Electronic Supplementary Information for Dalton Transactions

Electronic Supporting Information

Aqueous coordination chemistry and photochemistry of uranyl(VI) oxalate revisited: a density functional theory study

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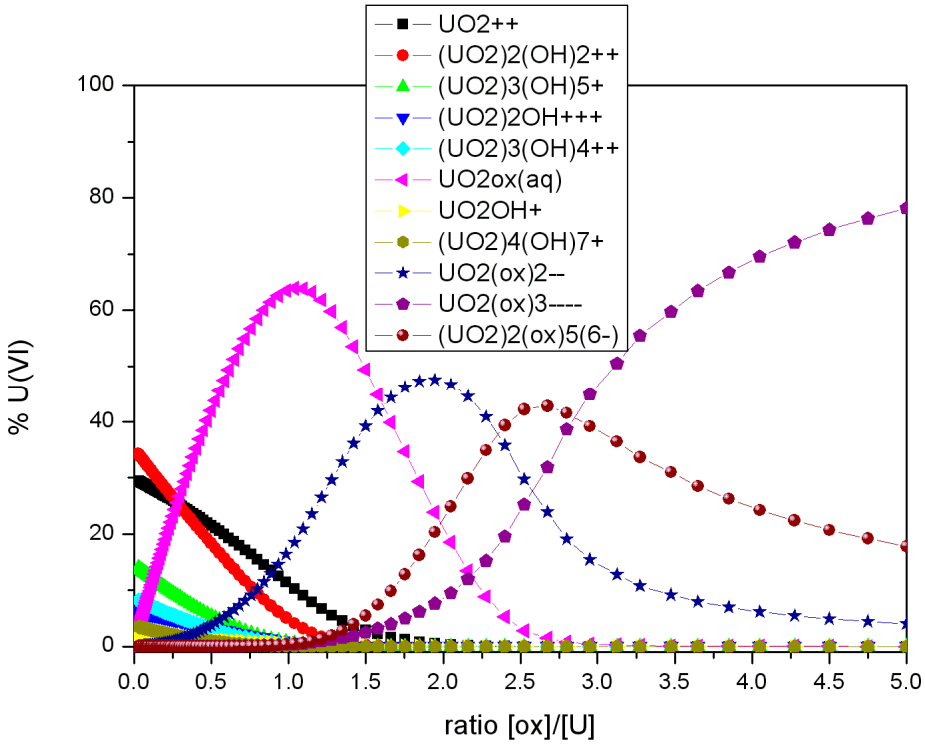
1. Aqueous uranyl(VI) oxalate speciation in previous experiments.

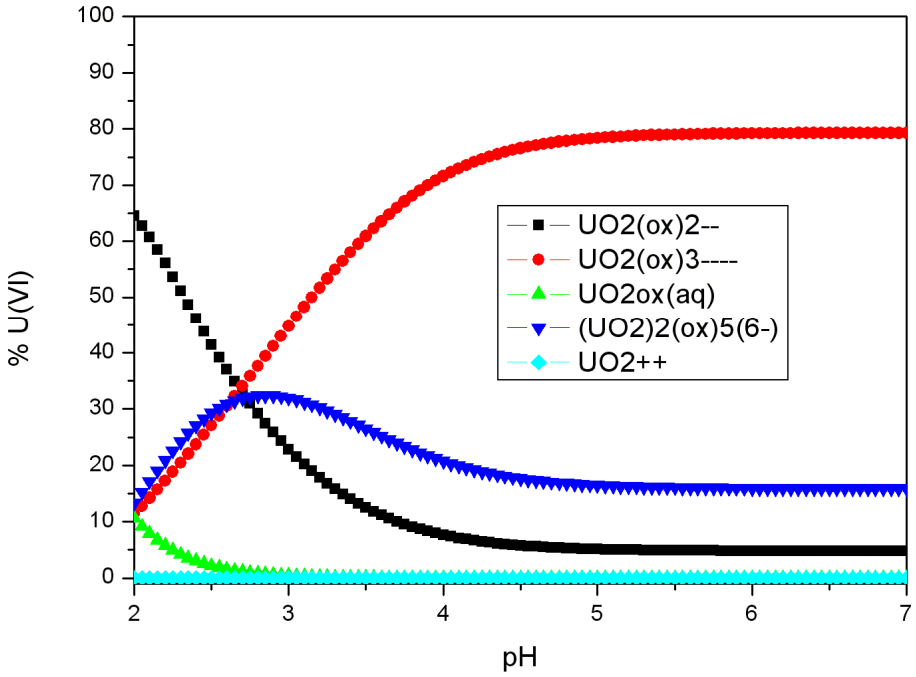
1-1. Brits et al. (A.G.Brits, R.Van Eldik, J.A.Van Den Berg, *J. Inorg. Nucl. Chem.* 1977, **39**, 1195.)

pH 4.5, [UO22+]=0.004M, [ox2-/UO22+] varied, Ionic Strength: 0.5M (by HClO4)



1-2. McCleskey et al. (T.M.McCleskey, T.M.Foreman, E.E.Hallman, C.J.Burns, N.N.Sauer, Environ. Sci. Technol. 2001, 35, 547)

[UO22+] = 0.01M, [ox2-] = 0.04M, pH varied



2. Coordinates and energies of the complexes S1-S17, T1-T10, T11, T15, S18a, S18b, S18c, T18, T19

S1
E(RB+HF-LYP) = -654.040858217

U	-0.72178300	0.02052400	0.00273700
O	-0.80853800	0.06411200	-1.76591200
O	-0.79471400	0.05669100	1.77195400
O	-0.98124700	2.50016000	0.01373600
O	-3.19490800	0.50673400	-0.05100900
O	-2.16470700	-2.07851000	0.04033200
H	-0.83190500	3.04002900	-0.78533200
H	-0.69186400	3.04191100	0.77232700
H	-3.62336800	0.90902200	-0.83034900
H	-3.67680100	0.83869000	0.73044700
H	-3.13625600	-2.01366600	0.04482600
H	-1.93159900	-2.85320700	0.58371400
C	2.69788500	0.82621300	0.00097600
C	3.61409100	-0.45559900	0.00671400
O	3.02223000	-1.59090400	-0.02733400
O	1.40148000	0.58636400	0.03654900
O	3.17863400	1.95274800	-0.02914000
O	4.84252700	-0.26560200	0.04418100
H	0.37269000	-2.75621100	-0.67561800
O	0.55826700	-2.03974500	-0.04453600
H	1.57905300	-1.85489000	-0.04853100

