Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Modeling Intermediates in Carbon Monoxide Coupling Reactions Using Cyclooctatetraene Thorium Derivatives

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Supporting Information

Tables S1 to S16: Optimized coordinates of the reported $(C_8H_8)_2Th_2(CO)_n$ (n =1 to 7) structures.

Tables S17 to S32: Harmonic vibrational frequencies and infrared intensities (in for the studied $(C_8H_8)_2Th_2(CO)_n$ (n = 1 to 7) structures.

Complete Gaussian09 reference (Reference 44).

Table S1. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_2$ structures **2S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.16177700	0.69513500	-0.00072000	-0.15963800	0.69415300	-0.00035600
C	-0.16171300	-0.69545100	-0.00072400	0.15961300	-0.69495900	-0.00021900
O	0.87235900	-1.65645200	-0.00063100	-0.85529000	-1.64824200	-0.00031200
O	-0.87228700	1.65611200	-0.00092300	0.85506500	1.64756100	-0.00022400
Th	2.41102400	-0.14063000	-0.00034400	-2.40214100	-0.14287600	0.00001900
Th	-2.41096000	0.14027000	-0.00038800	2.40201100	0.14219700	-0.00005400
C	-4.36414000	-0.20830000	-1.85307000	4.37224000	-0.20590600	1.83925200
C	-4.13272300	-1.51599800	-1.34429500	4.14011300	-1.50301900	1.33538800
C	-4.05389000	-2.08717000	-0.04986600	4.05962800	-2.07046700	0.05159000
C	-4.12068800	-1.58668900	1.27397700	4.12974900	-1.57522200	-1.26211000
C	-4.34142600	-0.30785400	1.85476800	4.35213100	-0.30750800	-1.83903900
C	-4.64686000	0.98489300	1.34592800	4.65045900	0.97623200	-1.33497700
C	-4.80533800	1.54066100	0.05156900	4.80304500	1.52976800	-0.05127600
C	-4.66760600	1.05393300	-1.27226200	4.66916300	1.04683000	1.26224100
H	-3.76585700	-3.14153100	-0.07963900	3.77333700	-3.11537900	0.08178600
H	-3.87483000	-2.34649200	2.02120200	3.88954400	-2.32948500	-2.00284100
H	-4.23406300	-0.31613100	2.94341600	4.25161600	-0.31762300	-2.91872200
H	-4.71633000	1.73795000	2.13627900	4.72211400	1.72138400	-2.11942700
H	-4.96872300	2.62169900	0.08139600	4.96355500	2.60151900	-0.08157600
H	-4.74911400	1.84770100	-2.02048400	4.75149200	1.83356700	2.00384900
H	-4.27042700	-0.15814200	-2.94185900	4.28383300	-0.15649000	2.91891600
H	-3.89453100	-2.23417700	-2.13400600	3.90670200	-2.21488500	2.11905300
C	4.05760500	2.05255800	-0.36380100	-4.06264600	2.03525800	0.36841400
C	4.09282600	1.78195700	1.02616100	-4.09948100	1.77220500	-1.01149900
C	4.28125800	0.61837900	1.81888200	-4.29069500	0.62145200	-1.80229300
C	4.58350700	-0.74464900	1.54330800	-4.58797600	-0.73209800	-1.53408300
C	4.79604800	-1.50578500	0.36511000	-4.79453300	-1.49297800	-0.36806300
C	4.72110000	-1.24297000	-1.02464400	-4.72261300	-1.23678700	1.01145100
C	4.42985600	-0.09964700	-1.81715100	-4.43853300	-0.10433000	1.80211200
C	4.16948700	1.27201200	-1.54208200	-4.17805300	1.25683300	1.53446800
H	4.13718500	0.80848700	2.88649500	-4.15276500	0.81496900	-2.86031000
H	4.61677200	-1.35640100	2.44956700	-4.62432500	-1.33419800	-2.43518200
H	4.95388100	-2.56661100	0.57957600	-4.95018900	-2.54376400	-0.58484200
H	4.83404000	-2.14863700	-1.62752300	-4.83606900	-2.13628700	1.60611200
H	4.37507800	-0.33124700	-2.88491400	-4.38957500	-0.33683800	2.86016000
H	3.95501500	1.84613200	-2.44803800	-3.96936700	1.82321200	2.43515300
H	3.77188900	3.08614000	-0.57743900	-3.77857500	3.05872700	0.58422500
H	3.82920200	2.65632000	1.62772200	-3.83965600	2.64136900	-1.60490100

Table S2. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_2$ structures **2S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	-0.18410800	0.56663200	-0.86637000	-0.19226300	-0.57675500	-0.85348200
C	-0.18290100	-0.85321800	-0.59143700	-0.14989300	-1.00031800	0.51558000
O	0.90469400	-1.63109500	-0.89171800	0.93343400	-1.63953800	1.02994200
O	0.90228400	1.17810600	-1.43509200	0.84972200	-0.78261200	-1.69345000
Th	2.33414600	-0.05295100	-0.27192200	2.31892100	-0.31645900	-0.09256700
Th	-2.37401800	-0.04016400	-0.18435400	-2.33946200	-0.22735800	0.08276300
C	-4.90713500	-0.58334300	-1.07957700	-4.95586600	-1.07580400	0.00044200
C	-4.64681600	-1.59443200	-0.11608400	-4.84149800	-0.48118500	1.27232700
C	-4.14048600	-1.61028300	1.20858200	-4.31995100	0.72955100	1.76012000
C	-3.67429400	-0.62351600	2.11816200	-3.69680400	1.85286900	1.18004900
C	-3.55775300	0.79411200	2.09094100	-3.37661100	2.24691900	-0.13686200
C	-3.87021500	1.80907700	1.14534000	-3.54383600	1.67507100	-1.41516400
C	-4.39695100	1.82581700	-0.17223100	-4.06892100	0.46309900	-1.90348500
C	-4.81138900	0.83490000	-1.09980400	-4.64071100	-0.68319500	-1.31693600
H	-4.00029900	-2.62571300	1.58992900	-4.33629300	0.78175100	2.84312400
H	-3.25962700	-1.05881300	3.03188300	-3.34351700	2.56150200	1.92090400
H	-3.07437600	1.19165200	2.98799300	-2.83057900	3.18297000	-0.16942300
H	-3.57031700	2.80337100	1.48827600	-3.08919800	2.27269100	-2.19665800
H	-4.40869500	2.83122400	-0.60267300	-3.92564000	0.35331000	-2.97223400
H	-5.07119100	1.25736300	-2.07494500	-4.84316400	-1.46298100	-2.04266800
H	-5.22435600	-0.99476000	-2.04247100	-5.34925900	-2.08536800	0.04796100
H	-4.80816700	-2.60081500	-0.51324800	-5.16768000	-1.14189600	2.06795200
C	4.10389500	1.96828400	0.41341200	3.94465700	1.41433300	-1.51790500
C	3.43274700	1.62372200	1.61358500	3.19335900	2.22260900	-0.64547800
C	3.15244800	0.40799000	2.29470100	2.91502800	2.20697600	0.73710700
C	3.46215400	-0.96084900	2.07024400	3.30058400	1.38900200	1.81931400
C	4.14230500	-1.68130600	1.05664100	4.09246800	0.23525300	1.96128900
C	4.75642100	-1.34278200	-0.17496600	4.79374300	-0.60571200	1.07952100
C	4.98660700	-0.13270600	-0.88432100	5.03006400	-0.61830300	-0.31047100
C	4.73104000	1.24204400	-0.62929300	4.69102300	0.23083700	-1.38372200
H	2.52837300	0.55744300	3.18067300	2.21550100	2.98226700	1.02964900
H	3.01735100	-1.61782900	2.82321700	2.82492600	1.68205500	2.74854900
H	4.09082800	-2.76273500	1.21090200	4.07644800	-0.15169400	2.97381000
H	5.07010700	-2.22403800	-0.74194500	5.19730300	-1.48163300	1.57518300
H	5.43904200	-0.30082200	-1.86597900	5.57730200	-1.49757000	-0.63185100
H	5.02959600	1.88278500	-1.46401500	5.03381900	-0.15304700	-2.33811700
H	4.02988400	3.03600400	0.18883600	3.84158800	1.72097100	-2.55255700
H	2.97104500	2.48909300	2.09776700	2.65445100	3.00589900	-1.16663900

Table S3. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_3$ structures **3S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	-1.00728800	2.15090200	0.17424300	-0.82918100	2.18084400	0.04916000
C	-0.11310900	0.33770100	-0.92544900	-0.10552300	0.14551600	-1.10883900
C	-0.17354700	-0.93217200	-0.27747900	-0.16601000	-1.05018400	-0.33224600
O	0.88435100	-1.80208800	-0.35308400	0.87591300	-1.91783100	-0.33329300
O	0.95111600	0.80845600	-1.61648000	0.95651900	0.51480800	-1.84013800
O	-0.27251800	3.04850100	0.16618800	-0.02064000	2.98675500	-0.02428300
Th	2.40746000	-0.19445500	-0.23748500	2.37550200	-0.28186000	-0.29622100
Th	-2.38250700	0.01169400	-0.08782500	-2.31534200	-0.00377700	-0.14816200
C	-4.82207300	1.06470500	-0.85841400	-4.78928000	1.12577600	-0.70648700
C	-4.68385600	-0.18295500	-1.52304800	-4.77641900	-0.13941600	-1.32526600
C	-4.39918500	-1.51555100	-1.10833900	-4.49908700	-1.45660200	-0.89584000
C	-4.07247600	-2.13480200	0.12227400	-4.07561000	-2.04213400	0.30941400
C	-3.85369100	-1.68076200	1.45062900	-3.71733900	-1.55661900	1.58349100
C	-3.92476800	-0.42189200	2.10448000	-3.67080200	-0.28416400	2.18622200
C	-4.26961900	0.89627100	1.69776700	-3.98690600	1.02478600	1.76476000
C	-4.66230500	1.50415500	0.47867200	-4.46826100	1.60268300	0.57581800
H	-4.35143600	-2.21107100	-1.95121300	-4.56745800	-2.17632400	-1.70397800
H	-3.82959500	-3.19414500	0.00269100	-3.88941100	-3.10513600	0.20864900
H	-3.48944700	-2.47465400	2.10826100	-3.32595700	-2.33549500	2.22747400
H	-3.60632800	-0.47129300	3.14961800	-3.25837100	-0.31201500	3.18844400
H	-4.15036500	1.62344000	2.50589400	-3.75499300	1.76691700	2.52046000
H	-4.77472400	2.58761900	0.57499300	-4.51964900	2.68395400	0.63774800
H	-5.03595800	1.88547800	-1.54895700	-5.04046800	1.92288800	-1.39720200
H	-4.81373800	-0.10075300	-2.60600700	-5.01918300	-0.09069300	-2.38095300
C	3.54348300	-0.40640600	2.24361100	3.02597300	0.17611600	2.30069200
C	4.12370900	-1.47155700	1.50971500	3.72004900	-1.00971000	1.99361100
C	4.71113300	-1.60276800	0.22718500	4.55020800	-1.43291800	0.94193800
C	5.00196000	-0.71202100	-0.84178100	5.05220000	-0.83961100	-0.23380200
C	4.86953100	0.68907200	-1.04240800	4.97180600	0.44362600	-0.81243100
C	4.35804400	1.76664600	-0.27660600	4.34117600	1.65268600	-0.46468900
C	3.71967300	1.88906400	0.98226100	3.48875200	2.06883000	0.57231200
C	3.36171300	0.98618800	2.01959500	2.92462200	1.45329300	1.70756400
H	4.92515300	-2.64416200	-0.02943400	4.80000900	-2.48560600	1.01143000
H	5.39099400	-1.22798800	-1.72431900	5.60291600	-1.54060100	-0.85113600
H	5.17822000	0.99750400	-2.04535900	5.47375600	0.49771700	-1.77205100
H	4.36090200	2.70824500	-0.83252700	4.46411400	2.41476900	-1.22576400
H	3.35019300	2.90161100	1.16610100	3.10601900	3.07085200	0.41612600
H	2.78895800	1.46852400	2.81690300	2.22022000	2.09697300	2.22299400
H	3.07488000	-0.74441600	3.17224800	2.38110300	0.06841800	3.16561600
H	3.98900800	-2.43727500	2.00458700	3.47640400	-1.81593000	2.67595300

Table S4. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_3$ structures **3S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.09936600	0.51029100	0.43647700	0.04489400	0.56400900	0.43251500
C	-0.20796600	-0.55399800	-0.46623400	-0.26268100	0.04563000	-0.86255300
O	0.78982700	-1.13912700	-1.21907300	0.80993200	0.10242000	-1.73969900
O	-0.92606200	1.11704600	1.16531400	-0.82947000	0.66912700	1.46398000
Th	2.39021700	-0.09498200	-0.11818800	2.38532700	-0.01196600	-0.25815700
Th	-2.48756200	0.02130600	0.13102700	-2.42335900	0.01569200	0.07463700
C	-4.51803800	1.25411100	-1.17564200	-4.70538900	1.44930900	-0.31300100
C	-4.21120500	0.11593700	-1.97269300	-4.48497300	0.78980700	-1.54128200
C	-4.06260300	-1.27192400	-1.72018600	-4.24369100	-0.54221100	-1.92375500
C	-4.09654900	-2.09051000	-0.56423000	-4.05906100	-1.75554500	-1.23978600
C	-4.30961100	-1.86422400	0.82152900	-4.06422300	-2.14841100	0.11397200
C	-4.64393300	-0.72994600	1.61326000	-4.32181800	-1.49541700	1.33833100
C	-4.88991200	0.64225200	1.34615000	-4.65534700	-0.18027100	1.71263700
C	-4.83045600	1.46458400	0.19465300	-4.80540800	1.03928100	1.03194500
H	-3.74806700	-1.82381300	-2.61005900	-4.05236900	-0.63623000	-2.98641700
H	-3.80169100	-3.12192700	-0.77600300	-3.76116300	-2.56122000	-1.90095000
H	-4.14809900	-2.76278900	1.42400600	-3.78006100	-3.18622200	0.24785100
H	-4.68037200	-0.96244100	2.68151200	-4.18756900	-2.14961600	2.19253700
H	-5.07111600	1.21669900	2.25902900	-4.71507600	-0.06192300	2.78858800
H	-4.97512300	2.52293200	0.42962100	-4.95298800	1.87461800	1.70713900
H	-4.48106900	2.18695500	-1.74569300	-4.79978800	2.52326400	-0.42918800
H	-3.98939700	0.38014800	-3.01058500	-4.44381200	1.47713300	-2.37871900
C	4.20820100	1.02279800	1.63705000	3.69933700	0.10449200	2.13922800
C	3.93279300	-0.28055100	2.12153300	3.28054200	-1.23274300	2.00581700
C	3.94802300	-1.58966700	1.55904900	3.39328600	-2.21983300	1.00296400
C	4.22598300	-2.12666700	0.27865300	3.96206500	-2.27185700	-0.28233200
C	4.56483100	-1.58086900	-0.98724500	4.64964800	-1.35870100	-1.10688300
C	4.77496500	-0.27366100	-1.48988500	5.04489400	-0.01499300	-0.98622600
C	4.75448000	1.03090000	-0.92655600	4.92163700	0.97309900	0.01199700
C	4.54521500	1.56515400	0.37189100	4.37657300	1.01930400	1.31083300
H	3.61455300	-2.35109500	2.27031400	2.86681200	-3.13196200	1.26122200
H	4.05856100	-3.20658900	0.23457300	3.77552800	-3.21747600	-0.77906200
H	4.59848500	-2.34120400	-1.77252300	4.86854900	-1.76950100	-2.08604900
H	4.93065800	-0.25928700	-2.57249800	5.49375800	0.36966700	-1.89526500
H	4.89790100	1.81139400	-1.67907400	5.29440900	1.93798700	-0.31324400
H	4.57449800	2.65807400	0.38143300	4.42795300	2.01139300	1.74532900
H	4.03403400	1.79497500	2.39147000	3.34791200	0.55832800	3.05862200
H	3.59224500	-0.27845700	3.16095500	2.68486000	-1.56540500	2.84825500
C	1.37602700	2.27190800	-0.58162400	1.60608400	2.58130900	-0.18390700
O	0.81091200	3.28104600	-0.59596000	1.15674100	3.61774400	-0.04014200

