

Supporting Information for:

New Evidence for 5f Covalency in Actinocenes Determined From Carbon K-edge XAS and Electronic Structure Theory

Stefan G. Minasian,^{1,2} Jason M. Keith,² Enrique R. Batista,² Kevin S. Boland, David L. Clark,² Stosh A. Kozimor,^{2*} Richard L. Martin,² David K. Shuh,^{1*} Tolek Tylliszczak¹

¹ Lawrence Berkeley National Laboratory, Berkeley, CA 94720

² Los Alamos National Laboratory, Los Alamos, NM 87545

Table of Contents:

Figure S1	Kohn-Sham Molecular Orbitals for (C ₈ H ₈) ₂ Th.....	S2
Figure S2	Kohn-Sham Molecular Orbitals for (C ₈ H ₈) ₂ U	S3
Figure S3	Normalized C K-edge NEXAFS Spectra and 2 nd Derivative for (C ₈ H ₈) ₂ Th.....	S4
Figure S4	Normalized C K-edge NEXAFS Spectra and 2 nd Derivative for (C ₈ H ₈) ₂ U.....	S4
Figure S5	N _{5,4} -edge and 2 nd Derivative for (C ₈ H ₈) ₂ Th.....	S5
Figure S6	N _{5,4} -edge and 2 nd Derivative for (C ₈ H ₈) ₂ U	S5
Table S1	Normalized C K-edge NEXAFS spectra of (C ₈ H ₈) ₂ Th and (C ₈ H ₈) ₂ U	S6
Table S2	DFT Atomic Coordinates and Mulliken Populations for (C ₈ H ₈) ₂ Th.....	S18
Table S3	DFT Atomic Coordinates and Mulliken Populations for (C ₈ H ₈) ₂ U.....	S19

