

Electronic Supporting Information

Evidence for 5d- σ and 5d- π Covalency in Lanthanide Sesquioxides from Oxygen K-edge X-ray Absorption Spectroscopy

Alison B. Altman,^{1,2} Joseph I. Pacold,² Jian Wang,³ Wayne W. Lukens,² and Stefan G. Minasian^{2*}

¹ Department of Chemistry, University of California, Berkeley CA 94720, United States

² Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley CA 94720, United States

³ Canadian Light Source, Saskatoon, Saskatchewan, S7N 2V3, Canada

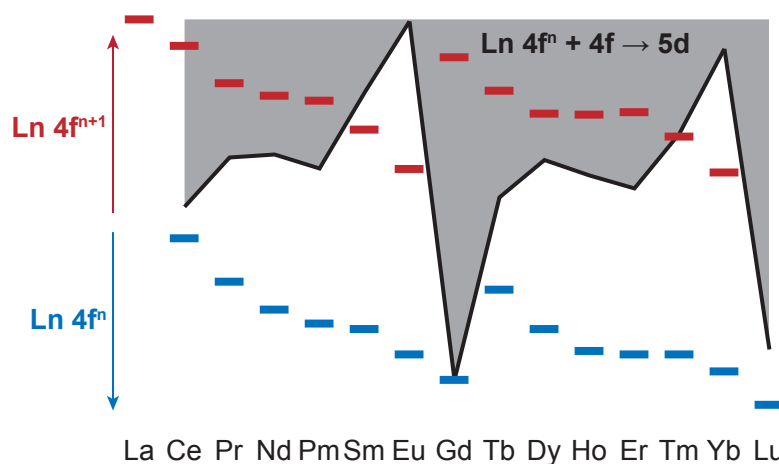


Figure S1. Qualitative diagram showing how changes in Ln_2O_3 band gaps are driven by periodic variations in the $4f^n$ and $4f^{n+1}$ states relative to the filled $5d^1$ states. For Sm, Eu, Tm, and Yb, the $4f^{n+1}$ states lie at or below the energy of the $5d^1$ states. Energies of the $4f^n$ and $4f^{n+1}$ states are given as $-IP_4$ and $-IP_3$, where IP_3 and IP_4 are the third and fourth ionization potentials, respectively.¹ Energies of the filled $5d^1$ states are estimated by adding the $4f \rightarrow 5d$ promotion energies² to the fourth ionization potential energies.

Normalized Oxygen K-edge X-ray Absorption Spectra for Lanthanide Sesquioxides, Ln_2O_3 (Ln = La to Lu, except Pm)

Spectra have been background-subtracted and normalized following the procedure developed by Weng et al.³ Errors in the raw intensities are typically 0.1% or less, determined by the total number of counts contributing to each data point. The background-subtracted data have not been rounded; the physical quantities of interest are derived from curve fitting as described in the main text and are rounded to reflect the precision of the fitting procedure.

La_2O_3

Energy (eV)	Intensity
524	-0.0164763
526	-0.00596482
528	-0.00353356
528.5	0.00309503
529	0.00825324
529.1	0.00486066
529.2	0.00778693
529.3	0.0140412
529.4	0.0172578
529.5	0.0172202
529.6	0.0224984
529.7	0.0259662
529.8	0.0246154
529.9	0.0242389
530	0.0269557
530.1	0.0322135
530.2	0.041715
530.3	0.0598892
530.4	0.0762451
530.5	0.0963922
530.6	0.1395
530.7	0.206021
530.8	0.325669
530.9	0.522769
531	0.777658
531.1	1.05127
531.2	1.27632
531.3	1.3976
531.4	1.45464
531.5	1.45797
531.6	1.41756
531.7	1.38115
531.8	1.37436
531.9	1.39351

532	1.41493
532.1	1.4178
532.2	1.40778
532.3	1.3862
532.4	1.33323
532.5	1.27151
532.6	1.20004
532.7	1.10902
532.8	1.05416
532.9	1.02357
533	0.986195
533.1	0.951189
533.2	0.935556
533.3	0.933112
533.4	0.929805
533.5	0.946336
533.6	0.962899
533.7	0.968904
533.8	0.993971
533.9	1.00978
534	1.01324
534.1	1.02735
534.2	1.04034
534.3	1.05243
534.4	1.06802
534.5	1.08606
534.6	1.11656
534.7	1.15189
534.8	1.18266
534.9	1.2367
535	1.28955
535.1	1.33058
535.2	1.3985
535.3	1.46
535.4	1.5063
535.5	1.5548
535.6	1.58866
535.7	1.61737
535.8	1.65016
535.9	1.67212
536	1.66874
536.1	1.64258
536.2	1.60956
536.3	1.58072
536.4	1.53995
536.5	1.48427

536.6	1.44339
536.7	1.42519
536.8	1.42301
536.9	1.42681
537	1.43237
537.1	1.42309
537.2	1.40162
537.3	1.39262
537.4	1.36309
537.5	1.31169
537.6	1.25954
537.7	1.19115
537.8	1.12528
537.9	1.06663
538	0.987228
538.1	0.912567
538.2	0.850213
538.3	0.786652
538.4	0.723466
538.5	0.674527
538.6	0.642038
538.7	0.609716
538.8	0.576586
538.9	0.549088
539	0.532184
539.1	0.521176
539.2	0.50535
539.3	0.491458
539.4	0.499242
539.5	0.49868
539.6	0.493624
539.7	0.503533
539.8	0.504663
539.9	0.504156
540	0.511193
540.5	0.549337
541	0.700057
541.5	0.850274
542	0.80741
542.5	0.78212
543	0.842635
543.5	0.897984
544	0.88393
544.5	0.882075
545	0.899209
545.5	0.91451