S2

E(RB+HF-LYP) = -636.752593746

U	-0.65237500	-0.03236800	0.00028300
O	-0.71019400	-0.07281700	1.76294300
O	-0.71225400	-0.06304500	-1.76198300
O	-1.41053300	-2.34846500	-0.00398200
O	-3.07071600	0.38916200	0.00920100
O	-0.90365300	2.44828200	0.01265400
H	-1.57776600	-2.89723700	0.78692000
H	-1.57429500	-2.90436800	-0.79055600
H	-3.64923100	0.37370600	0.79687000
H	-3.64955300	0.43982900	-0.77669200
H	-1.71898800	2.98230200	-0.00654600
H	-0.15457600	3.04573000	-0.16932100
C	3.70974900	-0.01936200	0.00355200
C	2.14855800	-0.02041100	-0.00569400
O	1.48437500	-1.11811800	-0.01392100
O	4.24645000	-1.15576600	-0.00585100
O	4.24440800	1.11808200	0.01944500
O	1.48124700	1.07475500	-0.00024400

S3

E(RB+HF-LYP) = -636.776793322

U	-0.51409500	-0.03006400	-0.00059700
O	-0.58760500	-0.08366800	1.77106800
O	-0.61293400	-0.04411100	-1.77159700
O	-1.42646500	-2.34182600	-0.00043200
O	-2.99371200	0.34231900	0.02129800
O	-1.03920300	2.43527600	0.03226400
H	-1.48772800	-2.91705800	0.78531000
H	-1.45200800	-2.92476600	-0.78253500
H	-3.56090600	0.17614200	0.79790800
H	-3.56691800	0.27365700	-0.76562900
H	-1.90013700	2.85979000	-0.13124500
H	-0.34599000	3.10047100	-0.12622400
C	2.63145900	-0.78849400	-0.00972000
C	2.62713100	0.77619400	0.00612700
O	1.41123000	1.26568100	0.00631500
O	1.41644700	-1.27876000	-0.04724300
O	3.67199500	-1.43555500	0.00931500
O	3.66760800	1.42457600	0.01637100

S4

E(RB+HF-LYP) = -712.642826586

U	0.01317800	-0.28442500	0.04839500
O	0.22988800	-0.27611600	1.81483000
O	-0.21056200	-0.34354300	-1.71584600
O	1.78142000	-2.01645900	-0.09544600
H	2.69103300	-1.56179000	-0.14948100
H	1.75066800	-2.69861600	-0.78705400
C	-4.13106700	1.20729300	-0.09310300
C	-3.49749100	-0.23131300	-0.01700000
O	-2.24669600	-0.26248000	0.35198200
O	-3.33080600	2.19736900	0.02148200
O	-5.36940400	1.28094300	-0.25579600

O	-4.17029500	-1.23387300	-0.26779500
C	3.15520700	1.33933500	-0.04801900
O	1.97180700	0.80566400	-0.18992800
C	4.36381700	0.33190900	-0.13514600
O	3.36124400	2.54029400	0.12693100
O	4.08557200	-0.91528600	-0.18068900
O	5.51398600	0.82230100	-0.15232700
H	-1.76770900	2.11621400	0.06508900
O	-0.75652900	2.06272900	0.01755900
H	-0.37356300	2.77179400	0.55864800
H	-0.52617200	-3.42437900	0.61878400
O	-0.91836700	-2.69385500	0.10779700
H	-1.85948400	-2.66098000	0.33923400

S5
E(RB+HF-LYP) = -695.357818216

U	-0.10162800	0.17728800	0.00096100
O	-0.13311100	0.23937000	1.77566800
O	-0.11942400	0.12573700	-1.77415100
O	0.82399000	-2.07442500	0.09687900
H	1.84434800	-2.01449800	0.05833700
H	0.53319900	-2.77995800	-0.50589700
C	-4.45095400	-0.53222300	-0.00435400
C	-2.91127300	-0.27596900	-0.00382200
O	-2.45152200	0.91696900	-0.02315600
O	-5.17881800	0.49607100	0.00164300
O	-4.80681600	-1.74063600	-0.00949000
O	-2.08923800	-1.25532500	0.01620200
C	3.41874700	0.52253000	-0.00987100
O	2.10776000	0.50864900	0.00584100
C	4.11403400	-0.89224700	0.00516300
O	4.09528900	1.54719500	-0.03620700
O	3.35870900	-1.92333600	0.03909500
O	5.36263900	-0.90402200	-0.01847200
H	-0.97444800	3.15041600	0.26720300
O	-0.17675800	2.70748100	-0.07837100
H	0.58171200	3.25119700	0.20539900

S6
E(RB+HF-LYP) = -695.371702261

U	0.24001800	-0.37996700	0.01513000
O	0.15201800	-0.37440500	-1.76655600
O	0.31660100	-0.44648600	1.79631700
O	1.07673300	-2.80291700	-0.10186000
H	0.57061500	-3.60315500	0.12776000
H	2.00461400	-2.96734700	0.14715900
C	2.64600700	1.83151400	-0.01965600
C	3.41032800	0.46615900	-0.07440500
O	2.61186100	-0.56150900	-0.08072700
O	1.35105600	1.68496600	0.01140800
O	3.25051900	2.90477600	-0.00786900
O	4.64240200	0.42709900	-0.10630900
C	-2.82786200	1.43247300	0.07512100

