

Extraction of uranyl from spent nuclear fuel
wastewater via complexation - a local vibrational
mode study
SUPPORTING INFORMATION

Bárbara M. T. C. Peluzo¹, Renaldo T. Moura Jr.^{1,2}, Elfi Kraka^{1*}

¹Computational and Theoretical Chemistry Group (CATCO),
Department of Chemistry, Southern Methodist University, 3215 Daniel
Avenue, Dallas, 75275-0314, Texas, United States.

²Department of Chemistry and Physics, Center of Agrarian Sciences,
Federal University of Paraíba, Areia, 58397-000, Paraíba, Brazil.

*Corresponding author(s). E-mail(s): ekraka@smu.edu;
Contributing authors: bmpeluzo@smu.edu, bmpeluzo.smu@gmail.com;
renaldo.mourajr@cca.ufpb.br;

1 Optimized Coordinates

1.1 UO_2^{2+}

U 0.000000 0.000000 0.000000
O 0.000000 0.000000 1.681700
O 0.000000 0.000000 -1.681700

1.2 a

U 0.000000 0.000000 0.000000
O 0.000000 1.065847 2.214806
O -1.746884 0.051235 -0.000000
O 1.746884 -0.051235 -0.000000
N -0.000000 -0.000000 2.908257
O -0.000000 -1.065847 2.214806
O -0.000000 -0.000000 4.097161
O 0.000000 1.065847 -2.214806
O -0.000000 -1.065847 -2.214806
N -0.000000 -0.000000 -2.908257
O -0.000000 -0.000000 -4.097161
O 0.046110 2.527021 -0.000000
H -0.302511 2.967230 -0.779616
H -0.302511 2.967230 0.779616
O -0.046110 -2.527021 -0.000000
H 0.302511 -2.967230 -0.779616
H 0.302511 -2.967230 0.779616

1.3 b

U -1.276604 -0.131304 -0.113136
O -2.153677 2.000122 0.739903
O -2.786035 -2.048600 -0.029395
O -1.819773 0.290007 -1.722814
O -0.659825 -0.487235 1.492209
N -3.325047 1.586079 1.039963
N -1.986559 -2.912810 -0.499934
O -3.514095 0.362767 0.803614
O -0.839804 -2.450733 -0.798059
N 0.508113 1.935849 -0.268806
O 1.010060 -0.532922 -0.888982
C 1.976629 0.105125 -0.435290
C 1.788071 1.595775 -0.462911
C 4.091022 0.214203 0.800283
C 5.425611 0.386187 0.081813
C 4.275979 -0.363630 2.196750
H 3.668959 1.205910 0.947376
H 5.292381 0.671191 -0.962906
H 5.998612 1.171445 0.578721
H 6.026726 -0.520606 0.103544
H 3.325616 -0.442464 2.723897
H 4.751200 -1.343511 2.183735
H 4.924294 0.306822 2.763612
N 3.075300 -0.507849 0.010409
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C 2.374438 -2.705782 0.990894
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H 2.180683 -3.736843 0.691316
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H 4.918174 -2.083725 -1.307745
H 5.119444 -2.535988 0.396657
H 4.303208 -3.621830 -0.712672
C 2.754471 2.523642 -0.813108
C 2.387683 3.854604 -0.939607
H 3.120198 4.596572 -1.231752
C 1.077711 4.210631 -0.691614
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1.4 c

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1.6 e

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C 2.614815 -0.030386 -2.374048

O 1.413399 0.003019 -1.999443
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1.7 f

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O 0.000000 -0.000000 -1.747795

1.8 g

U 0.000000 0.000000 0.004984
O -0.000000 1.742098 0.005945
O -0.000000 -1.742098 0.005945
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