546	0.913204
546.5	0.883089
547	0.863568
547.5	0.877811
548	0.897244
548.5	0.917828
549	0.93923
549.5	0.950428
550	0.933492
551	0.910227
552	0.907209
553	0.913455
554	0.912551
555	0.91404
556	0.922064
557	0.91129
558	0.929148
559	0.924132
560	0.914742
561	0.911278
562	0.958954
563	0.96377
564	0.962406
565	0.952428
566	0.93785
567	0.942517
568	0.929028
569	0.888139
570	0.860565
572.5	0.767673
575	0.762786
577.5	0.789635
580	0.807673
582.5	0.835881
585	0.825048

Ce₂O₃

Energy (eV)	Intensity
524	0.00887971
525	0.00764317
526	0.00955002
527	0.0108527
528	0.0176889
528.151	0.0279987
528.302	0.0202388
528.453	0.0200119

528.604	0.0315211
528.755	0.0365153
528.906	0.0372266
529.057	0.0323253
529.208	0.0380962
529.359	0.0614945
529.51	0.0816357
529.661	0.0973967
529.812	0.117302
529.963	0.145325
530.114	0.169566
530.265	0.177323
530.416	0.202423
530.567	0.203844
530.718	0.219815
530.869	0.238919
531.02	0.321188
531.171	0.502103
531.322	0.847247
531.473	1.17781
531.624	1.31091
531.775	1.33544
531.926	1.31219
532.077	1.29173
532.228	1.30033
532.379	1.34219
532.53	1.3743
532.681	1.33586
532.832	1.28142
532.983	1.2096
533.134	1.14191
533.285	1.07638
533.436	1.03077
533.587	1.00188
533.738	0.993678
533.889	1.00362
534.04	1.03155
534.191	1.06173
534.342	1.10679
534.493	1.12395
534.644	1.14916
534.795	1.19087
534.946	1.20257
535.097	1.21401
535.248	1.21543
535.399	1.21662

535.55	1.20659
535.701	1.21621
535.852	1.22761
536.003	1.24551
536.154	1.27807
536.305	1.32019
536.456	1.3481
536.607	1.39704
536.758	1.4485
536.909	1.49652
537.06	1.53722
537.211	1.52795
537.362	1.52845
537.513	1.49443
537.664	1.46186
537.815	1.39761
537.966	1.3257
538.117	1.23274
538.268	1.18246
538.419	1.08357
538.57	1.02393
538.721	0.966551
539.174	0.805315
539.325	0.776884
539.476	0.763437
539.627	0.731042
539.778	0.713275
539.929	0.712202
540.08	0.694579
540.231	0.685149
540.382	0.711553
540.533	0.71687
540.684	0.731402
540.835	0.737363
540.986	0.780344
541.137	0.804803
541.288	0.844248
541.439	0.870347
541.59	0.910197
541.741	0.932522
541.892	0.921723
542.043	0.921088
542.194	0.899866
542.345	0.866106
542.496	0.8626
542.647	0.850356

542.798	0.861835
542.949	0.852632
543.1	0.867769
543.251	0.893521
543.402	0.899944
543.553	0.931516
543.704	0.920654
543.855	0.923446
544.006	0.926596
544.157	0.922599
544.308	0.901719
544.459	0.908029
544.61	0.896553
544.761	0.902722
544.912	0.894953
545.063	0.901313
545.214	0.914631
545.365	0.932153
545.516	0.919851
545.667	0.93025
545.818	0.918258
545.969	0.935166
546.12	0.931818
546.271	0.917596
546.422	0.943576
546.573	0.921757
546.724	0.892387
546.875	0.898731
547.026	0.902416
547.177	0.907385
547.328	0.910217
547.479	0.907659
547.63	0.900068
547.781	0.894068
547.932	0.891631
548.083	0.899097
548.234	0.901482
548.385	0.90173
548.536	0.904567
548.687	0.916428
548.838	0.911692
548.989	0.907454
549.14	0.914568
549.291	0.932107
549.442	0.920938
549.593	0.927674

549.744	0.92959
549.895	0.922484
550.046	0.927108
551.034	0.938882
552.068	0.922316
553.102	0.89811
554.136	0.907816
555.17	0.904987
556.204	0.914533
557.238	0.901974
558.272	0.902643
559.306	0.937341
560.34	0.939793
561.374	0.93239
562.408	0.94681
563.442	0.946743
564.476	0.952017
565.51	0.94848
566.544	0.926869
567.578	0.931328
568.612	0.909663
569.646	0.878092
570.68	0.847061
571.714	0.842146
572.748	0.808041
573.782	0.809905
574.816	0.768544
575.85	0.792619
576.884	0.767437
577.918	0.780121
578.952	0.809489
579.986	0.8104
581.02	0.814695
582.593	0.814373
585.186	0.839172

Pr₂O₃

Energy (eV)	Intensity
524	-0.0264018
526	-0.0200356
528	-0.0167341
528.152	-0.0154923
528.304	0.019233
528.456	0.0251262
528.608	0.0373688
528.76	-0.00100797