O	-1.66140400	0.84967400	0.09536800
C	-4.06940600	0.47646600	-0.10421700
O	-2.99737500	2.64896600	0.18674200
O	-3.83842900	-0.78068200	-0.15683000
O	-5.19354100	1.01503600	-0.18459400
H	-2.51209200	-1.50111400	0.00520400
O	-1.63158900	-2.01443200	0.09148600
H	-1.73002900	-2.61179500	0.85424100

S7

E(RB+HF-LYP) = -678.068473565

U	0.00119800	-0.46980200	0.00371900
O	-0.00991500	-0.53925900	1.77235700
O	0.01128800	-0.49477700	-1.76601300
O	-0.03013900	-2.92093400	-0.03196400
H	-0.01345300	-3.48204100	-0.83134000
H	-0.12319000	-3.51339000	0.73911500
C	-4.02612200	1.25710200	-0.00793600
C	-2.59097300	0.64477600	0.00093700
O	-1.55586500	1.39719000	0.01376600
O	-4.08289500	2.51451600	-0.02133100
O	-4.97332600	0.42799400	-0.00041200
O	-2.42406900	-0.62494500	-0.00581100
C	2.59592600	0.63762500	0.01113400
O	2.42444000	-0.63197300	0.00935200
C	4.03294000	1.24560000	-0.00641200
O	1.56385800	1.39359400	0.02612800
O	4.97810800	0.41405200	-0.02090700
O	4.09298600	2.50286700	-0.00469300

S8

E(RB+HF-LYP) = -695.357511052

U	0.00059300	-0.00107800	0.00159000
O	0.00659700	-0.02325300	1.77344300
O	-0.00626900	0.03234200	-1.77031200
O	0.00096600	-2.52339700	-0.00429200
H	0.79408800	-3.03295000	-0.24231100
H	-0.78195600	-3.04072200	-0.25866300
C	-4.43721200	-0.00083400	0.01352200
C	-2.87673400	-0.00077700	0.00317000
O	-2.22517500	1.09626800	0.01751500
O	-4.98733200	1.13245800	-0.01461600
O	-4.98755300	-1.13390300	0.04560100
O	-2.22523800	-1.09766700	-0.01891900
C	2.87713200	-0.00104600	-0.00414000
O	2.22738400	-1.09914800	-0.02740100
C	4.43752500	0.00209300	0.01466100
O	2.22360200	1.09515700	0.00451400
O	4.99031200	-1.13013100	0.03155600
O	4.98538500	1.13671200	0.00538900
H	-0.78945500	2.98763900	-0.31514600
O	-0.01055300	2.53663200	0.05223300
H	0.78146400	3.01204100	-0.25112400

S9
E(RB+HF-LYP) = -678.082935131

U	-0.12921900	0.23315400	0.00169700
O	-0.10459800	0.25997900	-1.77777100
O	-0.10314000	0.22440800	1.78128200
O	-0.01232900	2.75533700	0.04456100
H	0.81229600	3.24521500	-0.14312500
H	-0.74941600	3.33175700	-0.23771800
C	-2.88781100	-1.46582900	-0.01109800
C	-3.37032700	0.02722600	0.00602200
O	-2.37734100	0.87645900	0.00557300
O	-1.58359000	-1.56978700	-0.01759800
O	-3.68671800	-2.39852700	-0.01679400
O	-4.56591100	0.31054100	0.01594300
C	2.65874400	-0.35548600	0.00045800
O	2.27170800	0.86129100	0.01324100
C	4.18134600	-0.70766400	-0.00151500
O	1.77688600	-1.28679200	-0.01195600
O	4.96770800	0.27580200	-0.01478800
O	4.45901900	-1.93579300	0.01099300

S10
E(RB+HF-LYP) = -678.101972003

U	0.00176800	-0.20244400	0.00110100
O	0.02711100	-0.22593000	-1.78600700
O	-0.01944800	-0.20207600	1.78834400
O	-0.02712000	-2.74988200	0.02687900
H	0.74213100	-3.29362700	-0.22537500
H	-0.82902600	-3.24553300	-0.22307500
C	2.87848800	1.34286200	-0.00348100
C	3.27822500	-0.17458900	0.01606900
O	2.24893300	-0.97141000	0.02999100
O	1.58848300	1.52812600	0.00103900
O	3.73522600	2.22834400	-0.02100600
O	4.46232800	-0.51842200	0.01718400
C	-2.87380800	1.34853400	-0.01008200
O	-1.58333200	1.53165200	-0.02839000
C	-3.27807500	-0.16687600	0.00337300
O	-3.72791400	2.23658700	-0.00211500
O	-2.25341700	-0.96900000	-0.01155800
O	-4.46394200	-0.50494100	0.02462700

S11
E(RB+HF-LYP) = -736.670276858

U	-0.33831400	0.03006100	-0.04162900
O	-0.40190000	0.04601700	-1.83330300
O	-0.31991000	0.01966000	1.74646600
C	-1.92574000	2.93824100	0.02202500
C	-0.41249100	3.33971700	-0.00413900
O	0.38746100	2.32039000	-0.03133300
O	-2.11676200	1.65670500	0.01243800
O	-2.80993400	3.80439800	0.04955800
O	-0.07131000	4.52975900	0.00285300
C	-2.44577100	-2.52371000	0.00709700

O	-2.38890300	-1.22904600	-0.00114300
C	-1.03711800	-3.20617400	-0.03376900
O	-3.47914900	-3.20456400	0.04202900
O	-0.05729400	-2.35863100	-0.07068600
O	-0.92957100	-4.43951300	-0.03030100
C	3.06206900	-0.43665600	0.49890400
C	4.39591100	-0.25938900	-0.25694400
O	1.99901300	-0.19033400	-0.21566400
O	4.80099300	-1.25649700	-0.92748200
O	4.97529700	0.85997800	-0.12968900
O	3.07493500	-0.79304900	1.69011200