Table S5. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_4$ structures **4S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.00000000	1.47176300	0.32471000	0.00000000	1.55856200	0.31593800
C	-1.47176300	0.00000000	0.32471000	-1.55856200	0.00000000	0.31593800
C	0.00000000	-1.47176300	0.32471000	0.00000000	-1.55856200	0.31593800
C	1.47176300	0.00000000	0.32471000	1.55856200	0.00000000	0.31593800
O	2.05402500	0.00000000	-0.75339000	2.10412700	0.00000000	-0.75978500
O	0.00000000	-2.05402500	-0.75339000	0.00000000	-2.10412700	-0.75978500
O	-2.05402500	0.00000000	-0.75339000	-2.10412700	0.00000000	-0.75978500
O	0.00000000	2.05402500	-0.75339000	0.00000000	2.10412700	-0.75978500
Th	0.00000000	0.00000000	-2.19328400	0.00000000	0.00000000	-2.16279300
Th	0.00000000	0.00000000	2.28404700	0.00000000	0.00000000	2.24953700
C	-1.85325800	0.00000000	4.32399500	-1.83895800	0.00000000	4.30210900
C	-1.31021500	-1.31021500	4.32297700	-1.30011800	-1.30011800	4.30182600
C	0.00000000	-1.85325800	4.32399500	0.00000000	-1.83895800	4.30210900
C	1.31021500	-1.31021500	4.32297700	1.30011800	-1.30011800	4.30182600
C	1.85325800	0.00000000	4.32399500	1.83895800	0.00000000	4.30210900
C	1.31021500	1.31021500	4.32297700	1.30011800	1.30011800	4.30182600
C	0.00000000	1.85325800	4.32399500	0.00000000	1.83895800	4.30210900
C	-1.31021500	1.31021500	4.32297700	-1.30011800	1.30011800	4.30182600
H	0.00000000	-2.94323600	4.23388900	0.00000000	-2.91956400	4.21419400
H	2.08106900	-2.08106900	4.23425800	2.06430200	-2.06430200	4.21462800
H	2.94323600	0.00000000	4.23388900	2.91956400	0.00000000	4.21419400
H	2.08106900	2.08106900	4.23425800	2.06430200	2.06430200	4.21462800
H	0.00000000	2.94323600	4.23388900	0.00000000	2.91956400	4.21419400
H	-2.08106900	2.08106900	4.23425800	-2.06430200	2.06430200	4.21462800
H	-2.94323600	0.00000000	4.23388900	-2.91956400	0.00000000	4.21419400
H	-2.08106900	-2.08106900	4.23425800	-2.06430200	-2.06430200	4.21462800
C	0.00000000	1.85176500	-4.18314500	0.00000000	1.83784900	-4.14900500
C	1.30889000	1.30889000	-4.18109800	1.29900100	1.29900100	-4.14621000
C	1.85176500	0.00000000	-4.18314500	1.83784900	0.00000000	-4.14900500
C	1.30889000	-1.30889000	-4.18109800	1.29900100	-1.29900100	-4.14621000
C	0.00000000	-1.85176500	-4.18314500	0.00000000	-1.83784900	-4.14900500
C	-1.30889000	-1.30889000	-4.18109800	-1.29900100	-1.29900100	-4.14621000
C	-1.85176500	0.00000000	-4.18314500	-1.83784900	0.00000000	-4.14900500
C	-1.30889000	1.30889000	-4.18109800	-1.29900100	1.29900100	-4.14621000
H	2.93823200	0.00000000	-4.06361100	2.91416600	0.00000000	-4.02365300
H	2.07756700	-2.07756700	-4.06422200	2.06072500	-2.06072500	-4.02655900
H	0.00000000	-2.93823200	-4.06361100	0.00000000	-2.91416600	-4.02365300
H	-2.07756700	-2.07756700	-4.06422200	-2.06072500	-2.06072500	-4.02655900
H	-2.93823200	0.00000000	-4.06361100	-2.91416600	0.00000000	-4.02365300
H	-2.07756700	2.07756700	-4.06422200	-2.06072500	2.06072500	-4.02655900
H	0.00000000	2.93823200	-4.06361100	0.00000000	2.91416600	-4.02365300
H	2.07756700	2.07756700	-4.06422200	2.06072500	2.06072500	-4.02655900

Table S6. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_4$ structures **4S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	1.24168000	-0.99727900	1.78788400	-1.35145100	0.77028400	1.63847600
C	-0.68009400	-0.12357700	0.71812100	0.89579000	0.14542000	0.72484300
C	-0.68009400	-0.12357700	-0.71812100	0.89579000	0.14542000	-0.72484300
O	-1.11564800	0.93767000	-1.43312100	1.33241900	-0.92150100	-1.40011800
O	-1.11564800	0.93767000	1.43312100	1.33241900	-0.92150100	1.40011800
O	1.63434700	-0.28549100	2.61125400	-1.75440500	-0.02818300	2.34978800
Th	-0.34471700	2.47229000	0.00000000	0.44492400	-2.42468500	0.00000000
Th	-0.01548500	-2.36655500	0.00000000	0.07654200	2.30971100	0.00000000
C	-0.90355600	-4.33560300	1.71692500	0.75257600	4.36472500	1.70382300
C	-1.89284200	-4.21673300	0.71358000	1.74185800	4.36111200	0.70690500
C	-1.89284200	-4.21673300	-0.71358000	1.74185800	4.36111200	-0.70690500
C	-0.90355600	-4.33560300	-1.71692500	0.75257600	4.36472500	-1.70382300
C	0.51119600	-4.48127000	-1.71479300	-0.65796600	4.36260200	-1.70292700
C	1.50319700	-4.57605100	-0.71082800	-1.64636400	4.36248400	-0.70464900
C	1.50319700	-4.57605100	0.71082800	-1.64636400	4.36248400	0.70464900
C	0.51119600	-4.48127000	1.71479300	-0.65796600	4.36260200	1.70292700
H	-2.88640100	-4.01877300	-1.12587100	2.74198400	4.27356000	-1.11631300
H	-1.31145800	-4.22020900	-2.72497700	1.16795000	4.28954300	-2.70233200
H	0.93418000	-4.45422200	-2.72262700	-1.07329400	4.28875700	-2.70159400
H	2.51515400	-4.59406400	-1.12530300	-2.64634100	4.27573700	-1.11503500
H	2.51515400	-4.59406400	1.12530300	-2.64634100	4.27573700	1.11503500
H	0.93418000	-4.45422200	2.72262700	-1.07329400	4.28875700	2.70159400
H	-1.31145800	-4.22020900	2.72497700	1.16795000	4.28954300	2.70233200
H	-2.88640100	-4.01877300	1.12587100	2.74198400	4.27356000	1.11631300
C	1.69612200	3.73065100	-1.31271100	-1.75119200	-3.37362100	-1.30215100
C	0.52426600	4.31644800	-1.85306600	-0.69199100	-4.12765200	-1.83747500
C	-0.67582800	4.84214700	-1.31257200	0.40222000	-4.83014200	-1.30175000
C	-1.18338700	5.04388100	0.00000000	0.86698400	-5.10880900	0.00000000
C	-0.67582800	4.84214700	1.31257200	0.40222000	-4.83014200	1.30175000
C	0.52426600	4.31644800	1.85306600	-0.69199100	-4.12765200	1.83747500
C	1.69612200	3.73065100	1.31271100	-1.75119200	-3.37362100	1.30215100
C	2.17562800	3.46988200	0.00000000	-2.18134400	-3.04267100	0.00000000
H	-1.41026000	5.08717100	-2.08501800	1.08104800	-5.18695600	-2.06808200
H	-2.21410600	5.40985600	0.00000000	1.81693500	-5.63151800	0.00000000
H	-1.41026000	5.08717100	2.08501800	1.08104800	-5.18695600	2.06808200
H	0.49246800	4.24809800	2.94383400	-0.65129700	-4.06613600	2.91889400
H	2.35276300	3.32128700	2.08515100	-2.32907400	-2.87046500	2.06813800
H	3.11698700	2.91314200	0.00000000	-3.01462700	-2.34766000	0.00000000
H	2.35276300	3.32128700	-2.08515100	-2.32907400	-2.87046500	-2.06813800
H	0.49246800	4.24809800	-2.94383400	-0.65129700	-4.06613600	-2.91889400
C	1.24168000	-0.99727900	-1.78788400	-1.35145100	0.77028400	-1.63847600
O	1.63434700	-0.28549100	-2.61125400	-1.75440500	-0.02818300	-2.34978800

Table S7. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_4$ structures **4S-3.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.12002900	0.54203200	0.46238500	0.00906400	1.08806200	0.40503900
C	-0.16585300	-0.29639900	-0.65139100	-0.17469700	0.40894800	-0.90418200
O	0.83197200	-0.48410000	-1.57399100	0.82583400	0.69905000	-1.76735600
O	-0.81233900	0.77788600	1.42437000	-0.84752800	1.16475800	1.35783500
Th	2.47185700	0.02668400	-0.18976100	2.33957800	-0.05413800	-0.31981200
Th	-2.46220700	-0.01496100	0.14302100	-2.42407500	0.01587500	0.05592300
C	-4.39415200	1.95167600	0.20025200	-4.64572900	1.32782100	1.04653200
C	-4.13910400	1.69338300	-1.16882400	-4.63032500	1.60842500	-0.32960000
C	-4.07691900	0.52444600	-1.97989400	-4.49263500	0.83484900	-1.50084600
C	-4.26042400	-0.86346800	-1.75577300	-4.36359400	-0.54146000	-1.77829100
C	-4.52733700	-1.66243400	-0.61520800	-4.26266700	-1.70611300	-0.99932800
C	-4.73147400	-1.40543400	0.76603900	-4.23261200	-1.98028000	0.38148900
C	-4.79999900	-0.24053600	1.57653100	-4.33884900	-1.20594100	1.55462900
C	-4.66469800	1.14962400	1.34014900	-4.51388000	0.16388500	1.82740600
H	-3.77141900	0.74626200	-3.00632400	-4.44120300	1.44385300	-2.39621400
H	-4.06699100	-1.46118700	-2.65070200	-4.22610600	-0.73726400	-2.83547200
H	-4.49363500	-2.73214700	-0.83862800	-4.06299600	-2.58726600	-1.59776600
H	-4.80992900	-2.32527100	1.35227900	-4.02078900	-3.02228700	0.59132600
H	-4.92098300	-0.47641600	2.63770100	-4.19184700	-1.79357100	2.45373200
H	-4.70865900	1.73692900	2.26155500	-4.47024000	0.38184700	2.88837800
H	-4.27592100	3.00895200	0.45374300	-4.68155700	2.22672600	1.65122800
H	-3.86728100	2.59706200	-1.72203000	-4.65719900	2.67200400	-0.53796200
C	3.73587800	-0.54892900	2.15284600	2.79218700	-1.19322400	2.09279000
C	3.81162400	-1.75170000	1.39565700	3.11208800	-2.22540800	1.18659400
C	4.21868600	-2.08495400	0.08029100	3.88890800	-2.32433600	0.02444900
C	4.70454100	-1.35477900	-1.03680400	4.67958000	-1.43682000	-0.73103800
C	4.98767400	0.00948800	-1.29438200	5.07020800	-0.09209200	-0.58412400
C	4.90533300	1.20987000	-0.53874600	4.84482100	0.90446100	0.38567600
C	4.53236200	1.54089700	0.79115200	4.07675500	1.00041400	1.55926700
C	4.05089200	0.81231400	1.90930500	3.20000000	0.14546300	2.25361700
H	4.04977900	-3.13989700	-0.15346800	3.76716700	-3.28283300	-0.46693400
H	4.82464100	-1.98207400	-1.92454100	5.03514200	-1.87654500	-1.65587800
H	5.27134300	0.19018300	-2.33519800	5.66119100	0.26611200	-1.41961500
H	5.13933600	2.09499900	-1.13685200	5.30323200	1.84975400	0.11709800
H	4.55419600	2.61872400	0.97363300	4.08767600	2.00136000	1.97633800
H	3.78474000	1.46029700	2.74881000	2.68175800	0.64631900	3.06306700
H	3.28151700	-0.70347100	3.13549300	2.03605900	-1.48766100	2.81190700
H	3.39967900	-2.60896500	1.93584800	2.52575600	-3.11923600	1.36345400
C	1.40050600	2.41060000	-0.44958500	2.37805900	2.75463500	-0.34098000
C	-1.19859200	-2.29901500	0.09685900	-0.36911900	-1.12766900	-0.60214100
O	0.86951200	3.43491500	-0.40333300	2.25437900	3.87344800	-0.20595900
O	-0.55324200	-3.24109600	-0.09827800	0.65397400	-1.80717900	-0.87682400

