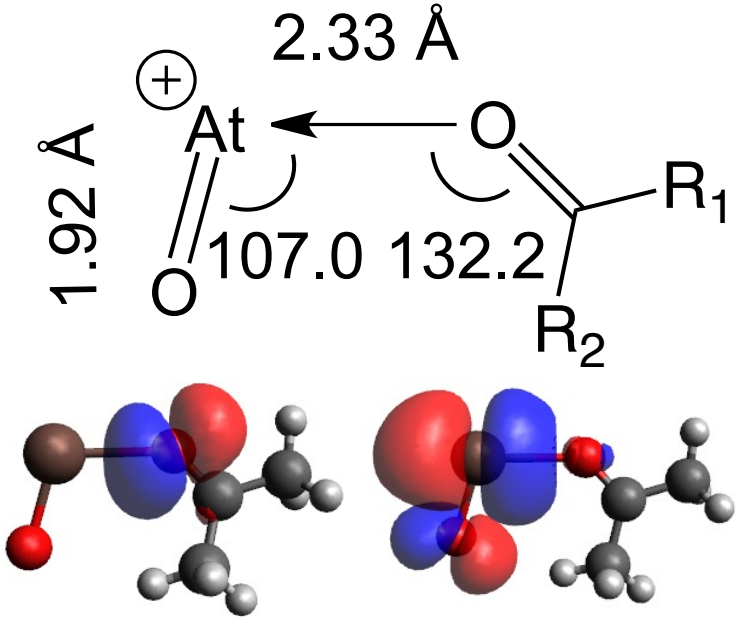
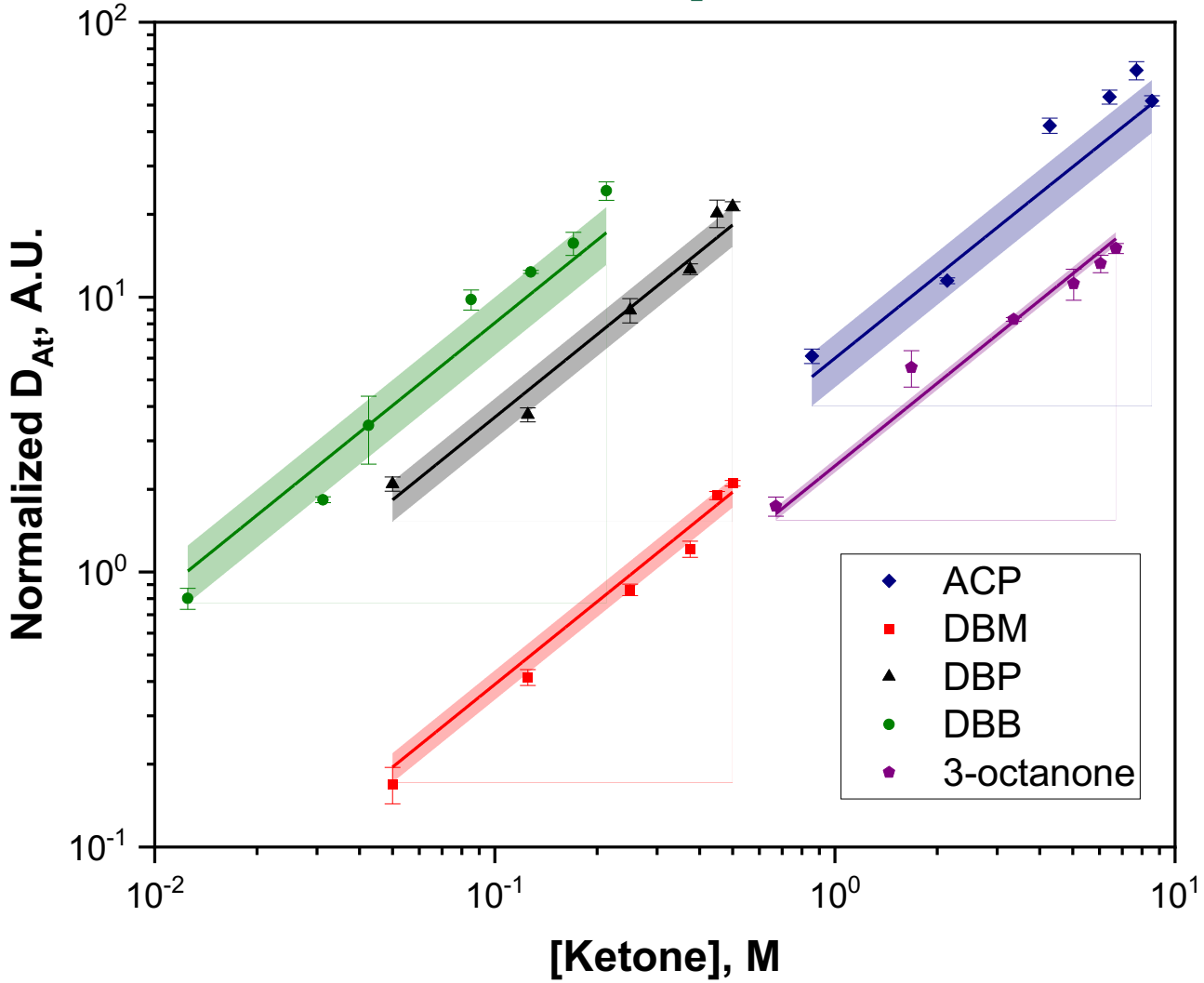
Astatine partitioning between nitric acid and conventional solvents: indication of covalency in ketone complexation of AtO^+†