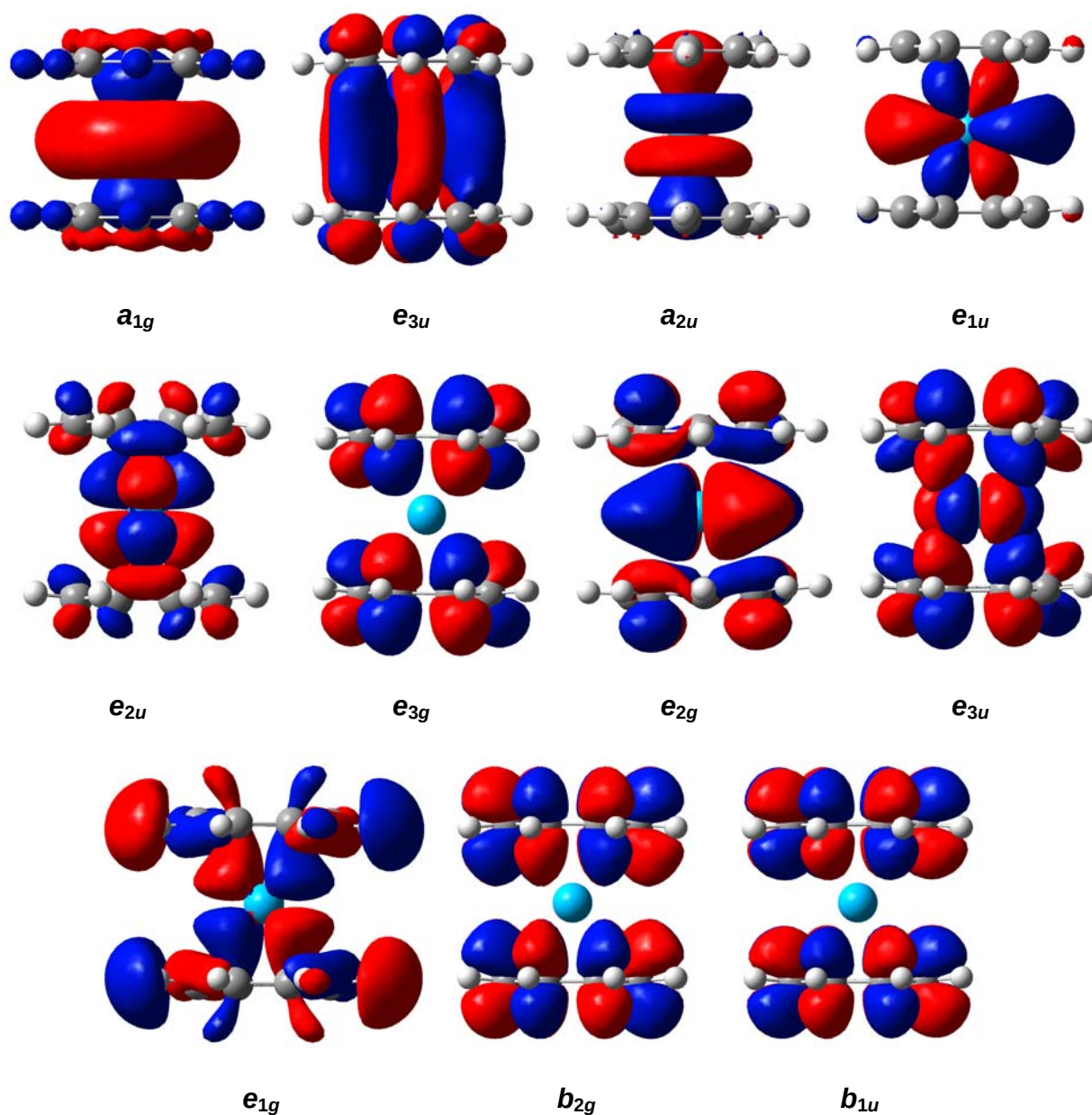


Figure S1. Kohn-Sham Molecular Orbitals for $(C_8H_8)_2Th$

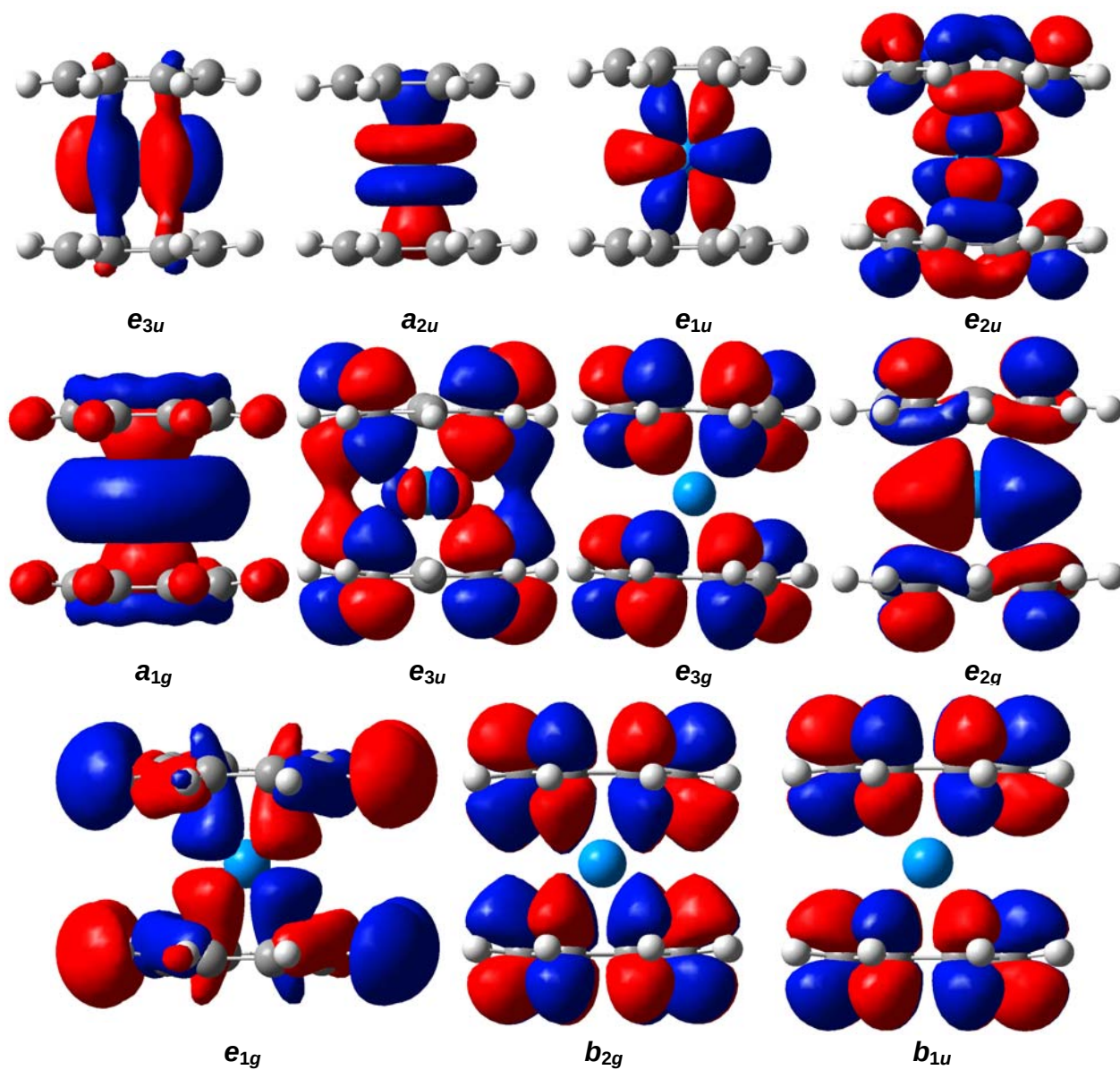


Figure S2. Kohn-Sham Molecular Orbitals for $(C_8H_8)_2U$

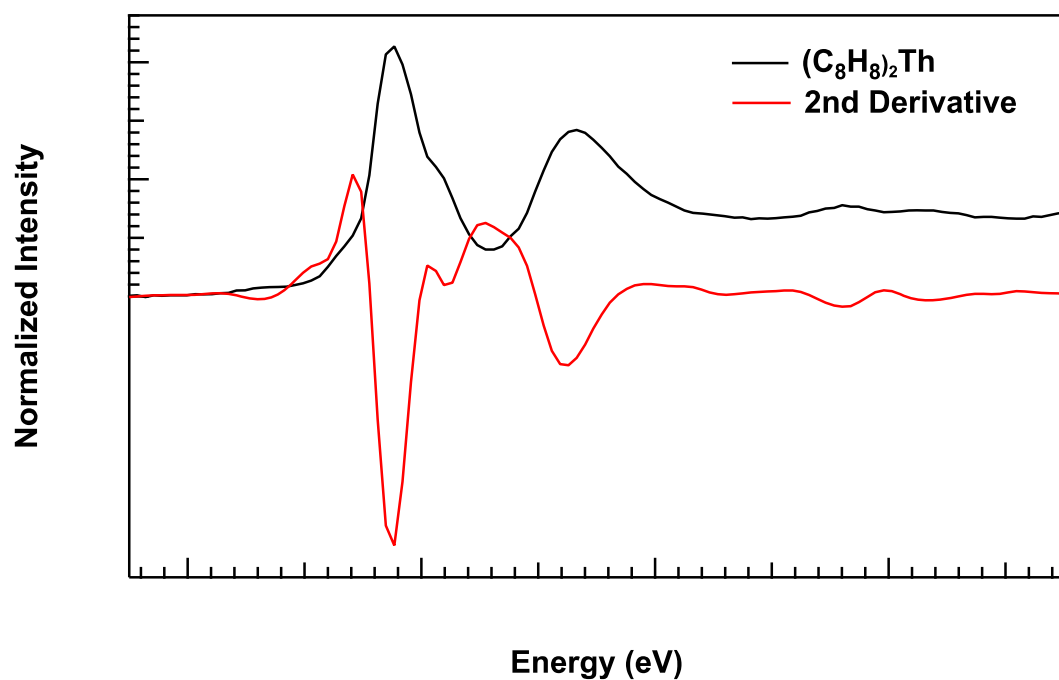


Figure S3. A plot of energy vs. normalized intensity for the C K-edge pre-edge