528.912	0.0140567
529.064	0.0249945
529.216	0.0435459
529.368	0.0409804
529.52	0.0406032
529.672	0.0404383
529.824	0.053074
529.976	0.073216
530.128	0.0739474
530.28	0.114752
530.432	0.140352
530.584	0.161775
530.736	0.187787
530.888	0.260289
531.04	0.356646
531.192	0.585996
531.344	0.908819
531.496	1.19641
531.648	1.38143
531.8	1.42128
531.952	1.40152
532.104	1.36508
532.256	1.39604
532.408	1.42739
532.56	1.41841
532.712	1.35531
532.864	1.32508
533.016	1.2563
533.168	1.24505
533.32	1.2044
533.472	1.2206
533.624	1.18873
533.776	1.15711
533.928	1.16096
534.08	1.16748
534.232	1.19172
534.384	1.1762
534.536	1.2181
534.688	1.18785
534.84	1.17835
534.992	1.21515
535.144	1.15253
535.296	1.20852
535.448	1.21504
535.6	1.18924
535.752	1.22083

535.904	1.23919
536.056	1.26233
536.208	1.32994
536.36	1.33164
536.512	1.40606
536.664	1.39146
536.816	1.41492
536.968	1.39224
537.12	1.43279
537.272	1.39145
537.424	1.37733
537.576	1.35261
537.728	1.3063
537.88	1.24007
538.032	1.23566
538.184	1.15884
538.336	1.07953
538.488	1.00979
538.64	0.97631
538.792	0.912808
538.944	0.864015
539.096	0.846156
539.248	0.810135
539.4	0.798296
539.552	0.759999
539.704	0.77763
539.856	0.749566
540.008	0.769815
540.16	0.756827
540.312	0.76038
540.464	0.776338
540.616	0.806036
540.768	0.813411
540.92	0.842927
541.072	0.878017
541.224	0.881154
541.376	0.952963
541.528	0.936054
541.68	0.97201
541.832	0.964602
541.984	0.961198
542.136	0.937172
542.288	0.955517
542.44	0.924242
542.592	0.909221
542.744	0.91914

542.896	0.938351
543.048	0.973578
543.2	0.976826
543.352	1.04074
543.504	1.0119
543.656	1.0246
543.808	1.03088
543.96	1.04096
544.112	1.01788
544.264	1.00462
544.416	0.993478
544.568	0.979928
544.72	0.964861
544.872	0.957619
545.024	0.996805
545.176	0.997703
545.328	0.97455
545.48	1.00175
545.632	1.01812
545.784	1.01766
545.936	1.01762
546.088	1.05379
546.24	1.00421
546.392	1.06005
546.544	1.03441
546.696	1.01883
546.848	1.0051
547	0.960076
547.152	0.976579
547.304	0.936369
547.456	0.932904
547.608	0.924676
547.76	0.959998
547.912	0.931201
548.064	0.898897
548.216	0.907944
548.368	0.90846
548.52	0.893405
548.672	0.929698
548.824	0.912157
548.976	0.89972
549.128	0.872053
549.28	0.882438
549.432	0.886203
549.584	0.887639
549.736	0.903338

549.888	0.92791
550.04	0.925579
550.192	0.948268
551.034	0.856499
552.068	0.886148
553.102	0.845291
554.136	0.913356
555.17	0.90835
556.204	0.935926
557.238	0.86727
558.272	0.855614
559.306	0.963376
560.34	0.909976
561.374	0.930772
562.408	0.920084
563.442	0.943261
564.476	0.947859
565.51	0.99543
566.544	0.944129
567.578	0.929129
568.612	0.907928
569.646	0.893115
570.68	0.875792
571.714	0.799692
572.748	0.810613
573.782	0.780109
574.816	0.767536
575.85	0.756693
576.884	0.780453
577.918	0.790033
578.952	0.789436
579.986	0.788164
581.02	0.816104
582.667	0.823053
585.334	0.845977

Nd₂O₃

Energy (eV)	Intensity
524	-0.0033575
525	-0.0108477
526	0.0120479
527	-0.00182028
528	0.0131415
528.5	0.00992833
529	0.0207566
529.5	0.0262073

530	0.0350809
530.15	0.0310504
530.3	0.0474045
530.45	0.0344916
530.6	0.0531185
530.75	0.0668212
530.9	0.0719201
531.05	0.153127
531.2	0.276501
531.35	0.433992
531.5	0.591795
531.65	0.693133
531.8	0.745671
531.95	0.773398
532.1	0.813685
532.25	0.849971
532.4	0.913415
532.55	0.984126
532.7	1.04994
532.85	1.07454
533	1.10447
533.15	1.0719
533.3	1.08664
533.45	1.12971
533.6	1.1949
533.75	1.23655
533.9	1.22973
534.05	1.24841
534.2	1.17562
534.35	1.1726
534.5	1.17585
534.65	1.15667
534.8	1.18206
534.95	1.21965
535.1	1.22586
535.25	1.2788
535.4	1.30072
535.55	1.34676
535.7	1.37307
535.85	1.40586
536	1.41044
536.15	1.46324
536.3	1.51128
536.45	1.50877
536.6	1.51404
536.75	1.49311