Table S8. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_4$ structures **4S-4.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.17909900	0.49744900	-0.63589900	0.18723100	0.34811600	-0.68796900
C	-0.11344500	0.17181400	0.72987900	-0.11637300	0.05519600	0.67981700
O	0.78778500	-0.28458400	1.62343800	0.75959100	-0.38458300	1.59369900
O	-0.90267600	0.99539000	-1.34596700	-0.87257300	0.86226900	-1.40320100
Th	2.41442600	-0.04785800	0.08088800	2.40116000	-0.10246700	0.08960200
Th	-2.47682500	0.06906100	-0.14949500	-2.47574800	0.02947300	-0.18852700
C	-3.98440500	-1.74997000	-1.56076500	-4.12441200	-1.84991900	-1.33258800
C	-3.51234400	-2.44814200	-0.42127600	-3.62457500	-2.44979300	-0.16241200
C	-3.49462600	-2.19531800	0.97873800	-3.53067700	-2.06853300	1.19293400
C	-3.95349900	-1.14575100	1.81553200	-3.90193800	-0.93239300	1.93608300
C	-4.58697900	0.10440200	1.59405900	-4.49492800	0.30618700	1.62601300
C	-5.02987000	0.81731400	0.44800700	-4.97273400	0.91562700	0.44822600
C	-5.05672400	0.56261500	-0.94979600	-5.08480700	0.52826500	-0.90298800
C	-4.62461800	-0.50109000	-1.78042300	-4.73471900	-0.61686700	-1.63903900
H	-2.95501800	-2.96707100	1.53471500	-2.99434200	-2.79642300	1.79083300
H	-3.68659500	-1.30018200	2.86455600	-3.58323300	-0.99232200	2.97027900
H	-4.69632600	0.68541800	2.51388600	-4.52746100	0.97455900	2.47913000
H	-5.39557400	1.81765400	0.69613400	-5.28838100	1.93984600	0.61242100
H	-5.43759100	1.41359400	-1.52178100	-5.46888100	1.32468500	-1.53051900
H	-4.75402600	-0.28042400	-2.84375900	-4.91604400	-0.49840500	-2.70134100
H	-3.73713700	-2.26122300	-2.49558300	-3.94646200	-2.45360400	-2.21549600
H	-2.98340000	-3.36894100	-0.68394800	-3.14655300	-3.40347700	-0.35656800
C	4.27312600	-0.35842900	-1.93261300	4.27956000	-0.20600100	-1.92851000
C	4.73069700	0.76049100	-1.19535400	4.66903900	0.89031300	-1.14094100
C	4.92063400	1.04663700	0.18219700	4.85591000	1.11111900	0.23754200
C	4.81203000	0.30564000	1.39057800	4.79954500	0.30795400	1.39545100
C	4.43893900	-1.02082700	1.71527500	4.50059900	-1.04041000	1.65068200
C	3.98821000	-2.14670700	0.97797700	4.10730200	-2.13994600	0.86360000
C	3.71043900	-2.40564500	-0.38551900	3.84735600	-2.34341600	-0.50195200
C	3.81573000	-1.65745300	-1.59411800	3.91066100	-1.53709100	-1.66119100
H	5.18676400	2.09272600	0.35728800	5.06198700	2.15102900	0.46508200
H	5.01015600	0.91668300	2.27580400	4.97221500	0.87604500	2.30262800
H	4.41688900	-1.19573300	2.79443400	4.49596500	-1.26984300	2.71009000
H	3.70141900	-2.97943500	1.62620200	3.87177000	-3.01221000	1.46277200
H	3.25895000	-3.38941700	-0.54378500	3.45856900	-3.33417100	-0.70949300
H	3.42792100	-2.20464500	-2.45804800	3.55858300	-2.05639900	-2.54527400
H	4.15829600	-0.13992800	-2.99785500	4.14390900	0.05887900	-2.97078400
H	4.89246400	1.63762400	-1.82749800	4.76612000	1.80152000	-1.72048800
C	1.79560700	2.25467400	-0.96282700	1.74022900	2.39703600	-0.72735400
C	-1.60467300	1.96759400	1.45199000	-1.51692900	2.18316200	1.15931000
O	1.37907800	3.16108000	-1.54197900	1.26233100	3.30625800	-1.21796100
O	-1.14059000	2.68553000	2.22576200	-0.96395200	2.97957300	1.75642500

Table S9. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_5$ structures **5S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	-1.15832400	-1.29530100	1.79587100	0.90324400	-1.34880700	-1.70611600
C	-0.20878700	0.59557100	0.71954500	0.21507600	0.83837200	-0.72759800
C	-0.20878800	0.59556900	-0.71954600	0.21506300	0.83826700	0.72759000
O	0.85901400	0.99204000	-1.44036600	-0.86941000	1.22340900	1.39348900
O	0.85901600	0.99204400	1.44036300	-0.86937500	1.22359200	-1.39348300
O	-0.47083700	-1.70926600	2.62891200	0.13447500	-1.72164100	-2.46515300
Th	2.37026100	0.14088700	-0.00000200	-2.32667200	0.18421800	-0.00008500
Th	-2.47188200	0.00910700	0.00000100	2.38924100	0.05577100	-0.00004200
C	-4.40304500	0.97952600	1.71681400	4.42862800	0.78103900	-1.70358400
C	-4.24200300	1.96292000	0.71355400	4.39738500	1.77007400	-0.70708100
C	-4.24200100	1.96292100	-0.71355200	4.39731300	1.77011500	0.70707700
C	-4.40304100	0.97953000	-1.71681400	4.42845400	0.78113800	1.70364000
C	-4.60886500	-0.42772100	-1.71469000	4.46215400	-0.62899000	1.70261700
C	-4.74550900	-1.41491100	-0.71083500	4.48397900	-1.61737400	0.70491300
C	-4.74550900	-1.41491300	0.71082900	4.48403900	-1.61741400	-0.70471500
C	-4.60886700	-0.42772500	1.71468700	4.46231800	-0.62908700	-1.70247900
H	-4.00203000	2.94713500	-1.12594300	4.28366300	2.76757400	1.11652200
H	-4.27050900	1.38210400	-2.72490600	4.34342000	1.19425400	2.70228300
H	-4.60013000	-0.85136900	-2.72258300	4.39929400	-1.04577500	2.70142400
H	-4.80695000	-2.42514600	-1.12538800	4.42240200	-2.61909300	1.11554500
H	-4.80694800	-2.42514900	1.12538000	4.42250100	-2.61915700	-1.11529600
H	-4.60013100	-0.85137500	2.72257900	4.39955000	-1.04592900	-2.70126800
H	-4.27051600	1.38209900	2.72490600	4.34370300	1.19410100	-2.70226000
H	-4.00203300	2.94713200	1.12594800	4.28378200	2.76751000	-1.11659500
C	3.06217400	-2.43116500	-0.70847600	-2.78356500	-2.42412600	0.70321200
C	3.63862400	-1.60757200	-1.71296900	-3.42818800	-1.66435600	1.70020000
C	4.45008700	-0.44777100	-1.71530400	-4.33328700	-0.58894300	1.70171000
C	5.00970400	0.38412800	-0.71089600	-4.95919700	0.18538700	0.70532300
C	5.00957500	0.38394800	0.71143700	-4.95941900	0.18543400	-0.70468500
C	4.44977900	-0.44820700	1.71553000	-4.33382600	-0.58883600	-1.70132000
C	3.63831000	-1.60800300	1.71275400	-3.42873500	-1.66425600	-1.70016100
C	3.06204400	-2.43134500	0.70794800	-2.78379800	-2.42408700	-0.70342700
H	4.62177700	-0.05861200	-2.72271200	-4.53310400	-0.21723300	2.70020500
H	5.53171000	1.24972700	-1.12825700	-5.53188500	1.00822800	1.11852200
H	5.53149800	1.24944600	1.12911100	-5.53223800	1.00830100	-1.11765000
H	4.62127600	-0.05929800	2.72306900	-4.53397000	-0.21707200	-2.69972900
H	3.32541500	-1.90046500	2.71864600	-3.09071800	-1.92249100	-2.69724700
H	2.42092400	-3.21166300	1.12738100	-2.07877700	-3.13521600	-1.11864400
H	2.42112700	-3.21137400	-1.12822300	-2.07841300	-3.13528200	1.11816100
H	3.32591100	-1.89977900	-2.71899100	-3.08985000	-1.92264400	2.69716200
C	-1.15832500	-1.29530000	-1.79587000	0.90345500	-1.34912400	1.70599400
O	-0.47083500	-1.70926600	-2.62890800	0.13487600	-1.72210700	2.46513800
C	3.01990200	2.81603200	0.00000100	-2.78711500	2.97518500	0.00015600
O	3.35647700	3.90643000	0.00000200	-2.77612100	4.10465600	0.00034800

Table S10. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_5$ structures **5S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.82089000	-2.12955500	0.45832200	0.65153200	-2.12684300	0.58331600
C	0.04817900	-0.31193100	-0.94826400	0.04638100	-0.24835700	-1.10190800
C	0.02720500	0.92528500	-0.23672900	0.02241200	0.99431900	-0.39869000
O	-1.03262300	1.76085800	-0.23944000	-1.01625800	1.83776200	-0.43943000
O	-1.01329800	-0.71373800	-1.69229800	-0.99792700	-0.63310500	-1.85569600
O	0.06408500	-3.00394800	0.48442300	-0.11113900	-2.97532900	0.60104300
Th	-2.54936300	0.10589600	-0.29641400	-2.50231800	0.15254500	-0.40230200
Th	2.29599100	-0.02734100	-0.01581600	2.22532500	-0.01642700	-0.02903500
C	3.98012900	-1.64307400	-1.50411300	3.86522500	-1.63966300	-1.52661500
C	4.25565100	-0.32917900	-1.93355300	4.22732200	-0.33410600	-1.88176400
C	4.60395400	0.88962400	-1.27540600	4.61744300	0.82207700	-1.16297800
C	4.79450800	1.29603300	0.06444200	4.79045100	1.14867900	0.19045000
C	4.66819500	0.67194600	1.33207300	4.59229800	0.48015300	1.41102800
C	4.36070300	-0.63892600	1.76021500	4.20189700	-0.82206300	1.76510000
C	4.08872500	-1.87239000	1.10622500	3.88363000	-1.99548400	1.05199300
C	3.92913000	-2.28806000	-0.23196600	3.73565100	-2.33387900	-0.30000300
H	4.70438600	1.71950200	-1.98040000	4.77493900	1.67283300	-1.81665600
H	5.01108000	2.36471500	0.14658700	5.04815500	2.19297500	0.32934400
H	4.80381700	1.37018600	2.16231800	4.73864400	1.12362900	2.27099300
H	4.29992800	-0.72340900	2.84880900	4.10639700	-0.95184000	2.83731300
H	3.86468700	-2.67328300	1.81649400	3.58906500	-2.80580100	1.70995000
H	3.63882000	-3.33877700	-0.31352900	3.38127900	-3.34911700	-0.43859300
H	3.70362700	-2.31065800	-2.32469900	3.57263400	-2.24207800	-2.37872000
H	4.13801300	-0.20091900	-3.01329900	4.14959000	-0.15212100	-2.94765900
C	-3.79137400	0.20434300	2.13702800	-3.29889100	0.00992100	2.19233200
C	-4.36465800	1.27920500	1.41262300	-4.02395200	1.10291800	1.68296200
C	-4.89674600	1.43989900	0.10897900	-4.79588800	1.33587100	0.53172400
C	-5.11820300	0.57828900	-0.99986000	-5.19190400	0.56051400	-0.57696700
C	-4.93916700	-0.81140100	-1.24048100	-5.01429900	-0.78371100	-0.96458600
C	-4.42874000	-1.90049300	-0.49047300	-4.34516700	-1.89531600	-0.42098300
C	-3.84045300	-2.04867500	0.79007200	-3.53610700	-2.11697100	0.70717900
C	-3.55723100	-1.17309400	1.87329400	-3.08566500	-1.32367400	1.78225900
H	-5.12569400	2.48380700	-0.12315000	-5.09808400	2.37290400	0.43924200
H	-5.48020400	1.11398000	-1.88207400	-5.73242600	1.13911500	-1.31770300
H	-5.19391100	-1.09255300	-2.26624900	-5.44861500	-0.99491900	-1.93532500
H	-4.37969700	-2.82143600	-1.07786000	-4.37877000	-2.75725300	-1.07741600
H	-3.44681800	-3.05521000	0.95496300	-3.09093800	-3.10509300	0.71051600
H	-3.00446600	-1.66647400	2.67771600	-2.38462500	-1.84890100	2.42179300
H	-3.37235700	0.52259200	3.09555000	-2.72312800	0.26900500	3.07323200
H	-4.27701900	2.23044000	1.94452100	-3.86452600	2.00534400	2.26196000
C	1.03756600	0.97185600	2.02330200	0.84547500	0.99505900	2.03725300
O	0.36243800	1.48181700	2.80728900	0.10638200	1.51592200	2.73166100
C	2.00373900	2.53481700	-0.61547100	2.09151200	2.67629800	-0.42604500
O	1.72281100	3.61755800	-0.87329300	1.84564400	3.77303200	-0.58411800

Table S11. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_5$ structures **5S-3.**

	BP86			M06L		
	x	y	z	x	y	z
C	-0.16283700	-0.99461400	-0.82205600	-0.16834600	-1.04830300	-0.84454500
C	-0.16283900	-0.99459300	0.82208300	-0.16836900	-1.04817700	0.84452200
C	-0.28939600	1.02427700	1.17995700	-0.26158200	1.07794500	1.21165500
C	-0.28939400	1.02423800	-1.17998700	-0.26154600	1.07790000	-1.21190500
O	0.79316600	1.39849200	-1.56224600	0.81677400	1.40956800	-1.59218000
O	0.79316400	1.39854000	1.56220400	0.81671300	1.40966900	1.59198200
O	0.89487700	-1.44480500	1.35966900	0.89191800	-1.47274500	1.35339200
O	0.89487400	-1.44484700	-1.35963200	0.89198700	-1.47290400	-1.35328600
Th	2.31617700	-0.06604000	-0.00000100	2.30297900	-0.06473200	0.00001000
Th	-2.22493400	0.02376300	-0.00000200	-2.18765500	-0.00021000	-0.00008600
C	-3.80036800	-1.47416700	1.71478600	-3.80512100	-1.45976800	1.70135400
C	-4.40175800	-0.19029400	1.71851700	-4.38946200	-0.17998000	1.70498700
C	-4.84597200	0.69957400	0.71152200	-4.82648600	0.70458000	0.70587700
C	-4.84597600	0.69957000	-0.71151700	-4.82685000	0.70486600	-0.70456100
C	-4.40176700	-0.19030400	-1.71850900	-4.39026600	-0.17922400	-1.70427600
C	-3.80037600	-1.47417600	-1.71477500	-3.80587100	-1.45899400	-1.70150800
C	-3.41392400	-2.39420800	-0.70792600	-3.43351400	-2.37717600	-0.70269200
C	-3.41392100	-2.39420500	0.70794100	-3.43321500	-2.37749800	0.70195200
H	-5.23629600	1.63382000	1.12500000	-5.19841900	1.63772400	1.11538800
H	-5.23630100	1.63381400	-1.12499700	-5.19901000	1.63817400	-1.11349100
H	-4.50521900	0.22526300	-2.72477100	-4.48891700	0.23436200	-2.70149800
H	-3.53520900	-1.81625600	-2.71881600	-3.54495800	-1.79985900	-2.69679400
H	-2.92014100	-3.27743000	-1.12173400	-2.94864100	-3.25543000	-1.11314000
H	-2.92013500	-3.27742300	1.12175100	-2.94817100	-3.25594300	1.11178700
H	-3.53519500	-1.81624100	2.71882800	-3.54373700	-1.80108800	2.69636000
H	-4.50520500	0.22527800	2.72477700	-4.48761500	0.23316000	2.70244300
C	4.37673600	-1.23477800	-1.31052300	4.37339300	-1.20230600	-1.30115500
C	4.31078300	0.07364400	-1.85129600	4.29369500	0.09596700	-1.83716600
C	4.24388500	1.38063300	-1.30895200	4.21603600	1.39199000	-1.29837400
C	4.21174000	1.92115300	0.00009600	4.17832200	1.92739200	0.00093500
C	4.24388900	1.38050000	1.30908700	4.21610600	1.39070300	1.29970500
C	4.31078800	0.07345600	1.85130000	4.29378600	0.09413900	1.83720600
C	4.37673800	-1.23491100	1.31039500	4.37345200	-1.20359700	1.29990000
C	4.40005800	-1.77659200	-0.00009200	4.40296700	-1.74023800	-0.00089800
H	4.09035900	2.14226300	-2.07793200	4.05042900	2.14508100	-2.05992100
H	4.04656100	3.00210500	0.00015000	4.00206500	2.99700000	0.00147100
H	4.09036700	2.14205300	2.07814600	4.05053400	2.14303600	2.06200900
H	4.19771700	0.06731600	2.93880000	4.17837100	0.08629200	2.91491900
H	4.29651900	-2.00835300	2.07857200	4.29732200	-1.97136300	2.06074500
H	4.33529800	-2.86800200	-0.00014700	4.34770000	-2.82264000	-0.00143400
H	4.29651500	-2.00814300	-2.07877800	4.29722600	-1.96931500	-2.06275900
H	4.19770900	0.06761300	-2.93879600	4.17822500	0.08919200	-2.91488000
C	-2.73317400	2.71401300	-0.00000700	-2.81383600	2.76923100	-0.00005500
O	-2.98192100	3.83110600	-0.00000100	-3.16755700	3.84637000	0.00007900