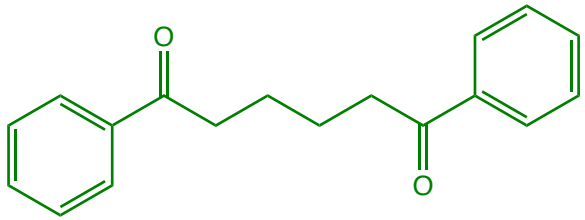
Jonathan D. Burns, *[a] Evgeny E. Tereshatov, [b] Mallory A. McCarthy,[bc] Lauren A. McIntosh, [b] Gabriel C. Tabacaru,[b] Xin Yang, [c] Michael B. Hall [c] and Sherry J. Yennello [bc]



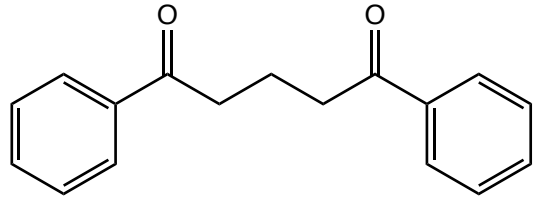
Champion, J. et al. *Inorganica Chim. Acta* **2009**, *362* (8), 2654-2661. Severo Pereira Gomes, A. et al. *Phys.Chem.Chem.Phys.* **2014**, *16*, 9238-9248. Burns, J. D. et al. *Chem. Commun.* **2020**, *56* (63), 9004.

^{211}At Extraction Speciation

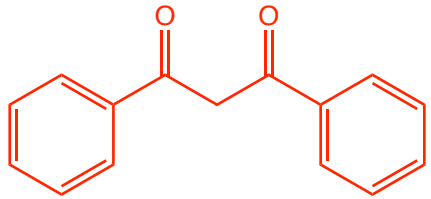




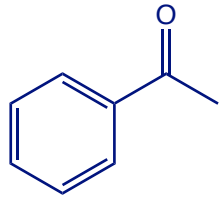
1,4-Dibenzoylbutane



1,3-Dibenzoylpropane



Dibenzoylmethane



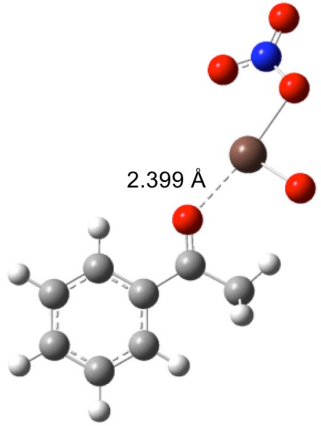
acetophenone

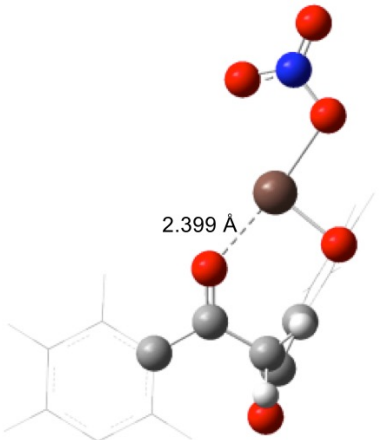
3-octanone

Burns, J. D. et al. *Inorg. Chem.* **2022,** *61* (31), 12087-12096.