536.9	1.50918
537.05	1.49875
537.2	1.42652
537.35	1.3996
537.5	1.36352
537.65	1.28228
537.8	1.26916
537.95	1.25647
538.1	1.22786
538.25	1.18047
538.4	1.12979
538.55	1.12296
538.7	1.11139
538.85	1.08272
539	1.07265
539.15	1.04415
539.3	1.01627
539.45	0.965427
539.6	0.953971
539.75	0.949326
539.9	0.911198
540.05	0.90573
540.55	0.894364
541.05	0.855171
541.55	0.873251
542.05	0.883963
542.55	0.872315
543.05	0.868592
543.55	0.875085
544.05	0.866018
544.55	0.876219
545.05	0.861391
545.55	0.834164
546.05	0.83071
546.55	0.83304
547.05	0.787585
547.55	0.785776
548.05	0.79032
548.55	0.796023
549.05	0.796518
549.55	0.789469
550.05	0.785612
551.05	0.825214
552.05	0.823429
553.05	0.845413
554.05	0.892956

555.05	0.892184
556.05	0.878926
557.05	0.902302
558.05	0.93632
559.05	0.939046
560.05	0.938274
561.05	0.938901
562.05	0.927787
563.05	0.920677
564.05	0.919862
565.05	0.915929
566.05	0.899637
567.05	0.882673
568.05	0.881063
569.05	0.871904
570.05	0.859549
572.55	0.853759
575.05	0.827701
577.55	0.832532
580.05	0.829301
582.55	0.797054
585.05	0.815722

Sm₂O₃

Energy (eV)	Intensity
525	-0.00350485
527	0.00932857
527.5	-0.00791966
528	0.00622344
528.5	-0.0067486
529	-0.00280317
529.1	0.0158691
529.2	0.00324203
529.3	-0.00359093
529.4	0.027815
529.5	0.00887391
529.6	0.00543006
529.7	0.00665155
529.8	-0.001829
529.9	0.0216352
530	0.0393302
530.1	0.00897129
530.2	0.0252758
530.3	0.0281698
530.4	0.0484715
530.5	0.081397

530.6	0.132666
530.7	0.199652
530.8	0.293695
530.9	0.422817
531	0.596665
531.1	0.740984
531.2	0.915304
531.3	1.06968
531.4	1.20736
531.5	1.30232
531.6	1.3841
531.7	1.43724
531.8	1.48567
531.9	1.53872
532	1.56842
532.1	1.61926
532.2	1.68122
532.3	1.7087
532.4	1.73668
532.5	1.74792
532.6	1.75634
532.7	1.74187
532.8	1.6895
532.9	1.65601
533	1.56639
533.1	1.50164
533.2	1.42128
533.3	1.35491
533.4	1.31284
533.5	1.26247
533.6	1.21532
533.7	1.20002
533.8	1.19811
533.9	1.18731
534	1.18864
534.1	1.17329
534.2	1.17489
534.3	1.16183
534.4	1.19154
534.5	1.17333
534.6	1.16049
534.7	1.16768
534.8	1.1564
534.9	1.14396
535	1.15967
535.1	1.13293

535.2	1.13183
535.3	1.12921
535.4	1.13252
535.5	1.14985
535.6	1.15652
535.7	1.13558
535.8	1.1366
535.9	1.15716
536	1.18221
536.1	1.19848
536.2	1.20268
536.3	1.23355
536.4	1.25022
536.5	1.28773
536.6	1.32084
536.7	1.31574
536.8	1.34035
536.9	1.32075
537	1.35565
537.1	1.34884
537.2	1.3787
537.3	1.35697
537.4	1.39622
537.5	1.37295
537.6	1.37202
537.7	1.37127
537.8	1.36837
537.9	1.3701
538	1.34605
538.1	1.35441
538.2	1.32298
538.3	1.29218
538.4	1.25107
538.5	1.22417
538.6	1.19842
538.7	1.16522
538.8	1.08799
538.9	1.09103
539	1.02762
539.1	1.00004
539.2	0.965779
539.3	0.912468
539.4	0.908276
539.5	0.886405
539.6	0.841839
539.7	0.82317

539.8	0.830681
539.9	0.836604
540	0.806191
541	0.903006
542	0.907972
543	0.852606
544	0.774411
545	0.703414
546	0.680804
547	0.716494
548	0.778965
549	0.878385
550	0.955155
551	0.946262
552	0.964623
553	0.942926
554	0.919286
555	0.914704
556	0.931489
557	0.909076
558	0.920857
559	0.930843
560	0.902939
561	0.889446
562	0.871911
563	0.844528
564	0.861148
565	0.841914
566	0.898365
567	0.91275
568	0.922111
569	0.921906
570	0.939294
575	0.834966
580	0.810528
585	0.805777

Eu₂O₃

Energy (eV)	Intensity
524	0.00997367
526	-0.0089689
528	-0.00569237
528.5	-0.00142252
529	0.0036652
529.5	0.0194393

530	0.0457511
530.15	0.0670211
530.3	0.0977168
530.45	0.123093
530.6	0.137806
530.75	0.145396
530.9	0.162992
531.05	0.189331
531.2	0.251771
531.35	0.351468
531.5	0.457509
531.65	0.559519
531.8	0.639082
531.95	0.698443
532.1	0.757549
532.25	0.811066
532.4	0.864731
532.55	0.904187
532.7	0.92258
532.85	0.922359
533	0.894282
533.15	0.850235
533.3	0.797955
533.45	0.763878
533.6	0.741125
533.75	0.729577
533.9	0.735152
534.05	0.745072
534.2	0.752513
534.35	0.762431
534.5	0.771879
534.65	0.768577
534.8	0.765013
534.95	0.776842
535.1	0.784071
535.25	0.800051
535.4	0.81736
535.55	0.840001
535.7	0.870451
535.85	0.906395
536	0.947476
536.15	1.00576
536.3	1.06459
536.45	1.15569
536.6	1.19688
536.75	1.22792