Table S12. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_6$ structures **6S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	-1.01158700	-2.11296000	-0.71230900	-0.83225500	-2.16703100	-0.68686200
C	-1.19880500	-0.26142300	2.26179100	-0.97044700	-0.24705200	2.28043100
C	-0.11013300	0.83830000	0.32424500	-0.08951300	0.99234900	0.20852900
C	-0.13156400	0.15320100	-0.92995100	-0.11518600	0.29736400	-1.04333800
O	0.93673600	0.15775900	-1.76035000	0.94889200	0.31805400	-1.85497300
O	0.95730100	1.52022600	0.78175800	0.97041900	1.68548700	0.62655700
O	-0.54754500	-0.25217300	3.21353200	-0.24965900	-0.16944400	3.16026900
O	-0.29392700	-2.90527700	-1.15225900	-0.11395200	-2.91499900	-1.16264900
Th	2.45147600	0.06914200	-0.09725800	2.41297800	0.10536700	-0.14162300
Th	-2.40191600	-0.01181800	-0.02473000	-2.31111000	-0.00579900	-0.02922800
C	-4.54059600	-1.37878600	1.14202500	-4.32435100	-1.57267700	1.10182800
C	-4.80397400	-0.02539500	1.44963800	-4.67838800	-0.26586700	1.47427300
C	-4.87408600	1.16865800	0.68667900	-4.85311300	0.94142300	0.77471300
C	-4.64766400	1.50751200	-0.66609900	-4.67844100	1.35607500	-0.55354700
C	-4.30426300	0.79354500	-1.85448300	-4.30853300	0.72952900	-1.76870500
C	-4.07386900	-0.56212800	-2.16344000	-3.98394900	-0.58049800	-2.14205200
C	-4.08133000	-1.77364900	-1.40908500	-3.88650900	-1.81209300	-1.45156600
C	-4.27512600	-2.10482500	-0.05202800	-4.03336200	-2.21657000	-0.11822900
H	-5.06944600	2.04770500	1.30703200	-5.08761700	1.76979200	1.43427100
H	-4.70575800	2.58550400	-0.84044400	-4.81011300	2.42586900	-0.67250700
H	-4.14749200	1.45759300	-2.70924300	-4.21800100	1.43459000	-2.58724100
H	-3.78572800	-0.71880000	-3.20648500	-3.70189600	-0.66415800	-3.18516600
H	-3.81392600	-2.64068200	-2.01873900	-3.56071700	-2.61959900	-2.09755400
H	-4.09434900	-3.16556100	0.14372300	-3.76672400	-3.25821800	0.02377100
H	-4.51834300	-2.01654400	2.03008200	-4.23897200	-2.24043900	1.95176000
H	-4.95175300	0.14722000	2.51904800	-4.81459600	-0.15520800	2.54393900
C	3.68697700	-2.32519600	-0.68399300	3.47227700	-2.39288100	-0.56701800
C	4.49903800	-1.34145500	-1.29761400	4.39088900	-1.51071500	-1.16195900
C	5.07798000	-0.11692100	-0.87504200	5.04062800	-0.32903500	-0.75591200
C	5.10542000	0.61531000	0.34399500	5.06395400	0.43993300	0.42549100
C	4.56342200	0.42659200	1.64213400	4.44510900	0.34652400	1.68759300
C	3.75242100	-0.56042600	2.25174600	3.52813700	-0.53803500	2.28149000
C	3.15755500	-1.77823000	1.82451800	2.85484700	-1.70432400	1.86526400
C	3.13083600	-2.50797600	0.61092800	2.83248700	-2.47260800	0.68641500
H	5.59171400	0.40507100	-1.68720200	5.61861100	0.12231800	-1.55467000
H	5.63650400	1.56638500	0.24766800	5.65450200	1.34313200	0.31941800
H	4.75483000	1.27759400	2.30166400	4.66713300	1.19825700	2.32036600
H	3.45931500	-0.28931700	3.26953700	3.20419300	-0.20305700	3.26031000
H	2.52548800	-2.22551200	2.59681600	2.14930900	-2.06129000	2.60716100
H	2.48136700	-3.38605100	0.66356900	2.11350800	-3.28259300	0.73229000
H	3.35495800	-3.09145500	-1.38960900	3.11798000	-3.14964000	-1.25776000
H	4.65066100	-1.52878200	-2.36425300	4.58034700	-1.75016500	-2.20209800
C	-2.03533700	2.47612200	0.79539200	-2.13261900	2.50608100	1.00261500
O	-1.71867300	3.52509500	1.13847100	-1.86890600	3.52449100	1.42975700
C	3.10921200	2.40323000	-1.39507200	2.86798200	2.55835900	-1.48732000
O	3.44165400	3.35660100	-1.92715800	2.84659700	3.55388500	-2.02052600

Table S13. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_6$ structures **6S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	0.90793800	-1.83041100	1.33581000	0.71052100	-1.89035500	1.29972600
C	-0.03086600	-0.71519200	-0.69940000	-0.05982300	-0.71537200	-0.90125500
C	-0.03093900	0.71473500	-0.69965300	-0.05982300	0.71538000	-0.90125100
O	-1.11808200	1.40561600	-1.11386900	-1.11853700	1.40235400	-1.35433900
O	-1.11795600	-1.40633500	-1.11333100	-1.11853700	-1.40234300	-1.35434700
O	0.21165800	-2.64090000	1.77231900	0.00991200	-2.71750200	1.65461600
Th	-2.63828400	-0.00026100	-0.27178900	-2.58497000	0.00000200	-0.40271800
Th	2.21909800	0.00000400	0.00478800	2.09780000	0.00000000	-0.00721400
C	4.49399800	-1.71530000	-0.07134800	4.38993500	-1.70283000	0.14431900
C	4.75953800	-0.71276100	-1.02311900	4.74204800	-0.70770800	-0.77057500
C	4.75938100	0.71361800	-1.02300400	4.74205000	0.70770300	-0.77057200
C	4.49353900	1.71593100	-0.07108600	4.38994000	1.70282300	0.14432700
C	4.09541000	1.71555600	1.29575300	3.86716800	1.70273200	1.45666500
C	3.81391600	0.71250600	2.24202200	3.50062100	0.70689200	2.36504300
C	3.81412700	-0.71241000	2.24192300	3.50061800	-0.70690600	2.36504000
C	4.09588000	-1.71523400	1.29549200	3.86716300	-1.70274300	1.45665800
H	4.98195900	1.12369300	-2.01201000	5.05004800	1.11461900	-1.72755800
H	4.57348000	2.72492600	-0.48417900	4.50280800	2.70288200	-0.25909900
H	3.93988500	2.72423100	1.68728600	3.67172700	2.70258100	1.82738000
H	3.46820700	1.12267200	3.19498800	3.06493800	1.11393500	3.27094400
H	3.46854100	-1.12281500	3.19482900	3.06493400	-1.11395000	3.27093900
H	3.94063700	-2.72401200	1.68687600	3.67171900	-2.70259200	1.82736800
H	4.57419800	-2.72420800	-0.48460000	4.50279900	-2.70288800	-0.25911000
H	4.98221000	-1.12262500	-2.01219200	5.05004500	-1.11462000	-1.72756200
C	-3.83019100	1.33538400	1.79434100	-3.03790500	0.70593500	2.16627200
C	-4.46031100	1.85356700	0.63533400	-3.70675800	1.70066200	1.42628100
C	-5.02566600	1.29060000	-0.53624900	-4.61244500	1.70006400	0.35154800
C	-5.23747800	-0.03131400	-1.01488400	-5.22746300	0.70508900	-0.43320900
C	-5.00781600	-1.33441800	-0.49491300	-5.22745300	-0.70512300	-0.43320400
C	-4.43268400	-1.85261800	0.69223700	-4.61242000	-1.70008300	0.35155900
C	-3.80864400	-1.28972100	1.83373200	-3.70673200	-1.70066200	1.42629100
C	-3.54306400	0.03224800	2.28444400	-3.03789300	-0.70592000	2.16627600
H	-5.30261100	2.04959700	-1.27335600	-4.81847100	2.69949600	-0.01420900
H	-5.64125400	-0.05004700	-2.03120600	-5.80255400	1.11966200	-1.25360900
H	-5.27415900	-2.11981800	-1.20785500	-5.80253900	-1.11971000	-1.25360000
H	-4.35741200	-2.94326800	0.67468300	-4.81843100	-2.69952200	-0.01419200
H	-3.37049700	-2.04885100	2.48734700	-3.37289000	-2.69879100	1.68616300
H	-2.95371600	0.05093100	3.20554900	-2.32181000	-1.12036000	2.86686900
H	-3.40432300	2.12072500	2.42467200	-2.32182800	1.12039000	2.86686200
H	-4.40129600	2.94417300	0.58435800	-3.37293100	2.69879800	1.68614700
C	0.90769700	1.83053100	1.33544500	0.71052400	1.89035200	1.29973200
O	0.21135400	2.64103200	1.77182500	0.00991300	2.71749800	1.65462500
C	1.90588700	1.84096600	-1.86078700	2.06452200	1.91124200	-1.92617200
O	1.60802100	2.64982800	-2.62103400	1.87938800	2.74293100	-2.67800300
C	1.90618200	-1.84150100	-1.86030900	2.06451900	-1.91123000	-1.92618400
O	1.60849200	-2.65058300	-2.62038800	1.87938400	-2.74291600	-2.67801900

Table S14. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_7$ structures **7S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	1.08215000	-1.38303900	-1.84073700	-0.87715100	-1.36303300	1.90759700
C	0.04805400	0.61517300	-0.71647900	-0.00107900	0.80984800	0.71717400
C	0.04796300	0.61580300	0.71554800	-0.00108000	0.80985200	-0.71717300
O	-1.04495800	0.98449200	1.41540600	1.07390400	1.21223000	-1.40010000
O	-1.04484300	0.98319700	-1.41676700	1.07390700	1.21222300	1.40010000
O	0.41691300	-1.84561800	-2.66212400	-0.21192700	-1.74633400	2.75055300
Th	-2.53905700	0.06261500	-0.00032600	2.49915600	0.13201300	-0.00000500
Th	2.32384700	0.00189800	-0.00000800	-2.18921800	0.00245200	0.00000000
C	4.59572200	0.16839500	-1.71525600	-4.48980700	-0.05950900	1.70288900
C	4.82275500	1.13055800	-0.71330400	-4.80567500	0.86826700	0.70763800
C	4.82257600	1.13118000	0.71297900	-4.80567500	0.86826800	-0.70763800
C	4.59525600	0.16990500	1.71571600	-4.48980700	-0.05950700	-1.70289000
C	4.25322000	-1.21209700	1.71604800	-4.02041800	-1.39199800	-1.70279100
C	4.00989100	-2.16954300	0.71371500	-3.69007800	-2.31418300	-0.70700600
C	4.01009900	-2.17017100	-0.71134700	-3.69007900	-2.31418400	0.70700300
C	4.25372100	-1.21361200	-1.71445900	-4.02041900	-1.39199900	1.70278900
H	5.00485000	2.12859600	1.12258700	-5.07532600	1.83679500	-1.11448200
H	4.65824300	0.58639300	2.72451900	-4.58678400	0.34802500	-2.70294100
H	4.11433100	-1.60916300	2.72500700	-3.84108100	-1.77066000	-2.70270400
H	3.70393600	-3.13578600	1.12443000	-3.29207100	-3.23729500	-1.11402200
H	3.70427700	-3.13678200	-1.12129700	-3.29207200	-3.23729600	1.11401800
H	4.11513100	-1.61157800	-2.72310400	-3.84108300	-1.77066300	2.70270200
H	4.65897900	0.58399400	-2.72440800	-4.58678300	0.34802200	2.70294100
H	5.00513300	2.12761600	-1.12373800	-5.07532600	1.83679400	1.11448300
C	-3.71585600	-1.75667900	1.69915500	3.44322900	-1.79960300	-1.69967200
C	-4.57025600	-0.62811100	1.73017800	4.43993900	-0.80788600	-1.70053600
C	-5.17203400	0.19872400	0.74629600	5.13025600	-0.08936800	-0.70488300
C	-5.18976000	0.22105900	-0.67568600	5.13025200	-0.08936000	0.70488900
C	-4.61266700	-0.57392000	-1.70009900	4.43993000	-0.80786800	1.70054500
C	-3.75921100	-1.70323900	-1.72615000	3.44322000	-1.79958600	1.69968500
C	-3.14053000	-2.52051900	-0.74179000	2.72998800	-2.49728700	0.70389000
C	-3.12255100	-2.54278400	0.67449300	2.72999200	-2.49729400	-0.70387300
H	-5.71728100	1.03975000	1.18372300	5.77476400	0.67809900	-1.11871100
H	-5.74613600	1.07469600	-1.07275600	5.77475600	0.67811300	1.11871300
H	-4.81128500	-0.17576800	-2.69902300	4.67332000	-0.45767000	2.69954400
H	-3.44934500	-1.96858800	-2.74049300	3.08588800	-2.02828500	2.69732500
H	-2.47642000	-3.26979800	-1.18152300	1.96484200	-3.14356200	1.11905500
H	-2.44829600	-3.30563400	1.07360800	1.96484700	-3.14357300	-1.11903500
H	-3.38086400	-2.05360800	2.69661900	3.08590200	-2.02831300	-2.69731100
H	-4.74276100	-0.26126900	2.74578400	4.67333700	-0.45770000	-2.69953800
C	1.08151600	-1.38152800	1.84141400	-0.87714400	-1.36302300	-1.90760100
O	0.41599700	-1.84338200	2.66298500	-0.21191500	-1.74631400	-2.75055600
C	1.93286200	1.85670000	1.83267700	-2.08103300	1.92100200	-1.90373900
O	1.59943600	2.60843200	2.63600900	-1.86450600	2.66980800	-2.73091300
C	-3.22332800	2.72885500	-0.00044800	2.99247100	2.92400700	0.00000900
O	-3.53246300	3.82707800	-0.00068900	2.93073600	4.05208400	0.00001400
C	1.93318200	1.85515300	-1.83435100	-2.08102900	1.92099500	1.90374400
O	1.59989100	2.60619400	-2.63838500	-1.86449800	2.66979700	2.73092200

Table S15. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_7$ structures **7S-2.**