S12
E(RB+HF-LYP) = -736.660664781

U	0.14797200	0.00033700	0.00915800
O	0.15011900	0.02315900	1.79663300
O	0.10981500	-0.02060500	-1.77766500
C	2.31289700	2.59313200	-0.02458900
C	0.92293500	3.29117200	-0.02476200
O	-0.05714700	2.45354300	-0.02471900
O	2.22773500	1.30599700	-0.02699200
O	3.36589400	3.25317600	-0.02459000
O	0.82438700	4.53025000	-0.02654300
C	2.36629000	-2.55035600	-0.00821500
O	2.26183300	-1.26486400	-0.00415400
C	0.98858200	-3.27131300	0.01646100
O	3.42904300	-3.19453700	-0.02834500
O	-0.00605400	-2.45079500	0.03887300
O	0.91008100	-4.51161000	0.01455700
C	-2.86034200	-0.03096600	0.01596700
C	-4.42276600	-0.03308500	-0.01847700
O	-2.21820600	1.06561800	0.02345100
O	-4.98927700	1.08200200	0.15798100
O	-4.97643600	-1.14999100	-0.22412900
O	-2.21415500	-1.12416300	0.03303000

S13
E(RB+HF-LYP) = -736.658241152

U	0.00183700	0.14680200	0.01658600
O	-0.01329900	0.09079900	1.80048100
O	0.01512800	0.15135100	-1.76797700
C	0.81578300	3.37580000	0.04989300
C	-0.73802700	3.38860300	-0.07380500
O	-1.25622600	2.20299100	-0.03752900
O	1.31018300	2.18237100	0.13184600
O	1.46331500	4.43213400	0.06421800
O	-1.36461300	4.45080100	-0.18921100
C	3.76389700	-2.32174600	-0.02913600
O	4.84721100	-1.68031400	-0.11339700
C	2.45590600	-1.46561000	-0.02074500
O	3.61232200	-3.57192100	0.05198600
O	2.51487900	-0.19391300	-0.03556100
O	1.31404900	-2.02732300	0.00078900
C	-2.49060000	-1.41311600	-0.00424600

C	-3.81494800	-2.24324600	-0.01436100
O	-2.52537700	-0.14093000	0.03572300
O	-4.88440000	-1.58554500	0.11209500
O	-3.68853100	-3.49232500	-0.14106200
O	-1.35978000	-1.99692000	-0.03384800

S14
E(RB+HF-LYP) = -736.656821838

U	0.00090200	-0.00513700	0.00111200
O	-0.01216100	0.00503500	-1.78518500
O	0.01112300	-0.00653800	1.78885700
C	-3.08307600	-1.54342900	-0.00645700
C	-3.44765400	-0.03467600	-0.00021700
O	-2.41275300	0.72608200	0.02709100
O	-1.81412300	-1.74946700	0.00908000
O	-3.96559000	-2.42348400	-0.02310600
O	-4.63564600	0.34379700	-0.01707400
C	1.76891900	-2.96288700	0.00040800
O	0.58347800	-2.46649500	-0.01036200
C	2.87633800	-1.87523400	0.00397100
O	2.05526700	-4.17618400	0.00582700
O	2.39723100	-0.68197500	-0.01118900
O	4.08416500	-2.17879700	0.01768500
C	0.19460500	3.43046200	0.01772500
C	1.68803100	3.00980300	-0.02292300
O	-0.14266500	4.62819800	0.04235400
O	2.59803700	3.86225200	-0.05469700
O	1.84921900	1.73693800	-0.01213600
O	-0.60383000	2.42168300	0.01568300

S15
E(RB+HF-LYP) = -1397.48677662

U	3.25633700	-0.33069600	-0.05630600
O	3.20024900	-0.39867600	-1.84043300
O	3.23029800	-0.27616500	1.72547100
C	-0.06013200	-0.77500000	-0.00076500
C	0.09749000	0.75964300	-0.05915500
O	1.28028000	1.20211800	-0.08518400
O	1.00497900	-1.45138200	0.00522700
O	-1.24336500	-1.21704900	0.03509700
O	-0.96817100	1.43602300	-0.07577800
C	4.79658500	-3.23282800	0.00069600
O	3.62113300	-2.68027400	0.02251800
C	5.96068900	-2.18875300	-0.06617900
O	5.02933900	-4.44530900	0.02766900
O	5.53686100	-0.95972700	-0.09034400
O	7.14130300	-2.54822600	-0.09048100
C	4.83559900	2.67245800	0.51020700
C	4.85979800	4.07659700	-0.13458800
O	4.22669600	1.75857400	-0.20538100
O	5.66974500	4.23437200	-1.09576000
O	4.08340900	4.94258000	0.36408900
O	5.38270100	2.48038800	1.60548200
U	-3.21448800	0.32167600	0.03304700

O	-3.11937800	0.40665400	1.81499200
O	-3.22533700	0.25561900	-1.74795000
C	-5.13385100	-3.97392400	0.34350700
C	-5.93126300	2.15987400	0.01853400
C	-4.77424200	3.21101000	-0.06506400
C	-4.86189500	-2.66715200	-0.43411600
O	-6.07598700	-3.93450300	1.18939800
O	-4.19211600	-1.76659300	0.24237300
O	-5.27902900	-2.53386800	-1.59381700
O	-4.40254200	-4.96637400	0.05616200
O	-5.49866600	0.93585100	0.09799200
O	-7.11484100	2.51035200	0.00833400
O	-3.59414400	2.66744000	-0.06193400
O	-5.01626300	4.42046100	-0.12506800