536.9	1.25251
537.05	1.26661
537.2	1.27169
537.35	1.2791
537.5	1.26648
537.65	1.27925
537.8	1.27932
537.95	1.2822
538.1	1.26571
538.25	1.25173
538.4	1.22892
538.55	1.20369
538.7	1.17333
538.85	1.1333
539	1.10226
539.15	1.0716
539.3	1.03545
539.45	1.01267
539.6	0.988881
539.75	0.96952
539.9	0.94947
540.05	0.944442
541.05	0.947932
542.05	0.929167
543.05	0.885795
544.05	0.859805
545.05	0.803199
546.05	0.788369
547.05	0.79095
548.05	0.788063
549.05	0.813824
550.05	0.845575
551.05	0.859829
552.05	0.837886
553.05	0.827014
554.05	0.823043
555.05	0.836562
556.05	0.862493
557.05	0.879224
558.05	0.889904
559.05	0.907618
560.05	0.916751
561.05	0.913927
562.05	0.914528
563.05	0.911012
564.05	0.909164

565.05	0.896398
566.05	0.877862
567.05	0.870659
568.05	0.867524
569.05	0.874502
570.05	0.870556
575.05	0.844824
580.05	0.822752
585.05	0.839524

Gd₂O₃

Energy (eV)	Intensity
524	-0.0121538
526	-0.00384667
528	0.0040069
528.5	-0.000780847
529	0.0070106
529.5	0.00232775
530	0.0118374
530.1	0.0143343
530.2	0.0197312
530.3	0.0283288
530.4	0.036604
530.5	0.0417136
530.6	0.0477806
530.7	0.058123
530.8	0.0740749
530.9	0.0964713
531	0.125426
531.1	0.160402
531.2	0.205156
531.3	0.262705
531.4	0.324135
531.5	0.387514
531.6	0.459735
531.7	0.530343
531.8	0.591371
531.9	0.656381
532	0.725802
532.1	0.790194
532.2	0.853072
532.3	0.917007
532.4	0.977937
532.5	1.03269
532.6	1.07749
532.7	1.10505

532.8	1.11532
532.9	1.11593
533	1.11397
533.1	1.11494
533.2	1.12174
533.3	1.13421
533.4	1.1508
533.5	1.17159
533.6	1.1945
533.7	1.21472
533.8	1.22997
533.9	1.24234
534	1.26077
534.1	1.28672
534.2	1.31502
534.3	1.34206
534.4	1.36389
534.5	1.37586
534.6	1.3793
534.7	1.37726
534.8	1.36826
534.9	1.35634
535	1.3503
535.1	1.34857
535.2	1.34784
535.3	1.34885
535.4	1.35257
535.5	1.36011
535.6	1.37353
535.7	1.39176
535.8	1.41014
535.9	1.42897
536	1.44914
536.1	1.46734
536.2	1.48242
536.3	1.49516
536.4	1.50392
536.5	1.5027
536.6	1.4825
536.7	1.4618
536.8	1.4589
536.9	1.44515
537	1.41575
537.1	1.39497
537.2	1.37443
537.3	1.34353

537.4	1.31201
537.5	1.28504
537.6	1.26302
537.7	1.24665
537.8	1.23424
537.9	1.22124
538	1.20624
538.1	1.19045
538.2	1.17735
538.3	1.16555
538.4	1.15087
538.5	1.13799
538.6	1.12873
538.7	1.11678
538.8	1.10538
538.9	1.10069
539	1.09903
539.1	1.09513
539.2	1.08533
539.3	1.07358
539.4	1.06525
539.5	1.06209
539.6	1.05804
539.7	1.04515
539.8	1.02961
539.9	1.01805
540	1.01251
541	1.01045
542	0.965594
543	0.928094
544	0.895242
545	0.856931
546	0.848626
547	0.831517
548	0.846451
549	0.847273
550	0.861483
551	0.87507
552	0.884344
553	0.892448
554	0.888043
555	0.894197
556	0.899056
557	0.913723
558	0.936986
559	0.943534

560	0.964255
561	0.954447
562	0.952176
563	0.939941
564	0.934142
565	0.913658
566	0.891082
567	0.88025
568	0.86662
569	0.852656
570	0.853479
575	0.8202
580	0.777715
585	0.796616

Tb₂O₃

Energy (eV)	Intensity
524	-0.00676351
525	0.0306259
526	-0.00135134
527	0.00704281
528	-0.00655657
528.254	-0.0131184
528.508	-0.0190439
528.762	-0.00357781
529.016	-0.00460703
529.27	0.000175158
529.524	0.0131867
529.778	0.0276738
530.032	0.0421098
530.286	0.0499271
530.54	0.0781685
530.794	0.121303
531.048	0.218481
531.302	0.49803
531.556	0.904767
531.81	1.17163
532.064	1.26819
532.318	1.34341
532.572	1.39894
532.826	1.40608
533.08	1.35641
533.334	1.24661
533.588	1.12713
533.842	1.06107
534.096	1.04043