	BP86			M06L		
	x	y	z	x	y	z
C	-1.22868800	-2.25972100	0.02047500	1.14144100	-2.31205900	0.32473200
C	-0.24744100	-0.20036400	0.87225300	0.22810300	-0.25657800	-0.98262400
C	-0.22709000	0.85116400	-0.09034400	0.20718900	0.93420100	-0.19865000
O	0.83972900	1.63619100	-0.32372400	-0.84317300	1.75322600	-0.10540600
O	0.82610300	-0.48592200	1.64587000	-0.83742500	-0.65135300	-1.69877600
O	-0.54867900	-3.17840900	0.19352500	0.49734900	-3.24757800	0.22137800
Th	2.37480100	0.01012900	0.07873100	-2.29486600	0.00678700	-0.10689200
Th	-2.53918600	-0.00540300	0.03955800	2.46775600	0.00283900	-0.06857800
C	-4.19848900	-1.16540500	1.93526800	4.11544300	-1.40152500	-1.78214000
C	-4.37937100	0.22420100	2.08538600	4.36398400	-0.05145900	-2.05714300
C	-4.71596300	1.29336800	1.20019500	4.73431200	1.07170800	-1.27647400
C	-4.97985100	1.41594700	-0.18212700	4.97903100	1.30953100	0.08335500
C	-4.96988400	0.53013100	-1.29041400	4.90011800	0.54445800	1.26059900
C	-4.75304000	-0.85717000	-1.44262800	4.61265300	-0.80111200	1.53794600
C	-4.49507300	-1.93734400	-0.55347400	4.32741100	-1.93959500	0.75596400
C	-4.26725800	-2.06780600	0.83195500	4.11986200	-2.18945900	-0.60650700
H	-4.72807600	2.25901100	1.71330700	4.79582800	1.97627600	-1.87143700
H	-5.15161900	2.45374800	-0.48081000	5.18439900	2.35528400	0.28467900
H	-5.12983900	1.04309900	-2.24257300	5.06272400	1.13355000	2.15589800
H	-4.77086600	-1.17484600	-2.48890100	4.59497000	-1.01465700	2.60081600
H	-4.35910800	-2.88352800	-1.08497100	4.13205900	-2.81503400	1.36571800
H	-4.02409900	-3.09323100	1.12232800	3.82996900	-3.21601100	-0.80083500
H	-3.89987200	-1.65946900	2.86388400	3.80975500	-1.96147900	-2.65833900
H	-4.18172600	0.57202500	3.10331300	4.20333500	0.20280500	-3.09873100
C	3.33600200	0.20274300	-2.52801200	-3.01612500	0.51349900	2.52354900
C	4.38353400	0.71762000	-1.72317900	-4.13734800	0.91660200	1.77467600
C	5.08213300	0.25664200	-0.57747900	-4.93808300	0.31390900	0.78567200
C	5.02763800	-0.90840000	0.23086600	-4.93978300	-0.92784700	0.12435000
C	4.22906300	-2.07844600	0.25630000	-4.13524100	-2.08158800	0.16184700
C	3.16284200	-2.58166600	-0.53412900	-3.00334700	-2.47905600	0.89877400
C	2.46279700	-2.11721900	-1.67001700	-2.21318200	-1.88206600	1.89264100
C	2.53711700	-0.96230000	-2.50004300	-2.21995900	-0.64051800	2.56788400
H	5.82523800	0.97576100	-0.22136200	-5.71054700	0.97959800	0.41562200
H	5.74113100	-0.87096600	1.05882000	-5.71393600	-0.98871100	-0.63321200
H	4.46028800	-2.72661800	1.10615000	-4.42919900	-2.81821200	-0.57782100
H	2.74344500	-3.50756200	-0.13213800	-2.61398900	-3.43921800	0.57983600
H	1.63313800	-2.77371200	-1.94536400	-1.36662100	-2.49738000	2.17399000
H	1.75129700	-0.94610600	-3.25966400	-1.37616600	-0.53538400	3.24001400
H	3.01560400	0.90955500	-3.29801300	-2.62846700	1.30788700	3.15120600
H	4.70345300	1.71447200	-2.03866400	-4.42937400	1.94054200	1.98033900
C	-1.40170300	0.49316700	-2.23439400	1.27460400	0.93818200	2.13689600
O	-0.78306700	0.81627000	-3.15299500	0.62694300	1.48302000	2.90080100
C	-2.08932000	2.59678400	0.06220900	2.18158600	2.69507700	-0.28660300
O	-1.72898400	3.68758500	0.07295800	1.87028000	3.78485500	-0.35897700
C	3.44564600	-0.14629600	2.66674800	-3.60141300	-0.62953600	-2.59383700
O	3.93501400	-0.33644200	3.68045800	-4.17601400	-1.04903800	-3.47255100
C	3.35296300	2.57238800	0.64478800	-3.53903900	2.44328600	-0.97580900
O	3.80574700	3.61709700	0.72109000	-4.08271800	3.42630600	-1.10272400

Table S16. Optimized coordinates of the $(C_8H_8)_2Th_2(CO)_7$ structures **1S-1.**

	BP86			M06L		
	x	y	z	x	y	z
C	-1.54189900	0.12913400	0.00000000	-1.63378600	0.09263900	0.00000000
O	-2.33652800	-1.03706300	0.00000000	-2.42304500	-1.06171500	0.00000000
Th	-0.47942000	-2.02619000	0.00000000	-0.53797300	-2.00389300	0.00000000
Th	-0.43153800	1.98603800	0.00000000	-0.47120400	1.90688300	0.00000000
C	-0.48398800	4.76189800	0.00000000	-0.32793500	4.69286500	0.00000000
C	-0.08313800	4.39796200	1.31278800	0.04411200	4.30701200	1.30253700
C	0.88581200	3.51456200	1.85828400	0.94555400	3.37091200	1.84514600
C	1.86062300	2.63479900	1.31407200	1.85960800	2.44337800	1.30413300
C	2.26602200	2.27343600	0.00000000	2.24358900	2.06837000	0.00000000
C	1.86062300	2.63479900	-1.31407200	1.85960800	2.44337800	-1.30413300
C	0.88581200	3.51456200	-1.85828400	0.94555400	3.37091200	-1.84514600
C	-0.08313800	4.39796200	-1.31278800	0.04411200	4.30701200	-1.30253700
H	0.83799700	3.46115000	2.94976300	0.89428900	3.32005500	2.92704300
H	2.38621700	2.06426500	2.08487000	2.34864700	1.84705900	2.06685800
H	3.03145700	1.49270900	0.00000000	2.96450000	1.25860100	0.00000000
H	2.38621700	2.06426500	-2.08487000	2.34864700	1.84705900	-2.06685800
H	0.83799700	3.46115000	-2.94976300	0.89428900	3.32005500	-2.92704300
H	-0.70246200	4.86558200	-2.08386600	-0.53846200	4.81066600	-2.06608600
H	-1.33832300	5.44536500	0.00000000	-1.12675800	5.42642600	0.00000000
H	-0.70246200	4.86558200	2.08386600	-0.53846200	4.81066600	2.06608600
C	1.51913800	-2.75040300	-1.71453500	1.54513000	-2.45792400	-1.70159400
C	2.15996200	-1.97837100	-0.71029500	2.05735300	-1.60401800	-0.70503100
C	2.15996200	-1.97837100	0.71029500	2.05735300	-1.60401800	0.70503100
C	1.51913800	-2.75040300	1.71453500	1.54513000	-2.45792400	1.70159400
C	0.63679400	-3.86522200	1.71290900	0.84409000	-3.68178500	1.69914600
C	0.04305300	-4.67339500	0.70858800	0.38188000	-4.56265600	0.70263500
C	0.04305300	-4.67339500	-0.70858800	0.38188000	-4.56265600	-0.70263500
C	0.63679400	-3.86522200	-1.71290900	0.84409000	-3.68178500	-1.69914600
H	2.72970200	-1.14347700	1.12698400	2.48631600	-0.69751400	1.11782700
H	1.70778900	-2.36720800	2.72135900	1.67474500	-2.05435100	2.69955500
H	0.31206900	-4.14144600	2.72032100	0.57204300	-4.00363700	2.69828000
H	-0.63254700	-5.42577400	1.12597200	-0.16323500	-5.40359700	1.11690100
H	-0.63254700	-5.42577400	-1.12597200	-0.16323500	-5.40359700	-1.11690100
H	0.31206900	-4.14144600	-2.72032100	0.57204300	-4.00363700	-2.69828000
H	1.70778900	-2.36720800	-2.72135900	1.67474500	-2.05435100	-2.69955500
H	2.72970200	-1.14347700	-1.12698400	2.48631600	-0.69751400	-1.11782700

Table S17 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_2$ structure **2S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
-2(0)	4(0)	699(0)	715(6)	1303(0)	1340(0)
5(0)	7(0)	741(13)	764(0)	1303(0)	1340(0)
16(0)	15(1)	741(0)	764(1)	1309(0)	1345(0)
23(1)	21(2)	742(1)	766(22)	1309(0)	1345(0)
35(0)	32(0)	743(1)	766(0)	1374(0)	1414(0)
41(0)	38(0)	745(0)	770(0)	1374(0)	1414(0)
90(18)	90(21)	745(0)	770(0)	1422(0)	1468(1)
100(0)	100(0)	753(1)	776(0)	1422(0)	1468(1)
206(30)	199(227)	753(2)	777(0)	1423(0)	1469(1)
213(0)	215(0)	760(0)	782(0)	1423(0)	1469(1)
215(132)	216(123)	761(1)	782(0)	1477(0)	1522(0)
227(20)	223(0)	818(0)	836(0)	1477(0)	1522(0)
227(0)	228(24)	818(0)	836(0)	1479(0)	1525(0)
230(0)	234(0)	820(0)	838(0)	1479(0)	1525(0)
240(0)	240(1)	820(0)	838(0)	1487(0)	1537(0)
243(0)	250(21)	882(3)	907(2)	1487(0)	1537(0)
244(0)	250(10)	882(3)	908(2)	1488(0)	1538(1)
247(1)	251(3)	888(13)	914(2)	1488(0)	1538(0)
249(0)	255(0)	889(16)	915(5)	1548(0)	1605(0)
275(0)	258(97)	890(4)	919(12)	1548(0)	1606(0)
287(242)	266(0)	891(3)	919(20)	3058(0)	3147(0)
334(2)	349(3)	894(13)	923(13)	3058(0)	3148(0)
373(0)	386(0)	894(10)	923(16)	3061(0)	3151(0)
373(0)	386(0)	911(0)	943(0)	3061(0)	3151(0)
375(0)	387(0)	911(0)	944(0)	3064(0)	3153(0)
375(0)	388(0)	960(0)	997(0)	3064(0)	3153(0)
450(0)	453(0)	960(0)	997(0)	3074(0)	3163(0)
467(493)	467(544)	984(117)	1031(142)	3074(0)	3163(0)
478(2)	496(0)	1018(0)	1046(0)	3075(0)	3164(0)
478(1)	496(0)	1134(0)	1179(0)	3075(0)	3164(0)
500(0)	517(0)	1170(0)	1207(0)	3087(0)	3176(13)
500(0)	517(0)	1170(0)	1207(0)	3087(39)	3176(33)
552(0)	572(0)	1171(0)	1207(0)	3088(0)	3178(18)
552(0)	572(0)	1171(0)	1207(0)	3088(36)	3178(23)
608(0)	624(0)	1297(0)	1333(0)	3095(5)	3184(2)
697(347)	714(294)	1297(0)	1333(0)	3095(0)	3184(2)

Table S18 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_2$ structure **2S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
3(0)	6(0)	740(7)	765(12)	1303(0)	1340(0)
5(0)	8(0)	741(5)	766(7)	1304(0)	1340(0)
7(1)	13(1)	744(1)	766(1)	1307(0)	1343(0)
15(1)	22(1)	745(0)	769(1)	1309(0)	1345(0)
27(1)	24(1)	746(0)	770(0)	1374(0)	1414(0)
51(2)	49(3)	746(0)	772(0)	1374(0)	1414(0)
66(6)	68(8)	752(0)	775(0)	1422(0)	1467(1)
133(16)	135(18)	753(2)	776(1)	1422(0)	1468(2)
209(18)	214(29)	756(1)	778(0)	1423(0)	1468(1)
217(2)	215(30)	759(1)	780(1)	1424(0)	1469(2)
217(75)	220(22)	782(14)	816(16)	1475(0)	1521(0)
225(7)	227(26)	816(0)	834(0)	1476(0)	1521(0)
226(7)	234(4)	817(0)	835(0)	1478(0)	1523(0)
232(1)	237(5)	822(0)	840(0)	1480(0)	1525(0)
237(1)	240(15)	823(0)	841(0)	1486(0)	1536(0)
244(0)	251(0)	880(1)	905(1)	1486(0)	1537(0)
244(0)	252(0)	887(5)	912(0)	1488(0)	1537(0)
245(1)	253(1)	888(5)	913(2)	1488(1)	1538(1)
247(2)	254(2)	888(4)	915(3)	1540(0)	1599(0)
273(37)	281(43)	889(16)	918(12)	1551(0)	1608(0)
369(238)	374(2)	890(5)	919(21)	3057(0)	3146(0)
372(0)	382(253)	891(10)	921(17)	3058(0)	3147(0)
374(45)	385(0)	892(35)	923(17)	3060(0)	3149(0)
376(0)	387(61)	893(14)	930(21)	3062(0)	3151(0)
377(48)	390(21)	910(0)	943(0)	3063(0)	3151(0)
378(1)	390(31)	913(0)	945(0)	3064(0)	3154(0)
480(0)	489(285)	957(0)	996(0)	3073(0)	3162(0)
485(14)	498(0)	959(0)	997(0)	3073(0)	3163(0)
490(309)	503(2)	1110(51)	1163(71)	3075(0)	3164(1)
492(3)	511(0)	1169(0)	1205(0)	3075(0)	3164(1)
501(0)	518(0)	1169(0)	1206(0)	3086(23)	3175(28)
551(0)	572(0)	1170(3)	1207(0)	3087(18)	3176(20)
553(0)	573(0)	1170(1)	1207(1)	3088(21)	3177(23)
575(6)	600(7)	1182(174)	1237(156)	3088(15)	3177(19)
697(272)	713(203)	1296(0)	1332(0)	3094(4)	3183(2)
699(71)	715(92)	1297(0)	1332(0)	3094(3)	3184(4)