S16
E(RB+HF-LYP) = -1397.47346727

U	-3.33208900	0.19265100	0.00266700
O	-3.32546300	0.19116700	-1.77871200
O	-3.31611700	0.14942000	1.78318000
C	0.04426200	0.75353100	0.08263700
C	-0.04438800	-0.76139400	-0.06304600
O	-1.20682600	-1.25079600	-0.11606700
O	-1.05276900	1.37675100	0.12911600
O	1.20623400	1.24342000	0.13969400
O	1.05244800	-1.38451200	-0.11289600
C	-4.34454200	3.38301400	-0.05401700
O	-3.30289900	2.61660700	-0.04181900
C	-5.67575200	2.58330700	0.01995800
O	-4.33600700	4.62106300	-0.11548400
O	-5.48598900	1.30517700	0.05825300
O	-6.77495200	3.15652900	0.03791700
C	-4.79866300	-2.38163600	-0.00994200
C	-5.57692400	-3.73696700	-0.01297400
O	-3.52774100	-2.36296900	0.02135900
O	-4.87255900	-4.78410400	0.00378800
O	-6.83629400	-3.65515100	-0.03140000
O	-5.42432000	-1.27480300	-0.03870800
U	3.33341100	-0.19439700	0.01640400
O	3.31990600	-0.20186500	1.79769600
O	3.32307500	-0.14561600	-1.76413200
C	5.56340700	3.74332800	-0.03557500
C	5.68308500	-2.57727700	-0.03215000
C	4.35275500	-3.38159400	-0.00095300
C	4.79114900	2.38554200	0.00377700
O	6.81964700	3.66608700	-0.13079200
O	5.42155000	1.28120400	0.02872100
O	3.51986300	2.36189100	0.00948800
O	4.85807700	4.78783100	0.03096400
O	5.49110000	-1.29923300	-0.00012200
O	6.78309200	-3.14711500	-0.07739600
O	3.30977300	-2.61718600	0.02098500
O	4.34618200	-4.62111100	0.00376500

S17
E(RB+HF-LYP) = -1397.47195630

U	3.72545200	-0.18120100	0.00036600
O	3.68524600	-0.13504600	-1.78143300
O	3.72981300	-0.18676500	1.78314500
C	0.76887400	-0.04398200	0.03012700
C	-0.76892900	0.02991500	0.03728800
O	-1.34018600	1.16088200	0.03398800
O	1.44572800	1.02643900	0.03621800
O	1.34131600	-1.17402300	0.01591300
O	-1.44701700	-1.03944800	0.04367700
C	4.65134700	-3.36940900	-0.05287600
O	3.62208500	-2.58262600	-0.03160000
C	6.00373800	-2.59443800	-0.05794700
O	4.61961700	-4.60673900	-0.06788600
O	5.84618100	-1.30856100	-0.03968200
O	7.08734700	-3.19240200	-0.07770800
C	5.04431700	2.43579100	0.02372900
C	5.74919000	3.83037900	0.03883500
O	3.77402900	2.35057100	0.04882600
O	4.99370300	4.83288700	0.16469500
O	7.00555900	3.81818200	-0.07543200
O	5.72984000	1.36269500	-0.01317900
U	-3.72513900	0.17957400	0.01176400
O	-3.74018600	0.17413700	1.79455600
O	-3.67423300	0.14427900	-1.76998300
C	-5.76476800	-3.82371000	0.02753300
C	-5.99198500	2.60223000	-0.07926700
C	-4.63696400	3.37222600	-0.05179600
C	-5.05618300	-2.43095000	0.01876300
O	-7.02079800	-3.80795300	-0.09028000
O	-5.73836700	-1.35583100	-0.01875900
O	-3.78570300	-2.34971900	0.04979200
O	-5.01224000	-4.82852100	0.15261600
O	-5.83917200	1.31590900	-0.05037700
O	-7.07316500	3.20330400	-0.12269800
O	-3.61205000	2.58181300	0.00681900
O	-4.59992100	4.60920700	-0.08151000

T1
E(UB+HF-LYP) = -653.999325949

U	0.83582500	0.02089200	0.01752100
O	1.02429000	0.02902600	1.82709400
O	0.69286900	0.07242400	-1.79588500
O	0.89992100	2.55021000	0.03288400
O	3.32395300	0.50834000	-0.15231800
O	2.20748600	-2.18332800	-0.14803600
H	0.83390100	3.10207800	0.83211300
H	0.69552600	3.12602700	-0.72515400
H	3.83980900	0.86466300	0.59323700
H	3.75302800	0.83312200	-0.96476500
H	3.14061900	-2.13037900	-0.41624600
H	1.81985300	-2.91700400	-0.65645700
C	-2.73121900	1.06592000	0.01394200

C	-4.08181300	-0.69280800	-0.03597400
O	-3.35150300	-1.65659500	-0.08995100
O	-1.60139100	0.65368000	0.25790100
O	-3.37437600	2.06278400	-0.18930800
O	-5.19319400	-0.25156000	-0.00024400
H	-0.53040800	-2.68700600	0.88700000
O	-0.62639300	-2.09119100	0.12339000
H	-1.58334400	-1.90253000	0.04633700

T2

E(UB+HF-LYP) = -636.688248909

U	-0.71139800	-0.00147500	0.00088800
O	-0.75521500	-0.00283800	1.82016900
O	-0.74088900	0.00041600	-1.81869400
O	-1.18092700	-2.47477000	-0.00187600
O	-3.23520900	0.02222500	-0.01153100
O	-1.15381200	2.48176600	-0.00000800
H	-1.28436700	-3.04554200	0.78000000
H	-1.25314100	-3.04894900	-0.78469200
H	-3.81840100	0.03075800	0.76767600
H	-3.80971200	0.06307400	-0.79618600
H	-1.09883500	3.06085700	-0.78107300
H	-1.10933500	3.06016300	0.78203200
C	3.77826100	-0.00590500	-0.00158500
C	2.25567000	-0.00434500	0.00419600
O	1.66985700	-1.11957400	0.00543200
O	4.46253600	-1.06658800	-0.00466600
O	4.46231000	1.05608200	-0.00369800
O	1.67369600	1.11288900	0.00673500

T3

E(UB+HF-LYP) = -636.690904594

U	0.50080900	-0.02876900	-0.00088400
O	0.61425000	-0.08693000	-1.82629500
O	0.59504500	-0.05140100	1.82627800
O	1.41249800	-2.35862700	0.02045600
O	3.01395800	0.31004900	-0.00798600
O	1.12843700	2.42012700	-0.01379100
H	1.45606200	-2.93440500	-0.76559600
H	1.39256700	-2.94587100	0.79892700
H	3.58360500	0.08925000	-0.76816100
H	3.56907700	0.22573600	0.78942000
H	2.02823300	2.78859200	0.01452200
H	0.50452800	3.15188000	0.13956400
C	-2.63453600	-0.77288700	0.00171300
C	-2.61458300	0.79167600	-0.00606600
O	-1.39321200	1.27882300	-0.01042400
O	-1.42802000	-1.28933900	0.00206200
O	-3.68530100	-1.40379400	0.00581500
O	-3.64688000	1.45095000	-0.00876400