534.35	1.00849
534.604	1.00383
534.858	0.986253
535.112	0.959612
535.366	0.965189
535.62	0.949509
535.874	0.996474
536.128	1.09391
536.382	1.16088
536.636	1.3075
536.89	1.3704
537.144	1.44939
537.398	1.50697
537.652	1.5493
537.906	1.59736
538.16	1.61544
538.414	1.591
538.668	1.51304
538.922	1.42887
539.176	1.33983
539.43	1.27596
539.684	1.21858
539.938	1.18526
540.192	1.17485
540.446	1.14368
540.7	1.13072
540.954	1.13096
541.208	1.13799
541.462	1.13874
541.716	1.1474
541.97	1.14998
542.224	1.11394
542.478	1.07375
542.732	1.02758
542.986	0.996465
543.24	0.988834
543.494	0.955187
543.748	0.935658
544.002	0.939431
544.256	0.934859
544.51	0.920338
544.764	0.880102
545.018	0.853387
545.272	0.838516
547.561	0.813679
550.122	0.94278

552.683	0.958127
555.244	0.921385
557.805	0.936957
560.366	0.952567
562.927	0.925277
565.488	0.894122
568.049	0.902732
570.61	0.906672
573.171	0.886356
575.732	0.852448
578.293	0.816312
580.854	0.80169
583.415	0.783923
585.976	0.826927

Dy₂O₃

Energy (eV)	Intensity
524	-0.0265217
525	-0.0166508
526	-0.00433616
527	0.0175237
528	0.00832662
528.254	0.0149471
528.508	0.0154803
528.762	0.0430676
529.016	0.0108576
529.27	0.0207352
529.524	0.0191513
529.778	0.0303579
530.032	0.0250131
530.286	0.0577167
530.54	0.0792241
530.794	0.133234
531.048	0.176017
531.302	0.299598
531.556	0.540067
531.81	0.86363
532.064	1.00005
532.318	1.1
532.572	1.15261
532.826	1.21152
533.08	1.22379
533.334	1.20985
533.588	1.11051
533.842	0.981499
534.096	0.912912

534.35	0.899434
534.604	0.882724
535.112	0.912755
535.366	0.944487
535.62	0.952816
535.874	0.934105
536.128	0.969534
536.382	1.0571
536.636	1.12186
536.89	1.18222
537.144	1.28412
537.398	1.31425
537.652	1.32507
537.906	1.40815
538.16	1.41934
538.414	1.46515
538.668	1.5338
538.922	1.44247
539.176	1.3949
539.43	1.35885
539.684	1.30369
539.938	1.24087
540.192	1.23053
540.446	1.17175
540.7	1.16105
540.954	1.15466
541.208	1.15783
541.462	1.12072
541.716	1.11554
541.97	1.09838
542.224	1.07544
542.478	1.02399
542.732	1.0484
542.986	1.04041
543.24	1.01999
543.494	0.973404
543.748	1.00712
544.002	0.978998
544.256	0.970774
544.51	0.954165
544.764	0.929506
545.018	0.925195
545.272	0.916965
547.561	0.848187
550.122	0.860773
552.683	0.931223

555.244	0.903619
557.805	0.865488
560.366	0.950519
562.927	0.888382
565.488	0.847669
568.049	0.927983
570.61	0.854007
573.171	0.880382
575.732	0.849831
578.293	0.81624
580.854	0.789999
583.415	0.765216
585.976	0.766846

H₂O₃

Energy (eV)	Intensity
524	-0.00553312
525	-0.00518654
525.203	0.000462507
525.406	0.00233016
525.609	0.00204353
525.812	0.00358483
526.015	0.00831908
526.218	0.00143157
526.421	0.00406877
526.624	0.0108406
526.827	0.0112629
527.03	0.0175088
527.233	0.0239325
527.436	0.0291226
527.639	0.0293139
527.842	0.0254551
528.045	0.0324939
528.248	0.0331498
528.451	0.0342489
528.654	0.0319987
528.857	0.0347454
529.06	0.0372876
529.263	0.0400707
529.466	0.0419009
529.669	0.0490636
529.872	0.0584688
530.075	0.0603987
530.278	0.0655106
530.481	0.0784249
530.684	0.0942576

530.887	0.122597
531.09	0.152843
531.293	0.186696
531.496	0.267071
531.699	0.461036
531.902	0.739054
532.105	1.02588
532.308	1.18637
532.511	1.21213
532.714	1.26376
532.917	1.33436
533.12	1.39905
533.323	1.43569
533.526	1.40455
533.729	1.30497
533.932	1.19388
534.135	1.0947
534.338	1.02379
534.541	0.979445
534.744	0.953551
534.947	0.952796
535.15	0.957161
535.353	0.950048
535.556	0.945731
535.759	0.94106
535.962	0.941225
536.165	0.966881
536.368	0.986624
536.571	1.00894
536.774	1.08571
536.977	1.12675
537.18	1.21707
537.52	1.33845
538.04	1.46747
538.56	1.61065
539.08	1.58674
539.6	1.38054
540.12	1.22876
540.64	1.14017
541.16	1.09894
541.68	1.09167
542.2	1.05913
542.72	0.996679
543.24	0.91311
543.76	0.872446
544.28	0.867874

544.8	0.843987
545.32	0.802501
545.84	0.760872
546.36	0.733209
546.88	0.711374
547.4	0.697251
547.92	0.704961
548.44	0.700104
548.96	0.713903
549.48	0.747709
550	0.769679
550.52	0.80142
553.125	0.839594
556.25	0.811843
559.375	0.853744
562.5	0.874114
565.625	0.828905
568.75	0.818998
571.875	0.811427
575	0.78448
578.125	0.736683
581.25	0.692621
584.375	0.682073