spectrum of $(C_8H_8)_2Th$, (black) together with the second derivative (red) of the experimental data.

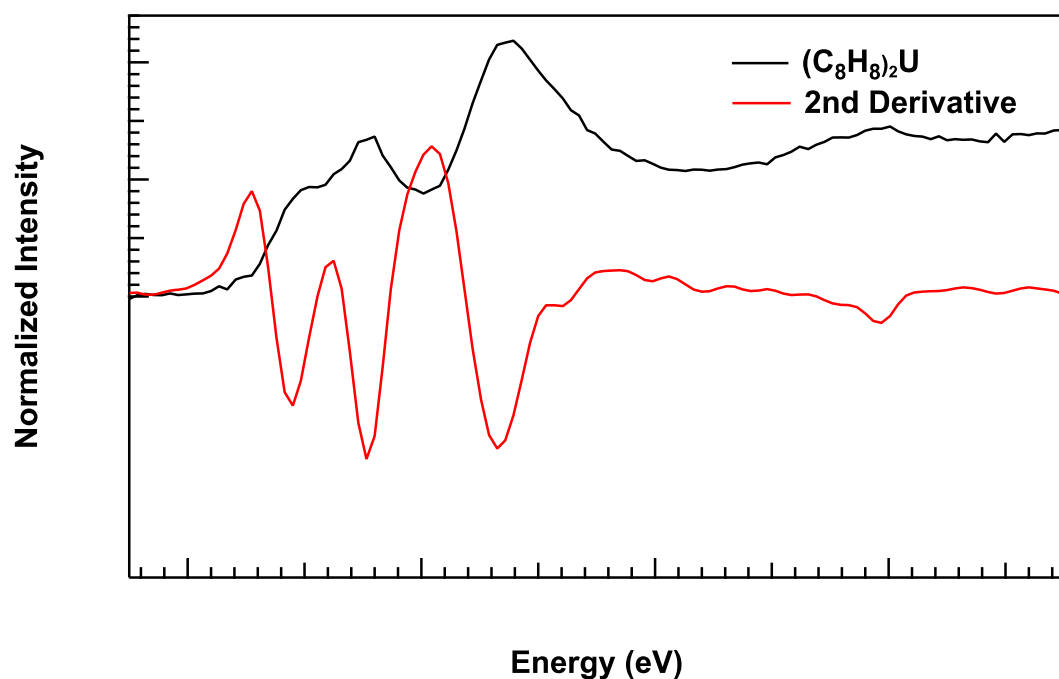


Figure S4. A plot of energy vs. normalized intensity for the C K-edge pre-edge spectrum of $(C_8H_8)_2U$, (black) together with the second derivative (red) of the experimental data.