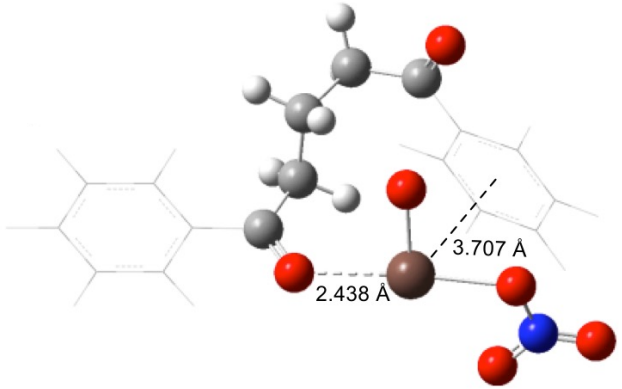
^{211}At Extraction Speciation Cont.

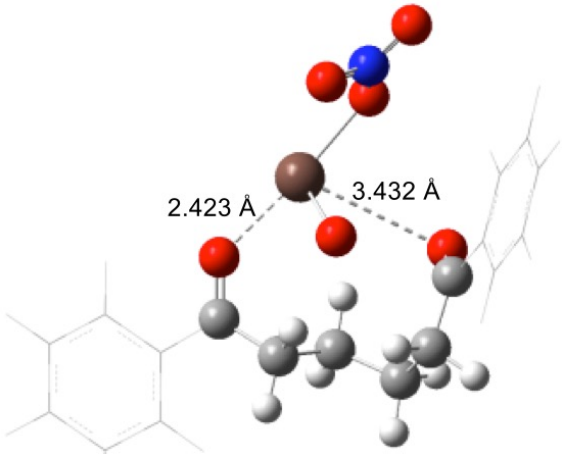
Monodentate





Bidentate

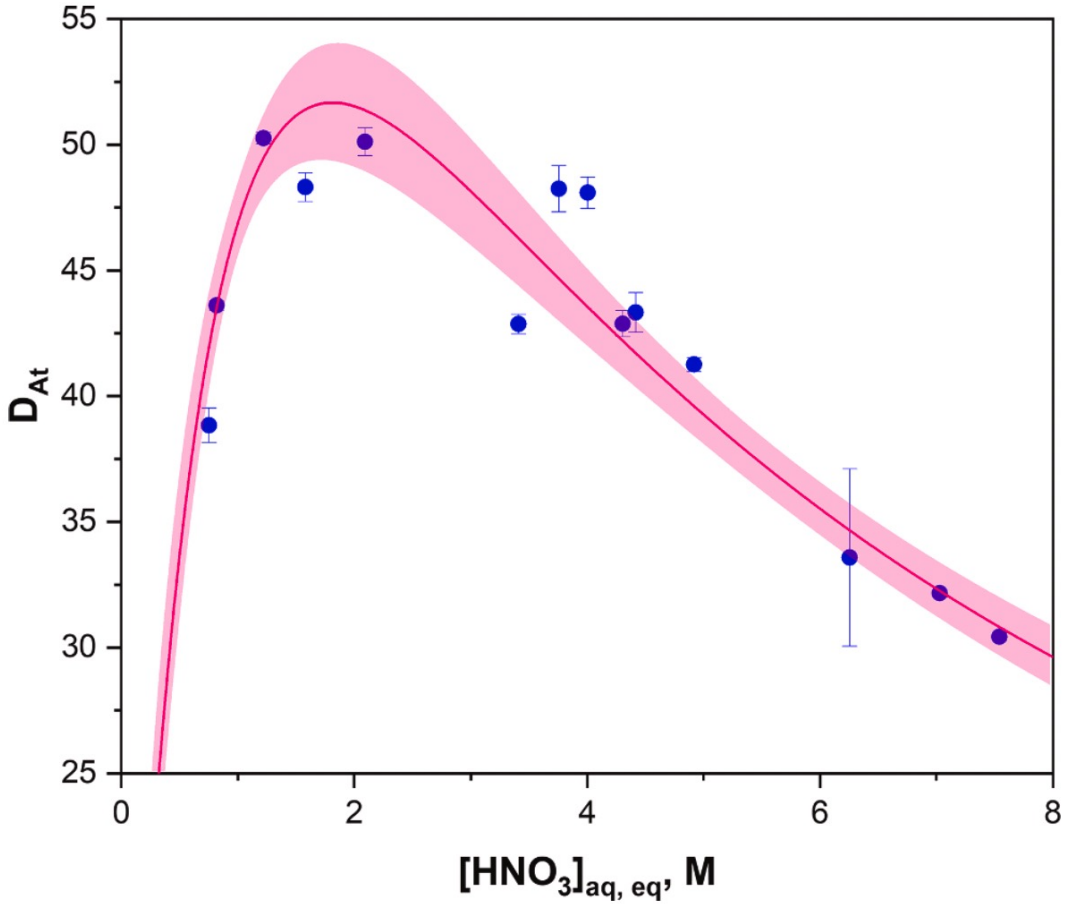




Solvent	Mode	ΔG(sol) / kcal•mol^{-1}	E_d / kcal•mol^{-1}
3-octanone	Mono	-11.91	4.21
acetophenone	Mono	-13.56	1.00
dibenzoylmethane	Mono	-12.06	3.23
1,3-dibenzoylpropane	Mono	-15.58	0.71
	Bi O O	-11.27	4.29
	Bi O phenyl	-14.32	7.99
1,4-dibenzoylbutane	Mono	-11.58	3.20
	Bi O O	**-19.04**	**4.52**