Er₂O₃

Energy (eV)	Intensity
524	0.00118726
525	-0.0131642
526	-0.0084489
527	0.0316565
528	-0.0124216
529	-0.028574
529.154	-0.0344616
529.308	-0.0455612
529.462	-0.0519374
529.616	-0.0256872
529.77	-0.00329471
529.924	-0.00757178
530.078	-0.00772226
530.232	0.0038719
530.386	0.0196156
530.54	0.0295117
530.694	0.0438074
530.848	0.0680339
531.002	0.0973036
531.156	0.127603

531.31	0.153168
531.464	0.174603
531.618	0.217278
531.772	0.307974
531.926	0.457124
532.08	0.63997
532.234	0.829719
532.388	0.991483
532.542	1.07618
532.696	1.09953
532.85	1.11422
533.004	1.16661
533.158	1.23169
533.312	1.28436
533.466	1.34055
533.62	1.38559
533.774	1.38089
533.928	1.29499
534.082	1.198
534.236	1.12169
534.39	1.04195
534.544	1.0033
534.698	0.988081
534.852	0.939627
535.006	0.908801
535.16	0.91259
535.314	0.92512
535.468	0.925815
535.622	0.931826
535.776	0.950804
535.93	0.926452
536.084	0.905327
536.238	0.927544
536.392	0.920289
536.546	0.925536
536.7	0.975092
536.854	1.00657
537.008	1.05447
537.162	1.13306
537.257	1.17021
537.514	1.24998
537.771	1.34119
538.028	1.4207
538.285	1.51412
538.542	1.58162
538.799	1.66844

539.056	1.74376
539.313	1.70747
539.57	1.62833
539.827	1.51668
540.084	1.43051
540.341	1.31817
540.598	1.25084
540.855	1.23691
541.112	1.20656
541.369	1.17618
541.626	1.15447
541.883	1.13947
542.14	1.13692
542.397	1.10735
542.654	1.08381
542.911	1.06013
543.168	1.04113
543.425	1.02403
543.682	0.993335
543.939	0.984516
544.196	0.968332
544.453	0.953258
544.71	0.934591
544.967	0.916931
545.224	0.897499
545.481	0.870332
545.738	0.857518
545.995	0.831083
546.252	0.818574
548.039	0.787387
550.078	0.816813
552.117	0.926822
554.156	0.928804
556.195	0.930016
558.234	0.933399
560.273	0.945101
562.312	0.938421
564.351	0.929072
566.39	0.900859
568.429	0.897763
570.468	0.906268
572.507	0.923
574.546	0.89618
576.585	0.879802
578.624	0.833824
580.663	0.781541

582.702	0.794227
584.741	0.796826

Tm₂O₃

Energy (eV)	Intensity
524	-0.0037603
526	-0.00311857
528	0.00079827
528.5	-0.0024899
529	0.00975518
529.5	0.0224075
530	0.0303857
530.15	0.0292415
530.3	0.0531311
530.45	0.0663753
530.6	0.0622102
530.75	0.0782732
530.9	0.0896373
531.05	0.105908
531.2	0.145189
531.35	0.217185
531.5	0.333468
531.65	0.527416
531.8	0.723431
531.95	0.950855
532.1	1.13428
532.25	1.22662
532.4	1.27127
532.55	1.24
532.7	1.24398
532.85	1.28278
533	1.35674
533.15	1.38633
533.3	1.46929
533.45	1.48044
533.6	1.42036
533.75	1.34154
533.9	1.22045
534.05	1.10802
534.2	1.02447
534.35	0.962832
534.5	0.946172
534.65	0.93465
534.8	0.931361
534.95	0.943785
535.1	0.955712

535.25	0.961432
535.4	0.945878
535.55	0.952692
535.7	0.9539
535.85	0.994015
536	1.00756
536.15	0.992843
536.3	0.958634
536.45	0.959853
536.6	0.963252
536.75	0.97261
536.9	1.01167
537.05	1.03904
537.2	1.08889
537.35	1.10064
537.5	1.13667
537.65	1.1913
537.8	1.22668
537.95	1.27374
538.1	1.32567
538.25	1.35284
538.4	1.42201
538.55	1.47842
538.7	1.49875
538.85	1.50251
539	1.43073
539.15	1.37783
539.3	1.32711
539.45	1.24891
539.6	1.1984
539.75	1.16198
539.9	1.11606
540.05	1.09109
540.55	1.04955
541.05	1.07135
541.55	1.06315
542.05	1.06124
542.55	0.981106
543.05	0.886163
543.55	0.865598
544.05	0.829015
544.55	0.826036
545.05	0.800494
545.55	0.75581
546.05	0.720756
546.55	0.71872

547.05	0.716452
547.55	0.731931
548.05	0.716975
548.55	0.708099
549.05	0.729543
549.55	0.767902
550.05	0.82353
550.55	0.889371
551.05	0.907331
551.55	0.93844
552.05	0.920393
552.55	0.926095
553.05	0.932152
553.55	0.937475
554.05	0.942207
554.55	0.917709
555.05	0.925456
555.55	0.930365
556.55	0.910035
557.55	0.90214
558.55	0.902115
559.55	0.926584
560.55	0.938598
561.55	0.942597
566.55	0.869536
571.55	0.883212
576.55	0.89182
581.55	0.785989
586.55	0.796364

Yb₂O₃

Energy (eV)	Intensity
524	0.00562239
525	-0.00327203
526	-0.00657437
527	-0.0180598
528	-0.0217301
528.5	-0.0152925
529	0.000382454
529.5	0.0098191
530	0.0108838
530.15	0.0154033
530.3	0.0251195
530.45	0.0358687
530.6	0.0566082
530.75	0.0867505