Table S19 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_2$ structure **3S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
6(0)	7(0)	582(9)	607(8)	1298(0)	1334(0)
7(0)	16(1)	699(280)	714(186)	1303(0)	1340(0)
18(1)	19(0)	701(70)	718(117)	1304(0)	1341(0)
24(1)	24(1)	741(4)	765(8)	1310(0)	1345(0)
33(0)	36(0)	742(5)	766(8)	1310(0)	1347(0)
39(0)	43(1)	743(1)	768(2)	1374(0)	1414(0)
51(1)	57(0)	745(1)	769(1)	1374(0)	1415(0)
67(6)	65(6)	746(0)	772(1)	1422(0)	1467(1)
88(4)	83(5)	747(1)	772(1)	1423(0)	1468(1)
144(13)	147(17)	753(1)	775(1)	1424(0)	1469(1)
208(20)	205(20)	754(3)	777(1)	1424(0)	1469(1)
213(13)	212(22)	759(1)	780(0)	1475(0)	1521(0)
218(0)	217(6)	760(2)	781(2)	1478(0)	1523(0)
224(53)	220(5)	793(10)	822(14)	1478(0)	1523(0)
226(10)	223(20)	820(0)	839(0)	1481(0)	1525(0)
228(3)	227(32)	820(0)	840(0)	1487(0)	1537(0)
236(3)	235(2)	822(0)	840(1)	1488(0)	1537(0)
238(1)	240(11)	825(0)	844(0)	1488(1)	1538(1)
243(1)	245(19)	884(3)	909(2)	1490(0)	1539(0)
245(0)	253(1)	884(4)	910(1)	1540(9)	1598(10)
247(6)	255(1)	889(7)	916(7)	1550(0)	1607(0)
251(3)	256(3)	890(19)	916(5)	1959(368)	2075(372)
255(3)	257(1)	891(5)	919(15)	3059(0)	3148(0)
299(42)	307(75)	892(14)	921(11)	3060(0)	3148(0)
339(222)	351(188)	894(10)	923(12)	3062(0)	3151(0)
372(0)	380(42)	895(2)	924(16)	3064(0)	3152(0)
373(0)	386(1)	913(0)	944(0)	3065(0)	3154(0)
374(0)	387(0)	913(0)	947(0)	3066(0)	3154(0)
374(4)	387(1)	939(6)	957(13)	3076(0)	3164(0)
377(5)	388(3)	959(0)	996(0)	3076(0)	3164(1)
451(15)	413(35)	959(0)	996(0)	3076(0)	3165(1)
480(14)	482(285)	1104(56)	1161(71)	3077(0)	3165(1)
483(122)	499(0)	1169(0)	1205(0)	3088(18)	3176(23)
485(217)	502(0)	1171(0)	1207(0)	3089(17)	3177(20)
499(0)	515(0)	1172(0)	1208(1)	3090(14)	3178(18)
501(0)	518(0)	1172(0)	1209(0)	3090(16)	3179(18)
553(0)	574(0)	1230(348)	1257(314)	3096(1)	3185(1)
554(0)	574(0)	1297(0)	1333(0)	3096(4)	3185(4)

Table S20 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_3$ structure **3S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
3(0)	6(0)	553(0)	572(0)	1297(0)	1333(0)
10(0)	7(0)	612(2)	626(7)	1304(0)	1340(0)
14(1)	13(0)	697(265)	713(291)	1306(0)	1342(0)
21(1)	23(2)	701(95)	715(23)	1308(0)	1343(0)
30(0)	29(0)	741(6)	764(1)	1310(0)	1346(0)
41(1)	32(0)	741(4)	765(9)	1374(0)	1414(0)
47(0)	47(1)	743(1)	766(10)	1374(0)	1414(0)
57(3)	59(1)	743(2)	769(1)	1423(0)	1468(1)
96(2)	87(4)	746(0)	770(0)	1423(0)	1468(1)
107(16)	119(18)	746(1)	771(0)	1423(0)	1468(1)
203(43)	189(13)	752(4)	775(1)	1424(0)	1469(1)
205(19)	205(19)	754(1)	776(0)	1477(0)	1522(0)
210(35)	212(49)	759(3)	777(1)	1477(1)	1524(0)
216(7)	215(45)	762(1)	781(0)	1479(0)	1524(0)
221(52)	224(31)	816(1)	835(1)	1480(0)	1526(0)
223(10)	227(2)	821(0)	835(0)	1487(0)	1536(0)
232(1)	233(1)	822(0)	838(0)	1487(0)	1538(0)
232(0)	236(11)	822(0)	840(0)	1487(0)	1538(0)
238(2)	242(2)	884(0)	907(2)	1492(0)	1540(0)
243(0)	252(1)	885(3)	910(0)	1546(13)	1604(5)
244(0)	253(0)	888(3)	913(0)	1546(0)	1607(0)
247(2)	253(1)	888(22)	914(4)	1969(556)	2111(670)
253(2)	259(1)	889(5)	919(13)	3058(0)	3147(0)
274(57)	331(51)	893(4)	919(18)	3060(0)	3148(0)
347(60)	337(2)	894(9)	922(17)	3062(0)	3150(0)
357(151)	380(45)	894(15)	924(15)	3063(0)	3152(0)
369(1)	383(13)	911(0)	943(0)	3064(0)	3153(0)
371(1)	384(1)	913(0)	943(0)	3065(0)	3153(0)
374(1)	387(4)	959(0)	996(0)	3075(0)	3163(0)
376(4)	390(85)	960(0)	997(0)	3075(0)	3164(0)
391(31)	395(210)	999(32)	1024(27)	3076(0)	3164(0)
426(87)	431(171)	1039(105)	1080(88)	3076(0)	3164(0)
469(291)	479(148)	1161(69)	1205(0)	3087(19)	3176(20)
478(3)	494(1)	1169(1)	1207(0)	3088(16)	3177(22)
483(2)	504(1)	1171(0)	1208(0)	3089(17)	3178(20)
499(0)	512(0)	1171(0)	1209(1)	3090(15)	3178(20)
499(0)	517(0)	1174(0)	1218(46)	3095(3)	3184(2)
552(0)	571(0)	1297(0)	1333(0)	3096(2)	3185(1)

Table S21 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_4$ structure **4S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
7(0)	11(0)	526(0)	508(0)	1308(0)	1344(0)
10(0)	16(0)	535(0)	512(0)	1308(0)	1344(0)
22(1)	24(1)	535(0)	512(0)	1315(0)	1350(0)
22(1)	24(1)	547(0)	567(0)	1315(0)	1350(0)
51(0)	49(0)	553(0)	572(0)	1374(0)	1415(0)
51(0)	49(0)	653(0)	606(0)	1377(0)	1416(0)
90(1)	87(1)	696(221)	710(192)	1424(0)	1469(1)
126(6)	113(8)	709(153)	724(134)	1424(0)	1469(1)
126(6)	113(8)	742(6)	766(11)	1427(0)	1471(0)
156(1)	161(0)	743(0)	768(3)	1427(0)	1471(0)
156(1)	161(0)	743(0)	768(3)	1481(0)	1525(0)
216(0)	185(0)	746(0)	768(0)	1481(0)	1525(0)
217(0)	219(89)	746(0)	768(0)	1487(0)	1531(0)
217(0)	220(0)	747(6)	772(13)	1487(0)	1531(0)
217(0)	220(0)	750(4)	773(0)	1490(0)	1540(0)
218(84)	222(0)	750(4)	773(0)	1490(0)	1540(0)
220(0)	223(0)	764(7)	783(6)	1494(0)	1542(0)
220(0)	223(0)	764(7)	783(6)	1495(0)	1543(0)
238(5)	238(9)	814(0)	830(0)	1527(448)	1614(0)
245(0)	253(0)	815(0)	831(0)	1527(448)	1618(0)
246(0)	254(0)	826(0)	844(0)	1557(0)	1627(588)
246(0)	255(0)	827(0)	845(0)	1562(0)	1627(588)
250(0)	258(28)	884(0)	906(0)	1563(0)	1660(0)
281(191)	259(0)	884(0)	906(0)	1661(208)	1771(236)
310(0)	307(0)	893(15)	919(0)	3057(0)	3146(0)
310(0)	307(0)	893(15)	919(0)	3061(0)	3150(0)
333(218)	316(321)	896(1)	922(16)	3061(0)	3150(0)
362(0)	369(0)	896(1)	922(16)	3066(0)	3155(0)
363(0)	375(0)	898(11)	928(11)	3070(0)	3158(0)
366(0)	378(0)	898(11)	928(11)	3070(0)	3158(0)
366(0)	380(0)	909(0)	940(0)	3073(0)	3161(0)
393(0)	385(0)	917(0)	947(0)	3073(0)	3162(0)
412(5)	430(9)	956(0)	993(0)	3080(0)	3168(0)
412(5)	430(9)	959(0)	994(0)	3083(0)	3171(0)
413(0)	435(0)	1173(0)	1209(0)	3087(20)	3175(24)
459(53)	477(50)	1173(0)	1209(0)	3087(20)	3175(24)
486(0)	496(0)	1179(0)	1215(0)	3094(9)	3182(9)
486(0)	504(0)	1180(0)	1216(0)	3094(9)	3182(9)
492(0)	504(0)	1297(0)	1333(0)	3094(1)	3183(1)
492(0)	508(0)	1303(0)	1339(0)	3101(0)	3189(0)

Table S22 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_4$ structures **4S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
5(0)	-4(0)	500(0)	518(0)	1298(0)	1333(0)
14(0)	8(0)	553(0)	573(0)	1298(0)	1334(0)
20(0)	21(1)	554(0)	575(0)	1305(0)	1340(0)
25(0)	21(0)	588(6)	611(4)	1306(0)	1341(0)
34(0)	29(0)	696(224)	708(186)	1310(0)	1346(0)
36(1)	35(0)	703(153)	721(152)	1311(0)	1347(0)
42(0)	41(1)	741(1)	764(1)	1374(0)	1414(0)
47(0)	53(2)	742(5)	765(5)	1375(0)	1415(0)
55(1)	54(0)	743(1)	767(9)	1423(0)	1467(1)
72(6)	71(6)	745(0)	770(1)	1423(0)	1467(1)
97(7)	82(6)	746(0)	771(0)	1424(0)	1469(1)
149(14)	154(31)	748(1)	771(1)	1425(0)	1470(1)
210(8)	201(0)	751(2)	772(2)	1477(1)	1523(1)
212(2)	210(35)	756(3)	777(1)	1478(0)	1523(0)
218(11)	213(23)	758(3)	778(2)	1480(0)	1524(0)
221(5)	215(0)	762(2)	784(2)	1481(0)	1526(0)
222(78)	223(65)	793(8)	814(11)	1486(1)	1535(1)
226(15)	224(1)	815(0)	830(0)	1488(0)	1537(0)
228(9)	228(12)	823(0)	842(1)	1489(1)	1539(0)
237(2)	233(16)	824(0)	843(0)	1497(0)	1544(0)
239(1)	235(8)	831(0)	846(1)	1536(83)	1595(54)
241(0)	239(7)	886(5)	908(3)	1548(0)	1605(0)
242(0)	245(0)	888(0)	910(0)	1964(527)	2069(431)
245(1)	252(0)	889(12)	912(23)	1981(267)	2090(316)
248(6)	255(4)	889(1)	913(18)	3060(0)	3146(0)
248(0)	258(1)	890(10)	919(17)	3061(0)	3150(0)
265(7)	262(2)	893(9)	920(3)	3063(0)	3150(0)
300(161)	302(216)	894(14)	920(22)	3065(0)	3151(1)
336(18)	348(23)	896(4)	923(15)	3065(0)	3152(0)
366(0)	376(1)	912(0)	924(12)	3067(0)	3156(0)
371(1)	379(1)	915(0)	941(0)	3076(0)	3163(0)
373(0)	383(1)	938(8)	948(0)	3076(0)	3163(0)
375(0)	387(0)	958(0)	995(0)	3077(0)	3164(0)
376(0)	389(0)	959(0)	996(0)	3078(1)	3170(4)
427(19)	391(2)	1117(30)	1178(56)	3088(17)	3175(21)
428(7)	403(29)	1165(0)	1202(0)	3090(14)	3177(20)
480(321)	477(315)	1172(0)	1207(0)	3091(15)	3179(17)
483(61)	501(0)	1172(1)	1209(4)	3092(11)	3183(11)
484(0)	504(0)	1179(0)	1213(0)	3096(5)	3183(5)
497(0)	513(0)	1219(563)	1239(507)	3098(1)	3187(1)

Table S23 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_4$ structure **4S-3.**

BP86	M06L	BP86	M06L	BP86	M06L
5(1)	9(0)	496(0)	572(14)	1298(0)	1335(0)
7(0)	11(0)	497(0)	573(0)	1298(0)	1340(1)
10(0)	16(1)	554(0)	574(7)	1307(0)	1344(0)
23(0)	24(1)	554(0)	604(13)	1307(0)	1347(0)
30(1)	28(0)	617(1)	715(227)	1308(0)	1350(2)
33(1)	38(0)	699(346)	718(91)	1309(0)	1358(297)
42(0)	48(0)	701(26)	730(24)	1375(0)	1415(0)
48(0)	73(1)	741(5)	767(10)	1375(0)	1415(0)
56(0)	88(2)	741(3)	767(3)	1423(0)	1467(0)
67(1)	98(11)	744(1)	767(3)	1423(0)	1469(1)
92(1)	143(6)	745(0)	769(1)	1424(0)	1469(1)
116(20)	157(6)	747(1)	769(3)	1424(0)	1471(1)
182(23)	200(47)	747(0)	771(2)	1477(0)	1494(80)
206(5)	211(1)	753(3)	775(1)	1477(1)	1524(0)
213(26)	217(44)	753(4)	778(1)	1479(0)	1525(0)
218(27)	220(3)	760(0)	779(1)	1480(0)	1526(0)
219(12)	231(10)	760(7)	782(3)	1487(0)	1527(1)
224(25)	232(22)	818(1)	838(0)	1487(0)	1538(0)
224(12)	235(13)	819(1)	839(2)	1491(0)	1538(0)
228(4)	238(9)	824(0)	840(0)	1492(0)	1540(0)
232(0)	252(0)	825(0)	845(0)	1545(6)	1543(1)
234(1)	253(1)	887(0)	875(8)	1546(11)	1600(4)
235(0)	253(0)	888(0)	909(2)	1958(794)	1606(1)
244(0)	264(2)	889(0)	910(1)	1988(312)	2154(541)
245(0)	291(87)	889(26)	916(1)	3060(0)	3147(0)
253(1)	314(106)	891(0)	920(10)	3060(0)	3151(0)
253(0)	324(107)	891(0)	921(18)	3063(0)	3153(0)
355(175)	361(57)	893(14)	923(9)	3064(0)	3154(0)
369(10)	380(5)	894(15)	924(7)	3065(0)	3154(0)
370(4)	381(4)	913(0)	925(18)	3066(0)	3156(0)
372(0)	382(10)	913(0)	945(0)	3076(0)	3163(0)
373(3)	384(0)	959(0)	946(0)	3076(0)	3166(2)
376(29)	385(2)	959(0)	996(0)	3076(0)	3166(0)
382(11)	428(120)	1019(1)	996(0)	3077(0)	3167(0)
395(4)	480(22)	1095(139)	1176(81)	3088(15)	3178(15)
412(13)	496(1)	1169(0)	1207(0)	3089(15)	3179(16)
421(138)	501(0)	1169(0)	1209(0)	3090(0)	3179(16)
455(229)	514(0)	1173(0)	1210(0)	3090(28)	3180(15)
484(1)	520(0)	1174(0)	1211(0)	3096(3)	3186(2)
486(1)	547(14)	1206(11)	1334(0)	3096(2)	3187(1)

Table S24 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_4$ structure **4S-4.**