	Bi O phenyl	-17.86	4.39

Burns, J. D. et al. *Inorg. Chem.* **2022,** *61* (31), 12087-12096.

^{211}At Extraction from HNO_3 to 1-octanol



$$D_{At} = \frac{K_{ext\_At} \cdot K_1 \cdot [NO_{3,aq}^-]}{1 + K_1 \cdot [NO_{3,aq}^-] + K_{redox} \cdot [NO_3^-]^2}$$

$$K_{ext\_At} = \frac{[AtO(NO_3)_{org}]}{[AtO(NO_3)_{aq}]} = 118 \pm 18$$

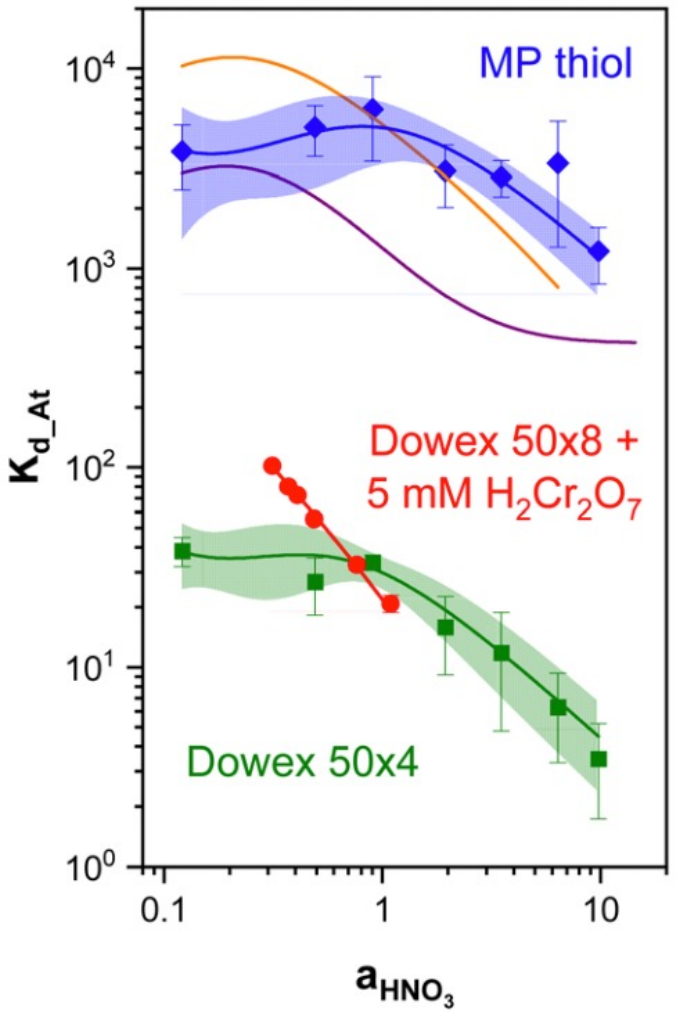
$$K_{redox} = \frac{[At_{aq}^+]}{[AtO_{aq}^+] \cdot [H_{aq}^+]^2} = 0.305 \pm 0.020$$