T4

E(UB+HF-LYP) = -712.583005289

U	0.07359700	-0.35744300	0.04523300

O	-0.02367100	-0.34511800	-1.78693200
O	0.10661500	-0.38116800	1.87923100
O	-1.92120000	-2.04441200	0.11807600
H	-2.78562900	-1.61012800	-0.01947500
H	-2.02165900	-2.58674100	0.92089100
C	4.18161000	1.36075100	-0.07711600
C	3.69400800	-0.14274100	-0.07454100
O	2.41900900	-0.32499500	-0.02117200
O	3.28395800	2.26868200	-0.01034200
O	5.41645900	1.56624400	-0.13948500
O	4.53875900	-1.05213600	-0.12243800
C	-3.17932100	1.58263800	0.08993300
O	-2.17204700	0.89129200	0.08619300
C	-4.89770500	0.22520000	-0.20234200
O	-3.59252100	2.70973000	0.18785700
O	-4.43419600	-0.89386400	-0.25297900
O	-5.87534700	0.91965100	-0.24338600
H	1.72119600	2.12108300	0.03395000
O	0.71061700	2.08685900	0.06789600
H	0.38397300	2.67408500	-0.63427400
H	0.44463400	-3.51125300	-0.55313300
O	0.90164900	-2.83866500	-0.01588000
H	1.83035000	-2.85416400	-0.29817700

T5

E(UB+HF-LYP) = -695.270432668

U	-0.08664500	0.18115700	0.01320900
O	-0.17454700	0.26079400	1.84243200
O	-0.11841100	0.10695900	-1.81803700
O	0.82770800	-2.05778000	0.11203600
H	1.84700500	-2.02030500	0.04351600
H	0.49555300	-2.84685000	-0.34852200
C	-4.46101900	-0.54451700	-0.02543800
C	-2.92195900	-0.27682600	-0.01800900
O	-2.47490900	0.91761200	-0.06448900
O	-5.19891900	0.47627700	-0.08139500
O	-4.81286100	-1.75408300	0.02280700
O	-2.09899700	-1.25471000	0.03369400
C	3.42524300	0.51885400	-0.01414900
O	2.10729600	0.51117600	0.02376300
C	4.11744800	-0.89560300	-0.02255700
O	4.09562600	1.54479400	-0.04537700
O	3.35941000	-1.92451800	-0.01541200
O	5.36561900	-0.90671400	-0.03880000
H	-1.06836400	3.15040700	0.09157200
O	-0.22017700	2.69532600	-0.06103800
H	0.48411300	3.31781800	0.19764700

T6

E(UB+HF-LYP) = -695.285838407

U	0.23940700	-0.37532800	0.01934000
O	0.14352800	-0.39208900	-1.81897500
O	0.33921800	-0.45763700	1.85517600
O	1.08584700	-2.81159000	-0.08632700

H	0.58672300	-3.61356700	0.15121800
H	2.01583600	-2.97012200	0.15676600
C	2.63860800	1.83087500	-0.04036800
C	3.41151500	0.46887800	-0.08910700
O	2.62607600	-0.56591900	-0.08598000
O	1.34055000	1.68412200	-0.00038600
O	3.23605900	2.90715700	-0.04282900
O	4.64533200	0.44517900	-0.12617500
C	-2.83359100	1.42448300	0.11273300
O	-1.66050000	0.84587900	0.12382700
C	-4.06807000	0.47634100	-0.14044000
O	-3.00795800	2.63119300	0.28831500
O	-3.83898700	-0.77991600	-0.18932600
O	-5.18364600	1.02366800	-0.26785900
H	-2.50853300	-1.51009100	0.00120900
O	-1.63401200	-2.02392400	0.10041600
H	-1.74229900	-2.62850600	0.85558500

T7

E(UB+HF-LYP) = -678.017380192

U	-0.20554600	-0.52907700	0.00866900
O	-0.18508600	-0.56717400	-1.81903300
O	-0.19286500	-0.57809500	1.83593600
O	-0.35221900	-3.03118700	-0.00139900
H	-0.39129100	-3.60544100	-0.78947200
H	-0.40376400	-3.61414200	0.77958800
C	5.74942800	1.32845300	-0.03340000
C	2.57225400	0.41915000	0.01298000
O	1.69218400	1.31104600	0.01486300
O	5.44408900	2.45258200	-0.06119300
O	6.07435400	0.20992500	-0.00611800
O	2.42603600	-0.82567700	0.01061600
C	-2.73414700	0.86347800	-0.00040000
O	-2.69919400	-0.41489300	-0.00066300
C	-4.11233900	1.60466900	-0.01926400
O	-1.64776800	1.53274600	0.01254600
O	-5.12956700	0.88140000	-0.20391700
O	-4.07320400	2.85434600	0.14996300

T8

E(UB+HF-LYP) = -695.301041319

U	0.16085500	0.00127200	0.02909500
O	0.15640400	0.00260800	1.87219800
O	0.11062200	0.00018800	-1.81360200
O	0.12161000	-2.59377700	0.05875400
H	0.92267700	-3.05021000	-0.25199000
H	-0.63898800	-3.07796600	-0.30678800
C	-6.14845700	0.00596400	-0.07110400
C	-2.85189800	-0.01365800	0.03254300
O	-2.31249500	1.11529200	0.04972000
O	-6.15160000	1.16681700	0.02976300
O	-6.17004000	-1.15468000	-0.17268000
O	-2.31592200	-1.14390600	0.02923000
C	3.11064200	-0.00494600	-0.02407100