BP86	M06L	BP86	M06L	BP86	M06L
7(0)	9(0)	500(9)	512(0)	1298(0)	1333(0)
10(0)	10(0)	501(43)	517(0)	1298(0)	1333(0)
15(0)	15(0)	553(0)	573(0)	1306(0)	1342(0)
28(1)	23(2)	554(0)	574(0)	1307(0)	1343(0)
28(0)	30(0)	614(6)	629(7)	1307(0)	1343(0)
37(0)	39(0)	698(301)	712(228)	1310(0)	1345(0)
44(0)	41(0)	700(76)	716(105)	1374(0)	1414(0)
53(0)	54(0)	741(5)	764(3)	1375(0)	1415(0)
65(0)	67(2)	741(2)	765(13)	1423(0)	1468(1)
76(2)	68(0)	743(2)	766(2)	1423(0)	1468(1)
92(0)	93(0)	746(0)	770(0)	1424(0)	1468(1)
123(22)	126(23)	746(1)	771(1)	1424(0)	1469(1)
201(17)	186(16)	747(0)	772(0)	1476(0)	1522(0)
204(4)	195(5)	753(2)	775(4)	1477(1)	1523(0)
209(7)	206(8)	753(7)	776(1)	1478(0)	1523(0)
215(31)	211(41)	759(3)	779(2)	1480(1)	1525(1)
219(58)	220(50)	760(3)	779(1)	1486(0)	1536(0)
223(1)	222(6)	818(2)	834(1)	1488(0)	1537(0)
227(11)	227(27)	819(1)	837(1)	1490(0)	1539(0)
230(2)	232(1)	824(0)	840(0)	1493(0)	1542(0)
235(5)	234(1)	824(0)	842(0)	1544(10)	1602(11)
237(3)	238(12)	884(1)	908(1)	1544(6)	1602(4)
238(3)	247(2)	888(0)	912(0)	1975(653)	2089(461)
245(1)	253(1)	889(8)	913(1)	2008(603)	2126(685)
245(0)	254(0)	889(19)	915(0)	3059(0)	3148(0)
255(1)	261(0)	890(0)	919(2)	3059(0)	3148(0)
259(1)	262(3)	892(1)	919(28)	3063(0)	3151(0)
324(2)	325(25)	892(15)	922(16)	3063(0)	3151(0)
357(70)	328(37)	895(14)	924(15)	3065(0)	3153(0)
363(30)	340(5)	912(0)	943(0)	3065(0)	3154(0)
368(3)	380(9)	913(0)	944(0)	3076(0)	3163(0)
370(8)	382(4)	959(0)	997(0)	3076(0)	3164(0)
373(2)	385(41)	959(0)	997(0)	3076(0)	3164(0)
375(2)	387(8)	986(11)	1005(16)	3076(0)	3165(0)
376(26)	390(19)	1062(99)	1087(103)	3088(11)	3176(19)
414(292)	413(362)	1169(0)	1205(0)	3088(20)	3176(19)
427(85)	421(61)	1169(0)	1206(0)	3090(15)	3178(18)
480(1)	489(81)	1173(0)	1209(0)	3090(16)	3178(21)
486(0)	500(2)	1174(0)	1210(0)	3096(3)	3184(3)
495(3)	505(2)	1205(109)	1238(132)	3096(3)	3185(2)

Table S25 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_5$ structure **5S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
4(0)	9(0)	484(0)	503(0)	1211(395)	1236(301)
13(0)	19(0)	489(0)	508(0)	1298(0)	1333(0)
20(0)	20(0)	493(1)	513(0)	1299(0)	1334(0)
24(0)	21(0)	497(0)	513(1)	1306(0)	1341(0)
26(0)	23(1)	553(0)	574(0)	1307(0)	1344(1)
27(1)	26(0)	554(0)	575(0)	1309(0)	1345(0)
35(0)	32(0)	584(5)	605(5)	1310(0)	1345(0)
42(0)	37(0)	696(240)	708(190)	1375(0)	1415(0)
43(0)	42(1)	701(149)	722(154)	1375(0)	1415(0)
50(0)	68(0)	741(1)	765(2)	1423(0)	1467(1)
59(1)	69(1)	742(2)	765(5)	1424(0)	1469(1)
78(8)	79(7)	743(1)	767(8)	1425(0)	1469(1)
103(7)	98(7)	747(0)	771(0)	1425(0)	1470(1)
147(15)	149(10)	747(1)	772(2)	1477(1)	1523(1)
174(1)	177(27)	748(1)	773(1)	1478(2)	1523(1)
201(2)	201(1)	751(2)	774(1)	1480(0)	1524(0)
210(11)	209(36)	753(5)	775(3)	1481(0)	1525(0)
212(2)	212(4)	757(3)	777(1)	1486(1)	1535(1)
216(66)	213(25)	761(4)	786(5)	1488(0)	1537(0)
217(16)	216(0)	789(6)	811(7)	1494(0)	1541(0)
223(1)	223(58)	815(0)	831(0)	1497(0)	1545(0)
224(5)	228(1)	823(2)	844(0)	1536(82)	1594(60)
227(3)	231(9)	828(0)	844(2)	1537(4)	1602(2)
228(6)	232(9)	830(0)	848(1)	1966(528)	2067(468)
236(6)	236(2)	888(0)	894(69)	1981(301)	2086(368)
238(1)	237(8)	888(2)	909(1)	2079(700)	2191(598)
241(0)	243(5)	889(2)	911(0)	3060(0)	3147(0)
242(0)	253(0)	889(10)	917(3)	3061(0)	3149(0)
248(0)	258(12)	889(13)	918(0)	3063(0)	3151(0)
253(0)	262(0)	893(1)	919(16)	3065(0)	3152(0)
265(8)	263(2)	894(13)	922(13)	3065(0)	3155(0)
279(2)	270(22)	895(11)	923(8)	3067(0)	3155(0)
308(195)	312(228)	912(0)	923(21)	3076(0)	3163(0)
339(19)	355(13)	915(0)	941(0)	3076(0)	3163(0)
365(0)	368(1)	927(23)	951(0)	3078(1)	3165(1)
369(0)	378(1)	958(0)	995(0)	3078(0)	3166(0)
370(1)	383(1)	958(0)	997(0)	3088(17)	3176(20)
371(0)	386(0)	1119(30)	1188(51)	3090(13)	3177(19)
372(0)	389(0)	1165(0)	1202(0)	3090(15)	3178(17)
424(20)	392(3)	1171(0)	1207(0)	3092(11)	3179(14)
425(7)	405(30)	1174(1)	1210(2)	3096(6)	3184(5)
468(236)	460(185)	1179(0)	1213(0)	3098(2)	3186(1)

Table S26 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_5$ structure **5S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
5(0)	10(0)	482(29)	500(1)	1223(624)	1244(548)
17(0)	16(0)	483(62)	501(0)	1298(0)	1334(0)
20(0)	18(0)	496(0)	517(0)	1300(0)	1335(0)
29(0)	24(0)	500(0)	517(2)	1304(1)	1339(1)
29(0)	30(0)	553(0)	574(0)	1305(0)	1342(0)
39(0)	37(0)	557(0)	576(0)	1311(0)	1347(0)
41(0)	40(0)	584(4)	607(5)	1313(0)	1348(0)
44(0)	44(0)	698(247)	712(194)	1374(0)	1415(0)
46(0)	46(1)	703(139)	721(145)	1377(0)	1416(0)
55(1)	51(0)	740(1)	763(0)	1423(0)	1468(1)
66(1)	67(2)	742(5)	766(2)	1424(0)	1468(1)
74(5)	79(4)	743(0)	767(10)	1424(0)	1469(1)
85(5)	81(5)	745(1)	770(1)	1428(1)	1471(1)
152(19)	157(22)	746(0)	771(1)	1477(0)	1521(0)
193(4)	181(2)	747(0)	772(1)	1478(0)	1523(0)
198(9)	190(15)	753(3)	773(1)	1481(0)	1526(0)
201(2)	196(2)	756(3)	778(2)	1483(6)	1527(6)
211(3)	201(1)	762(2)	781(2)	1488(0)	1537(0)
216(6)	204(2)	765(4)	785(4)	1489(1)	1538(1)
219(0)	209(8)	790(10)	817(13)	1490(0)	1539(0)
220(1)	219(13)	821(4)	836(4)	1504(0)	1549(0)
225(50)	223(1)	823(0)	843(1)	1520(103)	1581(80)
227(24)	225(2)	824(0)	845(1)	1548(0)	1605(0)
231(6)	229(62)	840(0)	851(1)	1966(443)	2086(397)
236(1)	233(3)	886(5)	910(2)	1993(435)	2103(434)
240(0)	241(9)	887(10)	914(3)	2030(516)	2143(498)
242(2)	244(12)	890(10)	917(12)	3061(0)	3146(0)
246(1)	256(4)	891(2)	918(5)	3061(0)	3148(0)
247(6)	258(3)	893(9)	919(1)	3064(0)	3150(0)
262(1)	258(1)	895(4)	921(13)	3065(0)	3153(0)
271(1)	269(1)	895(9)	924(7)	3067(0)	3154(0)
296(114)	304(117)	899(4)	924(19)	3067(0)	3155(0)
339(47)	336(37)	915(0)	944(0)	3077(0)	3162(1)
358(3)	368(14)	916(0)	949(0)	3077(0)	3163(1)
366(0)	370(5)	953(1)	965(15)	3078(0)	3164(0)
372(15)	378(4)	958(0)	995(0)	3078(1)	3167(2)
373(1)	379(3)	959(0)	997(0)	3089(15)	3174(19)
375(2)	386(5)	1105(32)	1157(41)	3090(15)	3178(20)
389(30)	388(1)	1162(1)	1200(1)	3092(10)	3178(19)
406(7)	388(46)	1172(0)	1208(0)	3092(16)	3180(14)
415(23)	399(86)	1172(1)	1208(2)	3098(9)	3184(7)
480(264)	476(269)	1182(1)	1216(1)	3098(0)	3186(1)

Table S27 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_5$ structure **5S-3.**

BP86	M06L	BP86	M06L	BP86	M06L
7(0)	8(0)	486(0)	504(0)	1302(0)	1338(0)
7(0)	14(0)	488(1)	505(0)	1306(0)	1341(0)
17(0)	24(0)	488(0)	507(0)	1313(0)	1349(0)
29(1)	32(1)	492(0)	514(0)	1314(0)	1349(0)
34(0)	35(0)	548(0)	544(1)	1314(0)	1350(0)
49(1)	48(0)	555(0)	568(0)	1376(0)	1416(0)
52(0)	48(1)	582(5)	574(0)	1377(0)	1416(0)
59(3)	69(2)	613(0)	600(0)	1377(150)	1469(0)
82(2)	84(4)	699(238)	714(210)	1391(429)	1470(57)
130(1)	122(8)	706(148)	715(0)	1424(0)	1470(7)
133(6)	127(8)	716(0)	721(126)	1427(0)	1471(76)
139(3)	138(2)	742(1)	766(3)	1427(0)	1473(48)
148(8)	154(3)	743(0)	766(2)	1427(0)	1479(495)
171(4)	155(1)	744(0)	769(0)	1480(1)	1526(0)
191(1)	185(1)	744(0)	769(0)	1483(1)	1528(1)
204(1)	196(23)	747(7)	771(10)	1486(0)	1530(0)
209(58)	210(52)	747(1)	771(6)	1486(0)	1530(0)
215(0)	212(0)	751(4)	772(1)	1493(3)	1542(0)
216(4)	219(5)	761(4)	780(5)	1494(0)	1542(2)
217(0)	221(0)	761(7)	780(6)	1495(0)	1543(0)
236(12)	238(18)	762(7)	781(1)	1495(0)	1544(0)
237(0)	239(0)	822(0)	839(0)	1529(22)	1589(15)
242(1)	246(5)	823(0)	841(0)	1562(0)	1618(0)
245(0)	249(4)	825(0)	843(0)	1632(229)	1730(293)
248(0)	254(1)	827(3)	844(3)	1689(449)	1797(441)
252(0)	259(0)	889(2)	909(0)	2052(640)	2149(600)
260(9)	261(0)	889(11)	915(1)	3059(0)	3143(0)
286(234)	278(46)	891(0)	916(0)	3064(0)	3152(0)
302(0)	297(304)	893(1)	917(0)	3065(0)	3152(0)
306(104)	301(1)	894(0)	919(15)	3066(0)	3153(0)
323(66)	328(50)	896(13)	926(14)	3068(0)	3157(0)
343(3)	353(3)	897(11)	927(12)	3068(0)	3157(0)
362(2)	359(3)	898(12)	927(13)	3077(0)	3162(1)
363(0)	370(0)	914(0)	944(0)	3077(0)	3164(1)
364(0)	375(0)	915(0)	946(0)	3079(0)	3167(0)
367(1)	376(0)	958(0)	995(0)	3082(0)	3170(0)
373(3)	378(0)	959(0)	995(0)	3089(12)	3175(16)
415(22)	422(36)	1172(1)	1209(1)	3091(15)	3178(19)
417(8)	428(5)	1175(0)	1211(0)	3093(11)	3181(12)
422(3)	435(0)	1178(0)	1214(0)	3093(11)	3181(12)
457(19)	459(1)	1179(0)	1215(0)	3098(5)	3185(5)
469(0)	468(21)	1299(0)	1335(0)	3100(0)	3188(0)

Table S28 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_6$ structure **6S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
8(0)	16(0)	404(6)	390(64)	1183(1)	1216(1)
14(0)	18(0)	413(32)	401(77)	1216(473)	1236(373)
19(0)	18(0)	469(207)	462(151)	1299(0)	1334(0)
22(0)	20(0)	481(2)	500(1)	1300(0)	1335(0)
26(0)	23(0)	489(0)	508(0)	1304(1)	1340(1)
30(0)	24(0)	493(2)	513(0)	1308(0)	1343(1)
34(0)	33(0)	496(1)	518(1)	1310(0)	1345(0)
40(0)	37(0)	553(0)	574(0)	1313(0)	1348(0)
45(0)	41(0)	557(0)	576(0)	1375(0)	1414(0)
46(0)	46(0)	580(3)	603(5)	1377(0)	1417(0)
49(0)	51(0)	698(279)	712(205)	1424(0)	1468(1)
58(1)	53(0)	701(120)	720(147)	1424(0)	1468(1)
68(1)	74(2)	740(1)	763(1)	1425(0)	1469(1)
79(7)	81(5)	742(2)	766(2)	1428(1)	1472(1)
93(5)	92(5)	743(0)	766(8)	1477(0)	1522(0)
149(19)	148(11)	747(0)	771(1)	1478(2)	1523(1)
174(1)	174(15)	747(1)	773(1)	1481(0)	1525(0)
194(5)	183(2)	747(0)	773(1)	1484(5)	1527(6)
197(10)	191(16)	753(2)	773(1)	1488(0)	1537(0)
200(4)	195(4)	753(6)	775(2)	1489(0)	1539(0)
202(0)	202(1)	761(3)	782(1)	1494(0)	1540(1)
211(7)	204(4)	765(4)	782(5)	1504(0)	1550(0)
215(5)	209(6)	787(9)	815(10)	1520(111)	1580(92)
218(27)	211(3)	821(5)	836(5)	1538(3)	1602(2)
220(14)	219(12)	823(2)	841(2)	1970(438)	2086(411)
221(2)	226(5)	828(0)	845(0)	1993(436)	2101(469)
226(6)	227(10)	840(1)	853(1)	2027(451)	2139(456)
227(11)	229(46)	887(9)	910(2)	2078(745)	2191(641)
230(1)	233(4)	888(1)	915(0)	3061(0)	3146(0)
236(3)	235(1)	889(12)	916(2)	3061(0)	3148(0)
238(1)	244(9)	890(1)	918(11)	3064(0)	3149(0)
242(2)	257(8)	893(1)	920(1)	3065(0)	3153(0)
253(0)	259(0)	895(10)	922(13)	3067(0)	3153(0)
263(1)	260(1)	895(8)	923(13)	3067(0)	3154(0)
271(2)	268(14)	899(4)	925(15)	3077(0)	3162(1)
281(3)	270(1)	915(0)	944(0)	3077(0)	3163(1)
303(128)	312(134)	916(0)	948(0)	3078(0)	3165(0)
340(53)	339(29)	944(9)	956(41)	3078(0)	3165(0)
357(3)	363(11)	958(0)	995(0)	3089(15)	3174(19)
365(0)	368(3)	958(0)	997(0)	3090(14)	3177(18)
369(2)	378(4)	1106(29)	1163(37)	3092(13)	3178(19)
369(16)	378(3)	1162(1)	1200(1)	3092(14)	3179(15)
371(1)	385(0)	1171(0)	1207(0)	3097(9)	3184(8)
389(36)	388(3)	1174(0)	1210(2)	3098(2)	3185(1)