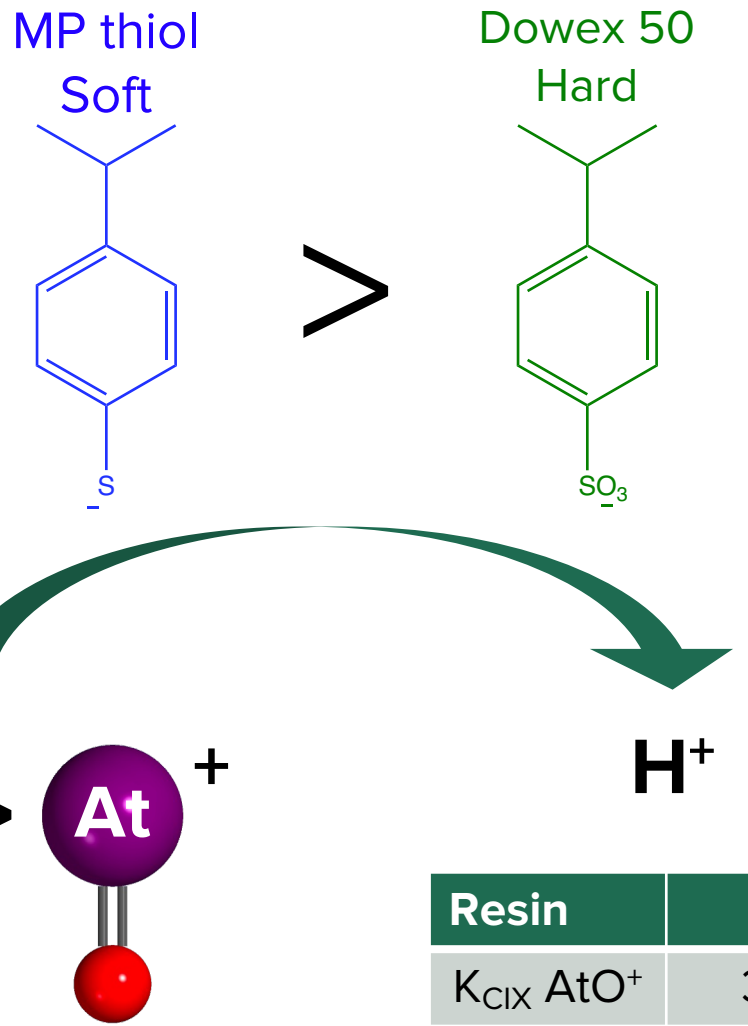
$$K_1 = \frac{[AtO(NO_3)_{aq}]}{[AtO_{aq}^+] \cdot [NO_{3,aq}^-]} = 0.86 \pm .23$$

Evgeny Tereshatov
CI TAMU

Tereshatov, E. E.; *et al*. *Sep. Purif. Technol*. **2022**, 282, 120088.