O	2.47815000	-1.11074000	-0.02108700
C	4.67723500	0.00048000	-0.06137000
O	2.47234000	1.09781300	0.00217200
O	5.24214600	-1.12734700	-0.00269300
O	5.23089100	1.13212200	-0.14747300
H	-0.62883100	3.08841800	-0.36066200
O	0.12429500	2.60877300	0.02586600
H	0.93010300	3.05039100	-0.29469300

T9
E(UB+HF-LYP) = -677.994605445

U	0.14024200	0.21616600	0.00087700
O	0.08926800	0.23631700	1.83849100
O	0.10683600	0.22147800	-1.83685600
O	-0.02152500	2.73512500	-0.01000300
H	-0.86913900	3.21558600	-0.06821300
H	0.67763500	3.34925500	-0.30487000
C	2.90214900	-1.44079100	0.01255600
C	3.37073700	0.05691500	-0.00149100
O	2.37378700	0.90414600	-0.00973900
O	1.59470500	-1.56374900	0.01926900
O	3.70713200	-2.36577700	0.01498800
O	4.56440800	0.34676300	-0.00264900
C	-2.67684400	-0.32578500	0.01007100
O	-2.30261800	0.88969900	0.01077800
C	-4.19676500	-0.69518200	-0.00525900
O	-1.79093900	-1.25908800	0.02142700
O	-4.99575000	0.27323200	0.09942800
O	-4.46361200	-1.92103200	-0.12049500

T10
E(UB+HF-LYP) = -678.014516679

U	0.00036300	-0.18195800	0.00696600
O	0.00442700	-0.18748300	1.85287700
O	-0.00386900	-0.22346000	-1.83805900
O	-0.00488400	-2.74146800	0.02498200
H	0.77437700	-3.24224500	-0.27962200
H	-0.79361800	-3.23104400	-0.27340900
C	-2.88593900	1.32111700	-0.01058900
C	-3.27985100	-0.19836100	0.00303200
O	-2.25614200	-0.99835000	0.01792600
O	-1.59410400	1.52042100	-0.00812200
O	-3.74465800	2.20323600	-0.02288700
O	-4.46723700	-0.53654800	-0.00006800
C	2.88700700	1.31982800	-0.01497400
O	1.59529500	1.51998000	-0.01016600
C	3.27987700	-0.19986900	0.00288600
O	3.74623100	2.20137800	-0.03122300
O	2.25541400	-0.99912700	0.00711800
O	4.46694100	-0.53893200	0.01137500

T11
E(UB+HF-LYP) = -736.608015586

U	0.44558900	0.06454300	-0.01904700

O	0.41410500	0.04442700	-1.87295300
O	0.45587100	0.07890400	1.83363300
C	2.87424200	-2.24546000	-0.00266900
C	1.56002700	-3.11167600	0.03075600
O	0.47072800	-2.42734900	0.00789700
O	2.67654700	-0.97105600	-0.02734600
O	3.98623200	-2.80586400	-0.00308600
O	1.64188000	-4.35457300	0.07677300
C	1.46474800	3.25559100	-0.06742300
O	1.90053200	2.04195400	-0.04605000
C	-0.10348200	3.38661300	-0.06473900
O	2.17319400	4.27957100	-0.08718400
O	-0.73214000	2.26536700	-0.02450900
O	-0.62765300	4.51765000	-0.09989000
C	-3.08391000	-0.58739900	0.69763300
C	-4.89870100	-1.01106400	-0.52773100
O	-2.10570600	-0.57934100	-0.04201000
O	-4.49694600	-1.62467600	-1.48013400
O	-5.80869700	-0.51994400	0.08521000
O	-3.43191400	-0.45227300	1.84932200

T15
E(UB+HF-LYP) = -1397.43253657

U	-3.22837400	-0.44397000	-0.01800000
O	-3.23025200	-0.36395800	1.82543400
O	-3.18979300	-0.48770500	-1.85924600
C	0.13622900	-0.80636000	-0.00753300
C	-0.04568300	0.73276800	-0.02292900
O	-1.21961800	1.17757800	-0.02341000
O	-0.90193800	-1.51454400	0.00233900
O	1.33771700	-1.21905600	-0.01326200
O	1.02781000	1.41304500	-0.03194600
C	-4.96672000	-3.27738900	0.03264600
O	-3.75636500	-2.82439400	0.03515900
C	-6.07565100	-2.16209200	-0.00302900
O	-5.29245400	-4.47641600	0.05557800
O	-5.61192000	-0.95747200	-0.00398400
O	-7.27721400	-2.47965600	-0.02497500
C	-4.94522100	2.85424600	-0.66471500
C	-5.20161900	4.24506400	0.73816500
O	-4.27736700	1.94132600	-0.18508000
O	-6.17428900	3.92633500	1.39266300
O	-4.33364100	5.08285700	0.59273400
O	-5.50247900	3.19143500	-1.68734900
U	3.26269100	0.34094100	-0.05920700
O	3.19785800	0.33171800	-1.84581700
O	3.25680600	0.37050500	1.72412600
C	5.23394100	-3.94907300	-0.09717700
C	5.96621000	2.21247200	-0.08613200
C	4.79752500	3.25387000	-0.06483000
C	4.94336400	-2.60279800	0.60202800
O	6.19260300	-3.95139500	-0.92568700
O	4.29265400	-1.74048900	-0.13646600

O	5.33654300	-2.40931900	1.76250700
O	4.50238500	-4.92911600	0.23019900
O	5.54869800	0.98286600	-0.12958600
O	7.14631800	2.57694300	-0.06819700
O	3.62340600	2.70046700	-0.07747200
O	5.02811200	4.46774500	-0.04025400