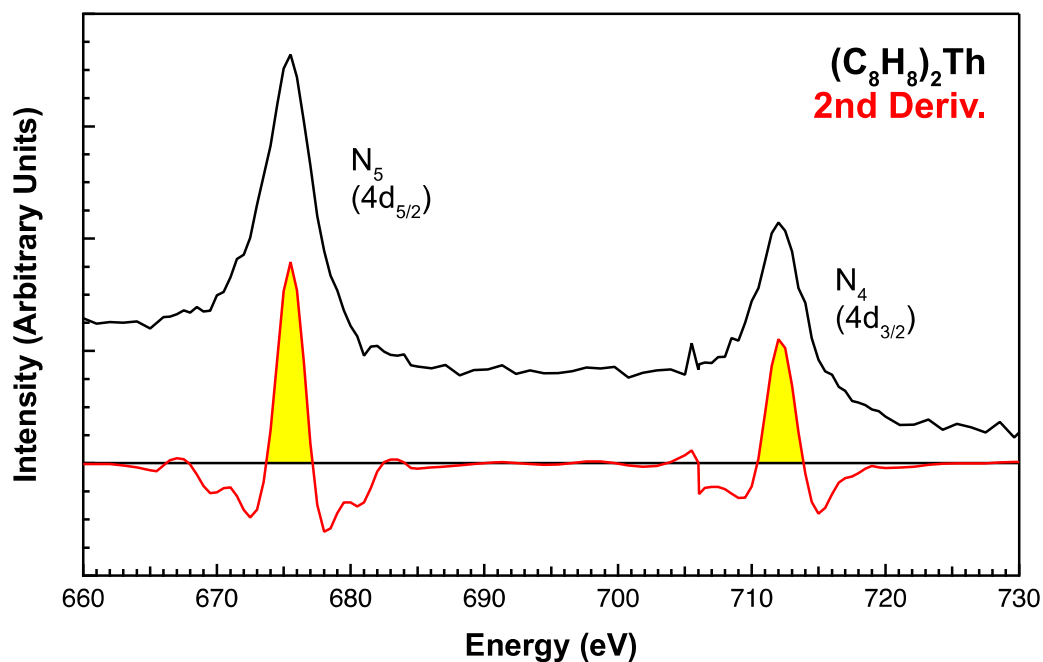


Figure S5. A plot of energy vs. intensity for the N_{5,4}-edge XAS (raw data) of (C₈H₈)₂Th (black), and second derivative (red) of the experimental data. The area of regions shaded in yellow were determined graphically and used in branching ratio determinations.

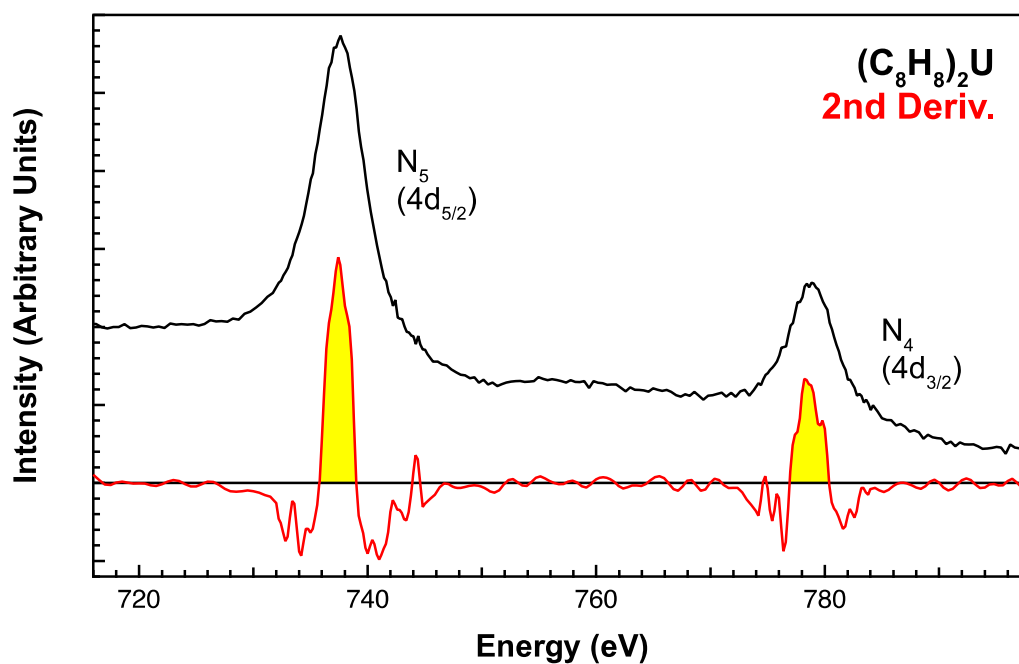


Figure S6. A plot of energy vs. intensity for the N_{5,4}-edge XAS (raw data) of (C₈H₈)₂U (black), and second derivative (red) of the experimental data. The area of regions shaded in yellow were determined graphically and used in branching ratio determinations.

Table S1. Normalized C K-edge XAS of (C₈H₈)₂Th and (C₈H₈)₂U.

COT2U_eV	COT2U_Int
260	-0.0029319635875387
261	-0.0111871187714129
262	-0.0142193907086876
263	-0.01699692895806
264	-0.00943197208191572
265	0.00652469962859191
266	0.00520861007473635
267	-0.00294579873604389
268	-0.00405096519546553
269	0.00494874780822558
270	-0.0103295462973909
271	0.00319243691234807
272	0.010033591041827
273	-0.00313945786169119
274	0.00116270992700096
275	-0.000473109934786815
275.263	-0.00418450590206642
275.526	0.000184231730628711
275.789	0.00505188302758382
276.052	-0.00696293191091596
276.315	0.00101464042313907
276.578	-0.0122830906985527
276.841	-0.00733199685656041
277.104	0.00261160822657996
277.367	0.00138812103214409
277.63	0.000482073723628011
277.893	-0.0088717004056416
278.156	-0.0040153710617602
278.419	0.00300459060453894
278.682	-0.0104325621702262
278.945	-0.000765816952235428
279.208	-0.00600554215203658
279.471	0.00683527610113807
279.734	0.00343472641157077
279.997	0.00256393423007511
280.07	-0.0018801815097382
280.14	0.000720803099824013
280.21	-0.000666502835086552
280.26	0.00261635809138581
280.28	-8.06156747428345e-06
280.35	0.000178119951510635
280.42	0.00195745549973064
280.49	0.00395795107858385
280.56	0.00463286246635856
280.63	0.00310735446566785
280.7	0.00269246642695763
280.77	0.00282156738320353