^{211}At Ion Exchange Behavior



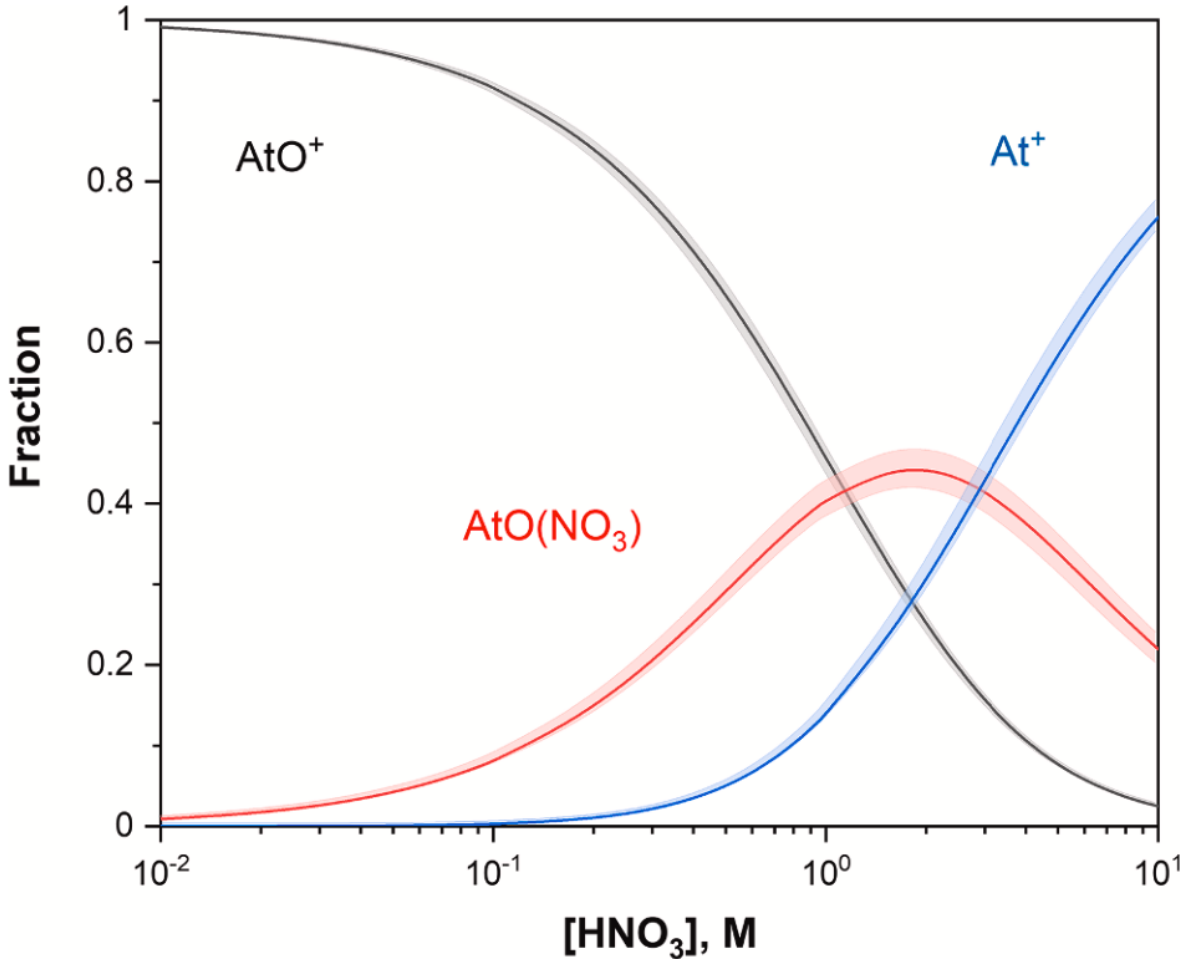


Evgeny Tereshatov
CI TAMU

Resin	MP thiol	Dowex 50
K_{CIX} AtO^+	300 ± 140	3.0 ± 1.0
K_{CIX} At^+	12,000 ± 1,800	45 ± 8

Tereshatov, E. E.; *et al*. *New J. Chem*. **2023**, *47* (25), 12037-12047.

^{211}At Speciation Diagrams



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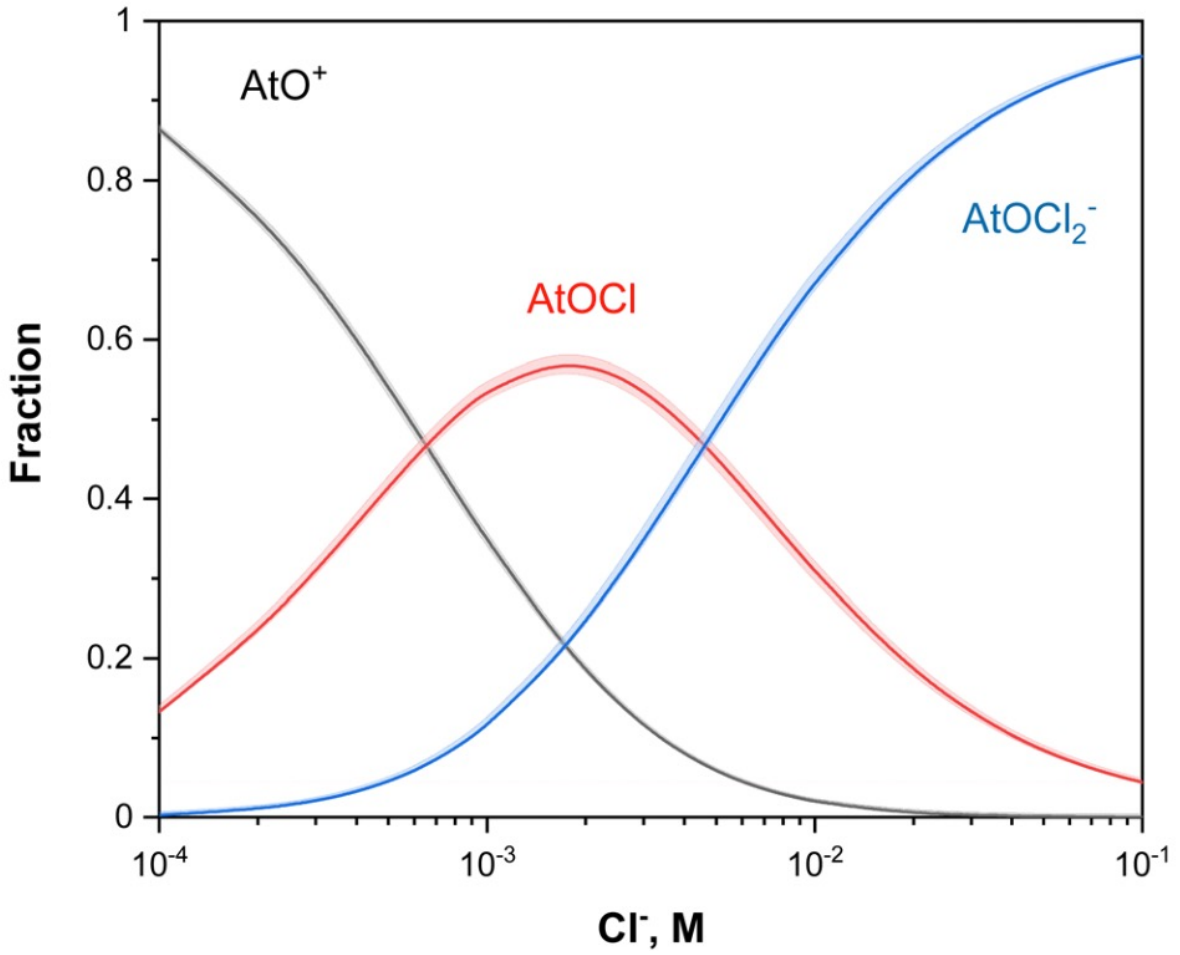