S18a
E(RB+HF-LYP) = -671.733608918

U	1.39033600	0.00403100	-0.01942000
O	3.14018700	0.01725700	-0.08138200
O	-0.37056100	-0.03534500	0.00021200
O	1.43764200	-1.74450600	-1.69904400
O	1.45403000	-2.06510700	1.26084300
O	1.44030200	0.44940200	2.41920700
H	2.23319900	-2.23489100	-1.98907700
H	0.66486200	-2.15308500	-2.13897500
H	2.25622600	-2.61232000	1.38683200
H	0.68387700	-2.62784500	1.48230400
H	1.55840400	-0.22899600	3.11022200
H	1.58794400	1.32116100	2.83156800
C	-5.71985700	0.20535200	0.00877900
C	-4.25407300	-0.35437900	0.00064700
O	-5.83967300	1.45712200	-0.01950500
O	-6.61736000	-0.67443600	0.04151600
O	-3.96486900	-1.53692000	-0.01506700
O	-3.30963800	0.62060100	0.01251100
H	-2.43207900	0.19814000	0.00855000
H	2.11153000	1.41076200	-2.70280100
O	1.33083400	1.13428500	-2.18275700
H	0.53566100	1.38278900	-2.69488400
H	0.51776700	2.93861400	0.59744700
O	1.31694800	2.39268900	0.44901800
H	2.07253900	3.00865100	0.35449400

S18b
E(RB+HF-LYP) = -633.892375544

U	-0.70562000	-0.00175500	-0.02115000
O	-2.46049300	-0.07427600	0.01457100
O	1.04924000	0.06347300	-0.11533000
O	-0.77274400	0.95497500	-2.26282300
O	-0.84871600	2.42944600	0.32407400
O	-0.62785300	0.62407400	2.40116600
H	-1.57339600	1.09411300	-2.80659300
H	-0.00889800	1.26500800	-2.78836000
H	-1.67317700	2.93865800	0.18843400
H	-0.10669300	3.05109700	0.18070000
H	-0.54730500	1.54684500	2.70523900
H	-0.25778600	0.05448600	3.10131900
C	5.44297300	-0.12727900	-0.00637200
O	5.14803100	1.06890800	-0.09474200
O	4.26042800	-0.99873700	0.03624600
H	3.46604700	-0.42672800	-0.00822200
H	0.08027500	-2.26721700	-2.02351000

O	-0.69898600	-1.93011200	-1.53885400
H	-1.35746200	-2.65246900	-1.51979800
H	0.17166400	-2.50867700	1.65657400
O	-0.61741700	-1.98276000	1.41718100
H	-1.38595600	-2.40989600	1.84634200

S18c
E(RB+HF-LYP) = -633.891221930

U	0.53294300	-0.16961400	-0.02075600
O	1.77384700	-1.40824700	-0.03139400
O	-0.69318300	1.08145600	-0.08398800
O	-0.03114100	-0.72286400	-2.32019000
O	-1.17687000	-1.93355400	0.12354800
O	-0.06905800	-0.71355800	2.32825600
H	0.42391000	-1.38121700	-2.88303200
H	-0.67014000	-0.24560700	-2.88715800
H	-0.96551700	-2.88122500	-0.00635100
H	-2.13247600	-1.83663200	-0.00168500
H	-0.71752700	-1.39172400	2.59409200
H	0.17130500	-0.19893400	3.12115700
C	-5.13066000	-0.70475600	-0.02198400
O	-4.00246300	-0.83526400	-0.02494900
O	-2.32310500	4.43096200	0.02124600
H	-1.92864100	3.54989800	-0.00594500
H	1.72799700	2.07918100	-1.81482200
O	1.97774000	1.24509500	-1.36843600
H	2.92678800	1.09062900	-1.54792400
H	1.75495600	2.07969400	1.75340100
O	1.84908600	1.12053300	1.57991700
H	2.72372800	0.85247300	1.92762300

T18
E(UB+HF-LYP) = -633.935723611

U	-0.60942600	0.02389700	-0.02206000
O	-2.40972100	0.21048700	-0.00405900
O	1.23389300	-0.16661900	-0.08873400
O	-0.52871000	1.04867600	-2.31521300
O	-0.39825400	2.51523000	0.39544200
O	-0.48036800	0.60062000	2.48231300
H	-1.29657900	1.31469900	-2.85194100
H	0.26809800	1.26346100	-2.83214000
H	-1.13824100	3.13136600	0.24356600
H	0.41869100	3.03242900	0.27321800
H	-0.24357400	1.49428200	2.78380100
H	-0.15368300	-0.02010900	3.15696400
C	4.57807500	-0.29322300	-0.00121400
O	4.61338300	0.90729600	-0.10226700
O	3.57999600	-1.14303500	0.04907200
H	2.64948500	-0.69779100	-0.01037200
H	-0.10492600	-2.35847000	-2.08658300
O	-0.84667300	-1.91774300	-1.63438500
H	-1.57273200	-2.56598400	-1.59662500
H	-0.11648700	-2.67202500	1.66469400
O	-0.82255800	-2.05514300	1.39983300

H	-1.63923000	-2.35918900	1.83621400

T19
E(UB+HF-LYP) = -651.643683628

U	-0.95411000	-0.03097400	-0.02276900
O	-2.73901600	-0.15389900	-0.06354000
O	1.00780900	0.09828600	-0.08917200
O	-1.01819500	1.24882200	-2.11970300
O	-1.15348200	2.33570400	0.68548700
O	-0.86804100	0.21391600	2.45882100
H	-1.81685600	1.42105700	-2.65441900
H	-0.25676800	1.61224400	-2.61104800
H	-2.00725000	2.80997100	0.64400100
H	-0.45562400	3.01871100	0.64761600
H	-0.91249900	1.05020600	2.95641100
H	-0.79175900	-0.51332500	3.10274300
C	4.52772800	1.17615900	0.01135300
O	4.20981000	2.32670500	-0.01678700
O	3.73911100	0.10063500	0.02840700
H	1.99358500	0.11490100	-0.01765500
H	0.02748300	-1.95112500	-2.31080000
O	-0.77049700	-1.73323200	-1.79221600
H	-1.50398200	-2.26768700	-2.15190200
H	-0.13992700	-2.83010900	1.17597800
O	-0.90048500	-2.21710900	1.14637100
H	-1.70353800	-2.76391800	1.25111100
H	4.29085400	-0.76388400	0.04397100
H	5.67489200	-2.22211900	0.75703400
H	5.58275600	-2.23737600	-0.79744700
O	5.07178600	-2.05543900	0.01121200