Table S29 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_6$ structure **6S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
3(0)	13(0)	407(3)	401(56)	1188(0)	1225(0)
18(0)	22(0)	415(21)	417(114)	1209(704)	1234(599)
22(0)	22(0)	479(0)	481(237)	1298(0)	1333(0)
30(0)	30(1)	482(11)	500(0)	1304(0)	1339(0)
37(0)	33(0)	489(356)	503(0)	1305(0)	1341(0)
39(0)	39(1)	493(4)	516(0)	1307(0)	1341(0)
42(1)	40(0)	500(0)	517(1)	1311(0)	1346(0)
43(0)	45(0)	554(0)	573(0)	1314(0)	1350(0)
44(0)	47(0)	560(0)	582(0)	1374(0)	1414(0)
55(0)	50(0)	588(2)	614(2)	1381(0)	1420(0)
60(1)	54(0)	701(272)	714(205)	1423(0)	1468(1)
65(2)	62(2)	704(118)	720(142)	1424(0)	1468(1)
67(0)	67(0)	742(0)	766(9)	1427(0)	1471(0)
71(4)	80(3)	742(5)	767(0)	1431(0)	1475(1)
88(3)	88(4)	743(3)	767(0)	1478(0)	1523(0)
162(26)	166(24)	745(0)	769(1)	1480(0)	1526(0)
188(0)	178(3)	746(0)	772(0)	1485(0)	1534(1)
193(2)	188(6)	747(0)	773(0)	1488(0)	1535(0)
196(8)	191(0)	756(3)	774(2)	1489(1)	1536(1)
198(3)	191(7)	758(4)	777(2)	1489(1)	1537(0)
200(3)	195(0)	762(1)	783(1)	1489(0)	1538(1)
207(2)	196(0)	767(5)	784(4)	1501(99)	1558(116)
214(4)	201(0)	792(10)	822(17)	1513(0)	1562(0)
221(2)	207(0)	824(0)	840(0)	1548(0)	1606(0)
224(10)	220(0)	825(0)	842(1)	1978(365)	2087(384)
225(14)	222(51)	827(0)	844(1)	1985(648)	2095(632)
227(51)	226(18)	853(1)	868(1)	2015(607)	2126(613)
233(6)	227(14)	887(6)	913(1)	2026(387)	2136(435)
237(3)	238(17)	890(7)	917(9)	3061(0)	3144(0)
240(0)	245(1)	890(9)	917(0)	3062(0)	3147(0)
246(1)	249(3)	893(10)	919(10)	3064(0)	3150(0)
248(7)	254(0)	895(8)	921(1)	3065(0)	3150(0)
265(1)	256(4)	896(3)	921(10)	3067(0)	3154(0)
273(1)	266(6)	898(1)	924(13)	3068(0)	3154(0)
275(8)	283(0)	903(2)	927(11)	3077(0)	3160(0)
287(108)	301(124)	915(0)	946(0)	3078(0)	3161(0)
344(37)	341(34)	918(0)	948(0)	3078(0)	3165(1)
346(0)	355(0)	956(0)	967(26)	3079(0)	3166(0)
359(0)	363(0)	958(0)	993(0)	3090(10)	3173(20)
369(1)	371(0)	959(0)	996(0)	3090(19)	3176(18)
374(0)	381(4)	1099(15)	1156(23)	3092(11)	3178(20)
375(0)	385(0)	1161(4)	1197(3)	3093(13)	3179(14)
394(51)	387(0)	1171(0)	1208(1)	3097(1)	3181(12)
398(1)	394(0)	1172(1)	1208(3)	3098(11)	3185(1)

Table S30 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_7$ structure **7S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
3(0)	13(0)	373(0)	386(0)	1174(1)	1209(4)
18(0)	21(0)	394(52)	388(0)	1188(0)	1224(0)
19(0)	22(0)	397(1)	391(0)	1203(535)	1228(407)
22(0)	25(0)	405(3)	400(61)	1299(0)	1333(0)
26(0)	25(0)	414(32)	418(128)	1304(0)	1339(0)
31(0)	29(1)	476(212)	466(113)	1307(0)	1341(0)
38(0)	33(0)	479(0)	502(0)	1307(0)	1341(1)
40(0)	36(0)	489(0)	506(0)	1309(0)	1346(0)
45(0)	39(1)	493(2)	512(0)	1314(0)	1350(0)
45(0)	43(0)	493(1)	516(1)	1375(0)	1414(0)
47(0)	45(0)	554(0)	573(0)	1381(0)	1420(0)
56(0)	47(0)	560(0)	582(0)	1424(0)	1467(1)
63(1)	54(0)	584(1)	609(2)	1425(0)	1469(1)
66(1)	62(2)	700(319)	713(227)	1427(0)	1471(0)
67(0)	67(0)	702(83)	717(132)	1431(0)	1475(1)
75(7)	81(3)	742(2)	766(6)	1477(2)	1522(0)
97(3)	97(4)	742(0)	766(3)	1481(0)	1524(0)
156(20)	154(8)	743(3)	767(0)	1485(0)	1533(1)
175(5)	176(15)	747(0)	773(1)	1488(0)	1534(0)
188(0)	183(2)	747(1)	773(1)	1489(0)	1535(1)
193(2)	187(9)	747(0)	773(1)	1489(0)	1536(0)
196(9)	192(2)	754(4)	774(1)	1493(1)	1539(1)
198(4)	193(3)	758(4)	776(3)	1501(107)	1556(128)
200(4)	197(0)	761(3)	776(1)	1513(0)	1562(0)
201(2)	198(7)	766(5)	783(3)	1538(2)	1601(1)
207(2)	202(0)	789(8)	818(12)	1980(352)	2091(380)
214(4)	211(1)	823(2)	840(0)	1987(623)	2097(632)
220(42)	212(4)	827(0)	840(0)	2013(618)	2124(625)
221(9)	222(26)	828(0)	843(0)	2023(239)	2133(286)
224(2)	225(11)	852(2)	868(2)	2081(797)	2190(734)
226(7)	228(0)	889(2)	910(0)	3061(0)	3144(0)
228(7)	230(43)	890(10)	917(4)	3062(0)	3147(0)
232(1)	234(2)	890(9)	917(0)	3064(0)	3149(0)
236(2)	244(1)	893(1)	918(10)	3065(0)	3150(0)
240(2)	249(3)	894(10)	921(2)	3067(0)	3152(0)
253(0)	254(2)	895(7)	922(14)	3068(0)	3154(0)
265(1)	257(0)	897(1)	922(10)	3078(0)	3160(0)
273(1)	266(4)	902(2)	927(10)	3078(0)	3161(0)
275(5)	269(25)	915(0)	946(0)	3078(0)	3164(0)
279(5)	282(0)	918(0)	946(0)	3078(0)	3165(0)
295(132)	311(127)	948(9)	957(55)	3090(10)	3173(20)
346(0)	342(32)	956(0)	993(0)	3090(19)	3176(18)
346(38)	354(0)	958(0)	996(0)	3092(11)	3177(19)
359(0)	359(0)	1102(15)	1162(23)	3093(14)	3178(15)
366(0)	369(0)	1160(3)	1196(2)	3098(2)	3181(13)
370(0)	379(4)	1170(0)	1206(0)	3098(12)	3184(1)

Table S31 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)_7$ structures **7S-2.**

BP86	M06L	BP86	M06L	BP86	M06L
9(0)	14(0)	365(0)	376(0)	1177(1)	1211(1)
11(0)	15(0)	373(16)	377(8)	1183(1)	1217(1)
18(0)	19(0)	391(19)	381(4)	1223(452)	1245(396)
21(0)	24(0)	408(7)	393(29)	1299(0)	1335(1)
28(0)	28(0)	414(18)	399(126)	1300(0)	1335(0)
36(0)	34(0)	455(201)	456(134)	1304(1)	1339(1)
38(0)	37(0)	481(1)	499(1)	1308(0)	1343(0)
39(0)	37(0)	486(0)	508(0)	1311(0)	1345(0)
42(1)	41(0)	491(1)	510(1)	1313(0)	1348(0)
47(1)	48(0)	497(0)	518(1)	1377(0)	1416(0)
48(0)	51(0)	554(0)	573(0)	1377(0)	1417(0)
53(0)	52(0)	557(0)	576(0)	1424(0)	1468(1)
56(0)	58(1)	584(3)	607(5)	1425(0)	1469(1)
62(3)	61(0)	697(232)	712(198)	1427(0)	1470(1)
72(0)	79(4)	704(165)	720(154)	1428(1)	1472(1)
82(9)	84(3)	740(1)	763(1)	1477(0)	1522(0)
88(7)	92(8)	742(1)	765(3)	1480(2)	1524(1)
140(9)	148(1)	743(1)	766(2)	1481(1)	1525(2)
142(9)	149(18)	745(0)	771(1)	1484(4)	1528(5)
150(1)	157(1)	746(0)	771(0)	1489(0)	1539(0)
187(5)	180(5)	747(0)	772(1)	1489(0)	1539(1)
193(4)	184(3)	752(3)	773(1)	1499(0)	1545(1)
196(14)	188(22)	756(4)	774(2)	1504(0)	1551(0)
199(1)	194(1)	764(3)	783(1)	1520(114)	1579(100)
200(3)	195(1)	764(4)	783(1)	1531(9)	1591(6)
207(1)	201(1)	786(10)	816(14)	1970(428)	2090(418)
212(3)	203(1)	820(5)	836(5)	1990(410)	2101(395)
214(5)	207(1)	825(4)	842(4)	2023(418)	2137(431)
217(16)	209(6)	831(0)	847(1)	2074(378)	2180(343)
221(1)	217(9)	839(0)	854(1)	2084(883)	2186(764)
223(7)	221(2)	887(9)	909(2)	3060(0)	3143(0)
228(36)	225(41)	889(9)	914(4)	3060(0)	3145(0)
230(4)	228(1)	890(2)	917(11)	3063(0)	3147(0)
236(3)	230(19)	894(2)	918(0)	3066(0)	3151(0)
242(1)	238(2)	895(11)	920(1)	3067(0)	3153(0)
249(4)	255(9)	895(8)	921(13)	3069(0)	3155(0)
251(2)	259(2)	896(2)	924(13)	3076(0)	3162(1)
263(1)	262(1)	898(5)	925(15)	3077(0)	3163(2)
272(2)	272(1)	915(0)	945(0)	3078(1)	3163(0)
281(14)	285(4)	918(0)	948(0)	3080(1)	3164(3)
287(37)	289(17)	948(5)	962(20)	3089(16)	3174(19)
311(61)	315(42)	958(0)	995(0)	3090(14)	3174(16)
326(83)	339(103)	958(0)	996(0)	3091(16)	3177(11)
357(1)	366(5)	1105(25)	1156(30)	3093(9)	3178(20)
360(0)	371(5)	1162(1)	1199(1)	3097(10)	3183(9)
364(0)	375(4)	1169(0)	1206(1)	3100(3)	3186(5)

Table S32 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the $(C_8H_8)_2Th_2(CO)$ structures **1S-1.**

BP86	M06L	BP86	M06L	BP86	M06L
4(0)	-12(2)	740(2)	763(9)	1304(0)	1341(0)
12(0)	11(0)	743(1)	765(4)	1305(0)	1341(1)
14(2)	15(2)	747(0)	768(0)	1373(0)	1413(0)
26(1)	49(0)	748(0)	772(1)	1373(0)	1415(0)
30(1)	60(0)	748(0)	774(1)	1421(0)	1466(2)
77(4)	82(14)	749(0)	774(1)	1422(0)	1466(2)
78(13)	85(4)	750(1)	775(0)	1422(0)	1467(2)
209(39)	201(37)	754(3)	776(2)	1422(0)	1469(0)
219(7)	215(10)	755(3)	777(0)	1473(0)	1519(0)
225(4)	226(1)	814(1)	831(1)	1473(0)	1520(0)
227(8)	232(16)	816(1)	833(1)	1476(0)	1520(0)
232(0)	232(0)	818(1)	838(2)	1476(0)	1521(0)
233(5)	235(3)	819(1)	840(1)	1485(0)	1536(0)
242(1)	252(0)	882(0)	905(0)	1485(0)	1536(0)
244(0)	253(0)	882(0)	908(0)	1487(0)	1537(0)
244(0)	255(1)	883(1)	909(1)	1487(0)	1537(0)
246(1)	260(0)	884(1)	912(3)	1540(0)	1599(0)
291(43)	318(47)	887(18)	917(23)	1547(0)	1604(0)
375(3)	387(1)	888(13)	919(35)	3057(0)	3145(0)
376(0)	388(0)	889(18)	920(18)	3057(0)	3146(0)
376(1)	388(0)	890(18)	921(0)	3061(0)	3149(0)
377(0)	389(0)	908(0)	941(0)	3062(0)	3149(0)
384(79)	403(126)	908(0)	942(0)	3063(0)	3150(0)
456(269)	464(204)	957(0)	996(0)	3063(0)	3151(0)
485(0)	502(0)	959(0)	996(0)	3074(0)	3159(0)
490(0)	506(0)	1045(176)	1077(172)	3074(0)	3161(0)
491(0)	510(0)	1166(0)	1203(0)	3074(0)	3162(0)
495(0)	514(0)	1167(0)	1204(1)	3074(2)	3162(1)
548(0)	570(11)	1168(0)	1204(1)	3087(23)	3173(20)
551(0)	572(73)	1169(1)	1207(0)	3087(0)	3174(38)
552(31)	572(0)	1295(0)	1331(1)	3088(27)	3175(27)
692(189)	706(148)	1295(0)	1331(0)	3088(36)	3176(19)
699(172)	716(172)	1302(0)	1337(0)	3094(3)	3181(1)
738(7)	759(0)	1303(0)	1340(0)	3095(1)	3182(4)

Complete Gaussian 09 reference (Reference 44)

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