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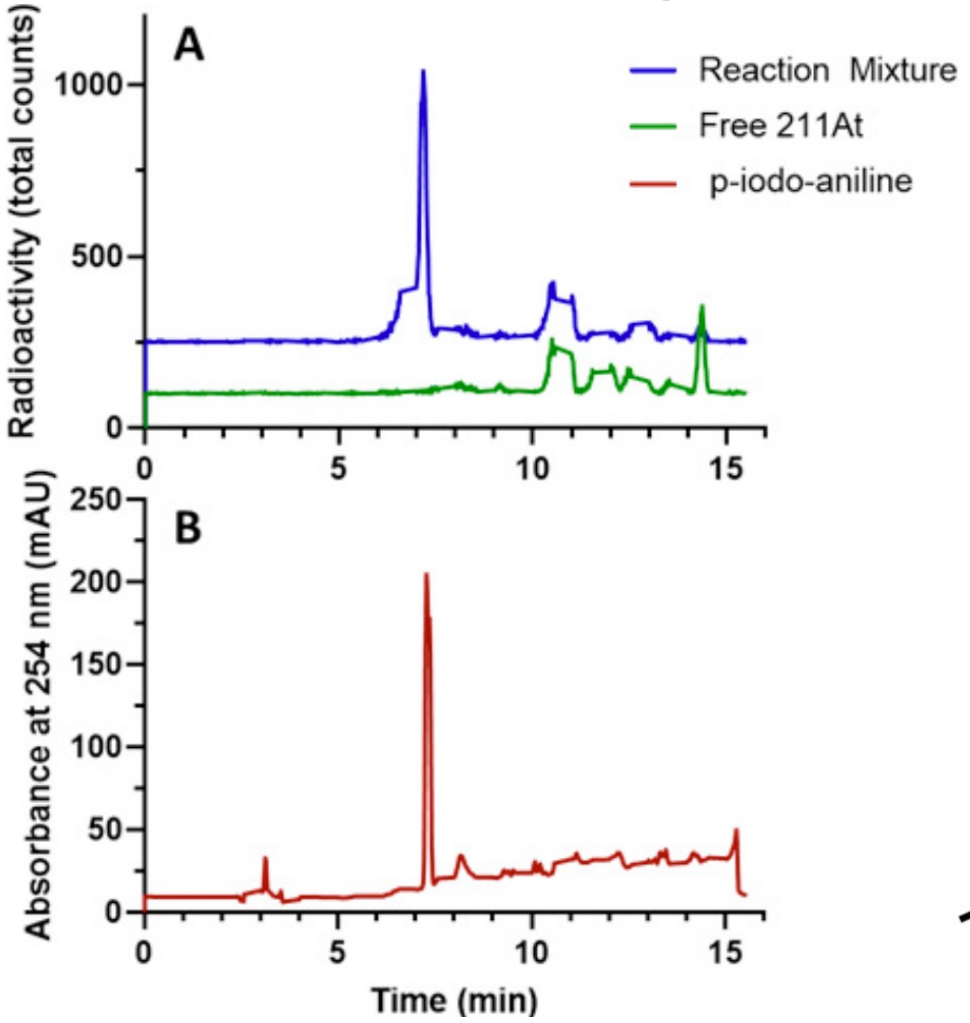
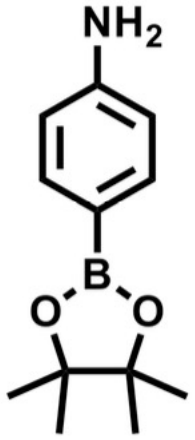
Aniline Labeling with ^{211}At