280.84	-0.00505671569173843
280.91	0.0138280148119169
280.98	-0.0078256265688501
281.05	0.00307465012936807
281.12	0.00341091652450728
281.19	0.00840712882131709
281.26	0.0109015653603202
281.33	0.00836897334508307
281.4	-0.00703929336090651
281.47	0.00996656922854322
281.54	-0.00104637851305209
281.61	0.00357542150687894
281.68	0.0143619382209378
281.75	0.00704861148118813
281.82	0.0113985963766404
281.89	0.0099957616930998
281.96	0.00223181428505035
282.03	0.00813785038733477
282.1	0.00177014444547358
282.17	0.0010272914097191
282.24	-0.00796655405340681
282.31	0.00896975639562485
282.38	0.0106677776502333
282.45	0.0047133497899034
282.52	0.0197928269585483
282.59	0.00736257292207868
282.66	0.00645816119468647
282.73	0.010835458279964
282.8	0.0163227124273479
282.87	0.0270814730139541
282.94	0.0196447889271623
283.01	0.015245312531946
283.08	0.0142878048679547
283.15	0.0181985864438754
283.22	-0.00125239951313594
283.29	0.00715689908200726
283.36	0.0203446171051569
283.43	0.0167173074947058
283.5	0.00523928546445443
283.57	0.0151052649618099
283.64	0.0243005459545168
283.71	0.0243672454343658
283.78	0.0238866894406991
283.85	0.0292294117264088
283.92	0.0390971997478246
283.99	0.0400816917474808
284.06	0.0585895629848096
284.13	0.0566936209801285
284.2	0.0693929504315708
284.27	0.107577336379646
284.34	0.105896258563327

284.41	0.145253816430635
284.48	0.18243670962125
284.55	0.228099533154247
284.62	0.318365624792555
284.69	0.459340587299212
284.76	0.599627586953794
284.83	0.750831032308252
284.9	0.823151948195411
284.97	0.864307924338241
285.04	0.896525341729565
285.11	0.914367286794961
285.18	0.939623617999375
285.25	0.986937648041185
285.32	1.02098603740564
285.39	1.0975905184554
285.46	1.20325611202166
285.53	1.22871430192414
285.6	1.19992428135752
285.67	1.09281434732426
285.74	1.00804070403065
285.81	0.917190695536106
285.88	0.877002526584865
285.95	0.840138847289997
286.02	0.823913046464784
286.09	0.858420567108536
286.16	0.904400906851852
286.23	1.00952894225798
286.3	1.14759016138861
286.37	1.28179815981981
286.44	1.44548119803683
286.51	1.57086349312747
286.58	1.68154711261057
286.65	1.76589004708275
286.72	1.77341771576246
286.79	1.78434719848697
286.86	1.75302507211308
286.93	1.69299283074156
287	1.6279229507085
287.07	1.59105373838529
287.14	1.53378535029242
287.21	1.48580119302159
287.28	1.42272295327315
287.35	1.36940167640446
287.42	1.28471635347977
287.49	1.26016339491066
287.56	1.19644474067565
287.63	1.1546474866583
287.7	1.13253480115417
287.77	1.08723070700145
287.84	1.05925814467427
287.91	1.06110238450803

287.98	1.03079841079327
288.05	1.0184641200946
288.12	0.999498408974264
288.19	1.00065178624931
288.26	1.00241055015597
288.33	1.00201958652639
288.4	1.00281146785092
288.47	1.00780461716975
288.54	1.01382514959238
288.61	1.00760980325512
288.68	1.01972152395755
288.75	1.03723777250314
288.82	1.04058047997367
288.89	1.06566655338945
288.96	1.05628054593599
289.03	1.08968639231314
289.1	1.10638974332438
289.17	1.11236191683322
289.24	1.14843834400758
289.31	1.14579514909004
289.38	1.1722497227604
289.45	1.19957683064372
289.52	1.20766633187525
289.59	1.23296907128236
289.66	1.24088890843963
289.73	1.25590181733449
289.8	1.26608571904503
289.87	1.28120198773896
289.94	1.28230076766362
290.01	1.28816595746598
290.08	1.25345402396303
290.15	1.24374477904717
290.22	1.25086761983938
290.29	1.23305439709787
290.36	1.21558940327771
290.43	1.2299923547789
290.5	1.21088651032145
290.57	1.20971471489743
290.64	1.20414682310486
290.71	1.21271852958011
290.78	1.20740229579511
290.85	1.20947470185109
290.92	1.22955234574985
290.99	1.21369910619551
291.06	1.23462660648525
291.13	1.2299016305887
291.2	1.242943024384
291.27	1.24660441304011
291.34	1.27474875343281
291.41	1.27210978402266
291.48	1.29002798504409