530.9	0.114869
531.05	0.148177
531.2	0.175166
531.35	0.189934
531.5	0.22516
531.65	0.287546
531.8	0.402262
531.95	0.551627
532.1	0.728941
532.25	0.901101
532.4	1.04786
532.55	1.13418
532.7	1.14439
532.85	1.15193
533	1.18771
533.15	1.23745
533.3	1.29287
533.45	1.36074
533.6	1.38307
533.75	1.34303
533.9	1.25495
534.05	1.12947
534.2	1.01537
534.35	0.926021
534.5	0.879391
534.65	0.855137
534.8	0.848622
534.95	0.872242
535.1	0.884085
535.3	0.915088
535.55	0.90858
535.8	0.915134
536.05	0.93354
536.3	0.951214
536.55	0.95553
536.8	0.953891
537.05	0.961435
537.3	1.00115
537.55	1.06553
537.8	1.12795
538.05	1.19268
538.3	1.27301
538.55	1.38172
538.8	1.46446
539.05	1.51044
539.3	1.47475

539.55	1.36414
539.8	1.252
540.05	1.16083
540.3	1.12372
540.55	1.09629
540.8	1.0862
541.05	1.06878
541.3	1.06546
541.55	1.05745
541.8	1.06038
542.05	1.05942
542.3	1.03699
542.55	0.998796
542.8	0.954131
543.05	0.896165
543.3	0.87606
543.55	0.854223
543.8	0.864719
544.05	0.861452
544.3	0.864474
544.55	0.866455
544.8	0.859668
545.05	0.846838
545.3	0.820409
545.55	0.796371
545.8	0.775962
546.05	0.741654
547.05	0.701999
548.05	0.690594
549.05	0.698911
550.05	0.784214
551.05	0.856955
552.05	0.903499
553.05	0.92082
554.05	0.923574
555.05	0.902825
556.05	0.902347
557.05	0.899771
558.05	0.899513
559.05	0.904603
560.05	0.917769
561.05	0.909172
562.05	0.925137
563.05	0.935176
564.05	0.92124
565.05	0.89757

566.05	0.883793
567.05	0.871732
568.05	0.87334
569.05	0.880049
570.05	0.880947
575.05	0.883744
580.05	0.781639
585.05	0.825671

Lu₂O₃

Energy (eV)	Intensity
524	0.0736886
526	-0.0376244
528	0.0606047
528.5	-0.0156428
529	0.0586793
529.5	-0.0865301
530	-0.0173534
530.15	-0.0300323
530.3	-0.102934
530.45	-0.0445512
530.6	0.0354239
530.75	0.00385989
530.9	0.0101246
531.05	0.0705845
531.2	0.0815325
531.35	0.0349457
531.5	0.118607
531.65	0.180994
531.8	0.384455
531.95	0.611948
532.1	0.854124
532.25	1.12871
532.4	1.55361
532.55	1.59552
532.7	1.672
532.85	1.76046
533	1.72475
533.15	1.69479
533.3	1.67757
533.45	1.81167
533.6	1.84789
533.75	1.65436
533.9	1.64111
534.05	1.39892
534.2	1.19933

534.35	1.15565
534.5	1.10286
534.65	1.05116
534.8	1.05561
534.95	1.00097
535.1	1.05796
535.25	1.02633
535.4	0.954376
535.55	1.00707
535.7	1.07537
535.85	1.02314
536	1.0458
536.15	0.980701
536.3	1.02524
536.45	1.00801
536.6	1.00322
536.75	0.899984
536.9	0.927307
537.05	1.04403
537.2	1.03268
537.35	1.11085
537.5	1.21797
537.65	1.26745
537.8	1.27952
537.95	1.38339
538.1	1.39646
538.25	1.4647
538.4	1.5761
538.55	1.63038
538.7	1.71958
538.85	1.71279
539	1.85369
539.15	1.78214
539.3	1.65891
539.45	1.70503
539.6	1.57589
539.75	1.43859
539.9	1.48342
540.05	1.40637
540.55	1.29687
541.05	1.19611
541.55	1.14728
542.05	1.13197
542.55	0.960276
543.05	0.809862
543.55	0.736949

544.05	0.760003
544.55	0.746143
545.05	0.769746
545.55	0.697552
546.05	0.653498
546.55	0.638553
547.05	0.580182
547.55	0.585734
548.05	0.467017
548.55	0.584719
549.05	0.534121
549.55	0.630473
550.05	0.668516
550.55	0.632558
551.05	0.79725
551.55	0.898341
552.05	0.906154
552.55	0.841357
553.05	0.839008
553.55	0.960022
554.05	0.923729
554.55	0.895985
555.05	0.915415
555.55	0.902963
556.55	0.943772
557.55	0.86471
558.55	0.823517
559.55	0.943974
560.55	0.997478
561.55	0.919907
566.55	0.853905
571.55	1.05427
576.55	0.812711
581.55	0.767174
586.55	0.783393

References

- 1 W. C. Martin, R. Zalubas and L. Hagan, *Atomic Energy Levels – The Rare Earth Elements* NSRDS-NBS 60, U.S. Department of Commerce, Washington, DC, 1978.
- 2 L. Brewer, *Journal of the Optical Society of America*, 1971, **61**, 1666-1682.
- 3 T. C. Weng, G. S. Waldo and J. E. Penner-Hahn, *J. Synchrotron Rad.*, 2005, **12**, 506-510.