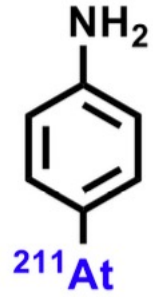




(1)

[^{211}At]
0.1M $NaOH_{MeOH}$

$Cu(OTf)_2(Py)_4$
3,4,7,8-Tetramethyl-1,10-phenanthroline
10min at RT



(2)

Labeling Yield
(non-decay corrected)
36 ± 22% (n = 4)

Riccardo Muzzioli
UTMDACC

McIntosh, L.A.; et al. *Nucl. Med. Biol.* **2023**, *in press*

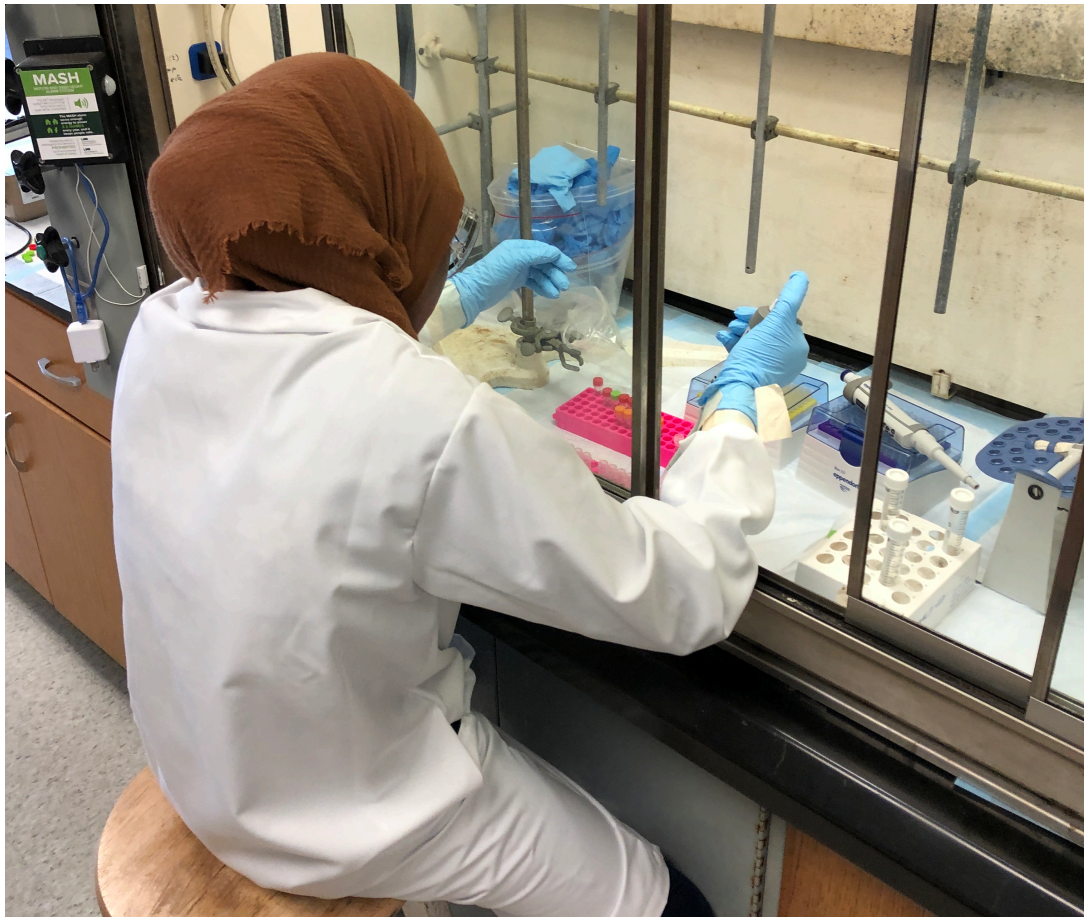
Future Work with At-211

- Investigate the At preference for ketone functionality more thoroughly
  - Electron donor groups on the hydrocarbon backbone
  - Electron withdrawing groups on the hydrocarbon backbone
- Expand fundamental understanding of binding affinity of At with N, S, and P groups
- Explore the chemical behavior of At post shipment

Collaborating with Texas A&M University on ^{211}At

Participated in a production run in June 2022

Received first shipment of At-211 October 2022



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Thank You for Your Attention!

Question?

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