291.55	1.31802078170074
291.62	1.32372147538022
291.69	1.34103473008273
291.76	1.35475208120003
291.83	1.37568341479036
291.9	1.37811883641269
291.97	1.42064382785641
292.04	1.40820581009054
292.11	1.44173692043077
292.18	1.46278722923312
292.25	1.46581430230641
292.32	1.48624834865268
292.39	1.48045343270498
292.46	1.49109301721427
292.53	1.49178123307063
292.6	1.50428197856745
292.67	1.49480064510682
292.74	1.48300622832544
292.81	1.51322131224978
292.88	1.50655166831963
292.95	1.49171711914696
293.02	1.49372068422737
293.09	1.47716132237557
293.16	1.46845780934361
293.23	1.47168534229951
293.3	1.45077450253484
293.37	1.42597139513069
293.44	1.434768142422
293.51	1.4207064494739
293.58	1.40502140095963
293.65	1.40389676702621
293.72	1.39051625423286
293.79	1.38531243719886
293.86	1.38751217618157
293.93	1.38112240964697
294	1.37053128620349
294.07	1.3680961431638
294.14	1.36871326261774
294.21	1.36030641177733
294.28	1.36343792280385
294.35	1.34683026351564
294.42	1.34686632766392
294.49	1.34060314813128
294.56	1.34729458471934
294.63	1.35232321804093
294.7	1.33119813885599
294.77	1.34733181157827
294.84	1.33430141748868
294.91	1.34430516203182
294.98	1.32214604625612
295.513	1.31710622759694

296.026	1.30706743910617
296.539	1.31770667883739
297.052	1.31363055084652
297.565	1.30453431410325
298.078	1.29832543779834
298.591	1.29586194758703
299.104	1.2872329680633
299.617	1.28038260572361
300.13	1.28349258379845
300.643	1.26838065375052
301.156	1.26484613118656
301.669	1.25727711019464
302.182	1.26228720740818
302.695	1.24245801900115
303.208	1.23279864699605
303.721	1.2331164625455
304.234	1.20965666725167
304.747	1.18052936856385
305.26	1.16197748800454
305.773	1.1340898374491
306.286	1.10844389916353
306.799	1.08364879774758
307.312	1.07262002414425
307.825	1.05943071183567
308.338	1.0286976688534
308.851	1.01772900707949
309.364	0.999440425596913
309.877	0.990993530251145
310.39	0.986394126326658
310.903	0.975415007533659
311.416	0.965937482299093
311.929	0.950557812153641
312.442	0.936556799401499
312.955	0.931373877471296
313.468	0.91667323961838
313.981	0.9178780612381
314.494	0.913201266440597
315.007	0.902504211637868
315.52	0.899553102728432
317.031	0.890237793434251
319.062	0.870350659260691
321.093	0.857121246919666
323.124	0.841838858399075
325.155	0.82134857094461
327.186	0.806869206120534
329.217	0.781127130035579
331.248	0.768629432147777
333.279	0.752696262940045
335.31	0.730008477953693
337.341	0.727015713434079
339.372	0.703562787461576

341.403	0.701576259303327
343.434	0.700078657904173
345.465	0.686031914408456
347.496	0.680437533988549
349.527	0.660377973611634
351.558	0.659912532173402
353.589	0.649883229442898
355.62	0.644878455867946
357.651	0.630660172289596
359.682	0.627856315272727
361.713	0.616932177802588
363.744	0.603144854916316
365.775	0.597566580704636
367.806	0.589381172296754
369.837	0.571689934111369
371.868	0.565790467027063
373.899	0.552960544226199
375.93	0.55284711581862
377.961	0.54501365314323
379.992	0.537012488334636
382.023	0.525802269656841

COT2Th_eV	COT2Th_Int
260	0.0145141196872323
261	0.0062198119988275
262	0.0100336891918743
263	0.000680611585637404
264	-0.0023599113278644
265	0.00810629360961417
266	-0.00496841962037841
267	5.65152940906046e-06
268	0.00257443751322289
269	-0.000415198490911033
270	0.0044431749599401
271	-0.00129905412347488
272	-0.00244069783067904
273	-0.00293658808980537
274	0.00612658417601143
275	-0.00483930012890312
275.258	0.00436646751324814
275.516	-0.00596694795562373
275.774	-0.00164062000200866
276.032	-0.0111400356131009
276.29	0.00638594974553424
276.548	-0.0124310525516216
276.806	-0.0112176048584227
277.064	-0.00968700942342789
277.322	-0.00487420287804869
277.58	-0.00720257108603999
277.838	-0.00310860775216567
278.096	-0.00574918590315012

278.354	-0.0137689425121903
278.612	-0.000275562176403905
278.87	-0.00995214698414339
279.128	-0.00352422927048524
279.386	-0.00117951651063138
279.644	-0.00871466047946902
279.902	-0.0102054290805167
280.16	-0.00480857904141874
280.418	-0.00656825499171784
280.676	0.00589950808852777
280.934	-0.00683038055026143
281.192	0.000163035945639688
281.45	0.00526110021583636
281.708	-0.00711698061289457
281.966	-0.00408581289087363
282.224	-0.0117653908448421
282.482	0.004996356215488
282.74	-0.00162579013709006
282.998	0.00530161977963035
283.071	-5.67810355744062e-05
283.142	0.0134038085584525
283.213	-0.000234468367542162
283.256	-0.00210765822490847
283.284	-0.000577254954588242
283.355	0.000346773158338325
283.426	0.006363106123458
283.497	0.00874331145499043
283.568	0.0128882824598734
283.639	-0.00540266670484823
283.71	0.0108846296741959
283.781	0.0107687205582586
283.852	0.0139269764312765
283.923	0.0159949334455376
283.994	0.0211136809252219
284.065	0.0398278222980082
284.136	0.0388914183224124
284.207	0.0510440232495474
284.278	0.0681015142509133
284.349	0.0800737284137896
284.42	0.11603975836538
284.491	0.13374230423576
284.562	0.166025924506301
284.633	0.185289496160205
284.704	0.19726934321334
284.775	0.20831309614361
284.846	0.212089604711965
284.917	0.232819233535379
284.988	0.255122650348069
285.059	0.306500208516121
285.13	0.392455072354841
285.201	0.553164581082201

285.272	0.743712096802701
285.343	0.918792733388422
285.414	1.10978848856849
285.485	1.41148641319555
285.556	2.1654360694615
285.627	3.30287475162074
285.698	4.06430557356992
285.769	4.18379469645427
285.84	3.91640128781934
285.911	3.45430572934628
285.982	2.86035780721043
286.053	2.46175702110601
286.124	2.28523167215765
286.195	2.09428350775911
286.266	1.74452053994814
286.337	1.40599642629026
286.408	1.12172315234221
286.479	0.939053193358292
286.55	0.865237531111266
286.621	0.867250782563343
286.692	0.929659710431611
286.763	1.09686170610209
286.834	1.25405915816717
286.905	1.52582520089326
286.976	1.8923111612236
287.047	2.23515515106281
287.118	2.54291821927522
287.189	2.74188959336587
287.26	2.85456882376798
287.331	2.89616160738409
287.402	2.84758864777248
287.473	2.72937345955112
287.544	2.60144746029018
287.615	2.46677425759693
287.686	2.30566415557835
287.757	2.17740224804295
287.828	2.04480016355232
287.899	1.93414443441077
287.97	1.83044333740429
288.041	1.75168804713094
288.112	1.68852640635639
288.183	1.62652549103858
288.254	1.56559114664388
288.325	1.52545954356452
288.396	1.50995213669311
288.467	1.49383737874604
288.538	1.47544098271509
288.609	1.46521617726733
288.68	1.43917749068507
288.751	1.44201666487315
288.822	1.41546049832614

288.893	1.42261200425336
288.964	1.41696067017482
289.035	1.42404108386685
289.106	1.44280753404177
289.177	1.44872469357002
289.248	1.47236752616085
289.319	1.51709602473463
289.39	1.55233190557679
289.461	1.59153338121242
289.532	1.60281126188101
289.603	1.64126536824145
289.674	1.62169471524761
289.745	1.62182017485543
289.816	1.57557330685479
289.887	1.55847773390061
289.958	1.53319747273834
290.029	1.53893607138426
290.1	1.53787261466706
290.171	1.55948718780704
290.242	1.55768689563568
290.313	1.54928461079599
290.384	1.55577217419014
290.455	1.53025144656505
290.526	1.51702430301075
290.597	1.50566954867418
290.668	1.48410718244423
290.739	1.45698030847943
290.81	1.45184896428682
290.881	1.45452258318189
290.952	1.44392246982318
291.023	1.4357340298191
291.094	1.42943353400127
291.165	1.43287797052212
291.236	1.46795908733597
291.307	1.46460323317749
291.378	1.49220730887762
291.449	1.51712013876235
291.52	1.54287192710395
291.591	1.57611974398936
291.755	1.64286079000622
292.01	1.78700398858993
292.265	1.90023971213109
292.52	1.97676435029116
292.775	1.95395906052726
293.03	1.89992794688691
293.285	1.82383475377491
293.54	1.74900305421274
293.795	1.67581078873683
294.05	1.62203667695703
294.305	1.60658785864363
294.56	1.58487269268477

294.815	1.57293432668886
295.07	1.58627768338224
295.325	1.58600131123226
295.58	1.57889540330804
295.835	1.57693494494476
296.09	1.58433491503679
296.345	1.56652065517745
296.6	1.56635215365521
296.855	1.5724991332938
297.11	1.56876746661633
297.365	1.56253958754176
297.62	1.56148554905453
297.875	1.55488908995273
298.13	1.54101096014677
298.385	1.53304808628332
298.64	1.51759194274407
298.895	1.51476362581625
299.15	1.50148187684939
299.405	1.49840275401607
299.66	1.49899045855372
299.915	1.50935197011524
300.17	1.49736180291523
300.425	1.50156445229919
300.68	1.49742547132542
300.935	1.49181665207805
301.19	1.49262527688565
301.445	1.49551659939958
301.7	1.46783876404848
301.955	1.4699736938539
302.21	1.46074249040988
302.465	1.45421946994067
302.72	1.43732341334264
302.975	1.42843212064356
303.23	1.41183254719369
303.485	1.42009276799553
303.74	1.39824263306897
303.995	1.38353031529503
304.25	1.3660618941229
304.505	1.36167133321059
304.76	1.34917782472918
305.015	1.31957847111036
305.27	1.31094192993952
307.027	1.20203450727379
309.054	1.12686346583695
311.081	1.05959183715329
313.108	1.01246225539556
315.135	0.97820396972532
317.162	0.963228021123082
319.189	0.934492332013866
321.216	0.91353758255002
323.243	0.889761122692175

325.27	0.860803379027435
327.297	0.824716504531687
329.324	0.806898680691117
331.351	0.78546456152616
333.378	0.759034295549816
335.405	0.746101640304237
337.432	0.7571324797123
339.459	0.738888709972827
341.486	0.721315190816911
343.513	0.707273109283152
345.54	0.70152829962971
347.567	0.700350856913287
349.594	0.68093780774084
351.621	0.666387247745758
353.648	0.644307113893848
355.675	0.634973720336438
357.702	0.625892634511459
359.729	0.614610146064757
361.756	0.609484978337372
363.783	0.607433339510646
365.81	0.595921931496199
367.837	0.591764276506066
369.864	0.582832008133953
371.891	0.57783928849589
373.918	0.568030333164251
375.945	0.559496270709099
377.972	0.555004964513963
379.999	0.545145438529532
382.026	0.539067149900903

Table S2. DFT Atomic Coordinates and Mulliken Populations for (C₈H₈)₂Th.

Center Number	Atom Type	Coordinates (Angstroms)			Mulliken Charges
		X	Y	Z	
1	C	-2.049356	-1.684185	-0.767035	-0.121126
2	C	-2.04969	-0.648456	-1.733508	-0.120967
3	C	-2.048917	0.767346	-1.684206	-0.121137
4	C	-2.049167	1.733892	-0.648543	-0.120948
5	C	-2.049526	-0.766876	1.684386	-0.121059
6	C	-2.049915	-1.733442	0.648749	-0.120992
7	H	-1.959386	-2.671696	-1.216656	0.078857
8	H	-1.958574	-1.028643	-2.74964	0.078924
9	H	-1.95905	1.216943	-2.671733	0.078846
10	H	-1.957861	2.749979	-1.02881	0.078913
11	H	-1.960084	-1.216532	2.671926	0.07883
12	H	-1.958751	-2.749546	1.029007	0.078919
13	C	-2.049617	0.648894	1.733692	-0.120941
14	C	-2.048727	1.684617	0.767217	-0.121108
15	H	-1.95892	1.029096	2.749856	0.078894
16	H	-1.958826	2.672117	1.216862	0.078833
17	C	2.049756	0.611388	1.747088	-0.121034
18	C	2.049613	-0.803049	1.66759	-0.12104
19	C	2.049379	-1.747111	0.611432	-0.121129
20	C	2.049191	0.803175	-1.667458	-0.121121
21	C	2.049329	1.74721	-0.611289	-0.121051
22	C	2.049364	1.667632	0.803127	-0.121082
23	H	1.959253	0.969739	2.771179	0.078868
24	H	1.959993	-1.273679	2.645295	0.078831
25	H	1.95824	-2.771151	0.969765	0.078896
26	H	1.958988	1.273775	-2.645124	0.078852
27	H	1.957976	2.771231	-0.969633	0.078895
28	H	1.959325	2.645263	1.273831	0.078833
29	C	2.049331	-1.667558	-0.803022	-0.121086
30	C	2.049443	-0.611299	-1.746979	-0.121083
31	H	1.95846	-0.969612	-2.771041	0.078899
32	H	1.959259	-2.645203	-1.273697	0.078854
33	Th	-0.000033	-0.000168	-0.000098	0.67496

Table S3. DFT Atomic Coordinates and Mulliken Populations for (C₈H₈)₂U.

Center	Atom	Coordinates (Angstroms)			Mulliken	Mulliken
Number	Type	X	Y	Z	Charges	Spin Densities
1	C	-1.946632	-1.771417	-0.530987	-0.133095	-0.01762
2	C	-1.945234	-0.877004	-1.627846	-0.133375	-0.017674
3	C	-1.94562	0.531191	-1.771163	-0.133218	-0.017687
4	C	-1.946467	1.628354	-0.876921	-0.133197	-0.017617
5	C	-1.945746	-0.531026	1.771217	-0.133248	-0.017576
6	C	-1.946773	-1.628214	0.876948	-0.133193	-0.017805
7	H	-1.827979	-2.807778	-0.84175	0.073483	0.000922
8	H	-1.827098	-1.39004	-2.580474	0.073468	0.00092
9	H	-1.826655	0.841818	-2.807493	0.0735	0.000921
10	H	-1.828574	2.581041	-1.38996	0.073457	0.000921
11	H	-1.826818	-0.841692	2.807571	0.073498	0.000916
12	H	-1.8291	-2.580953	1.390002	0.073465	0.000929
13	C	-1.945047	0.87719	1.627869	-0.133379	-0.017641
14	C	-1.946263	1.771577	0.530973	-0.133021	-0.017779
15	H	-1.826796	1.390207	2.580507	0.073465	0.000919
16	H	-1.827405	2.807904	0.841741	0.073485	0.000929
17	C	1.945051	0.84237	1.646173	-0.133293	-0.017659
18	C	1.945567	-0.568563	1.759539	-0.133238	-0.017679
19	C	1.946643	-1.646501	0.84206	-0.133263	-0.017605
20	C	1.945471	0.568725	-1.759492	-0.13324	-0.017552
21	C	1.94629	1.646628	-0.84204	-0.133175	-0.0178
22	C	1.946336	1.759935	0.568589	-0.133019	-0.017619
23	H	1.826493	1.334962	2.609483	0.073481	0.00092
24	H	1.826573	-0.901269	2.78902	0.073521	0.00092
25	H	1.828579	-2.609896	1.334696	0.073488	0.00092
26	H	1.826391	0.901398	-2.788942	0.073516	0.000915
27	H	1.828054	2.609977	-1.334663	0.073488	0.000928
28	H	1.827464	2.789391	0.901407	0.073496	0.000922
29	C	1.946677	-1.759774	-0.568589	-0.133033	-0.017761
30	C	1.945219	-0.842174	-1.646155	-0.133322	-0.017642
31	H	1.82678	-1.334795	-2.609449	0.073484	0.000919
32	H	1.828035	-2.789265	-0.90141	0.073507	0.000928
33	U	0.000057	-0.000096	-0.000014	0.955504	2.267967