Tetranuclear Iron Carbonyl Complexes with a Central Tin Atom: Relationship to Iron Carbonyl Carbides

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Supporting Information

Tables S1 to S15: Theoretical Cartesian coordinates for the structures of $SnFe_4(CO)_n$ (n=16-12) using the M06-L/TZP and BP86/DZP methods.

Tables S16 to S30: Theoretical harmonic vibrational frequencies for the structures of $SnFe_4(CO)_n$ (n=16-12) using the M06-L/TZP and BP86/DZP methods.

Tables S31 to S34: Metal- Metal Distances, Natural Population Analysis Natural Charges, Metal Electron Configuration, Formal Metal-Metal Bond Orders, and WBIs for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures Using the M06-L/TZP and BP86/DZP Methods.

Table S35. $\nu(CO)$ Frequencies (in cm-1) and IR Intensities (in km/mol) in Parentheses for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures are calculated by using the BP86/DZP Method except for 14S-3 and 12S-2 which are calculated by M06-L/TZP because the corresponding isomers are not optimized by BP86/DZP. Bridging $\nu(CO)$ frequencies are given in bold type, whereas weakly semibridging $\nu(CO)$ frequencies are given in italic type.

Complete Gaussian09 reference (reference 15).

Table S1. Theoretical Cartesian coordinates (in Å) for the structure **16S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP				BP86/DZP			
Fe	0.00000000	-1.43623800	2.07011100	Fe	0.00000000	-1.44895800	2.04725400
Fe	0.00000000	1.43623800	2.07011100	Fe	0.00000000	1.44895800	2.04725400
C	1.77805400	1.39340400	1.77220900	C	1.79073000	1.43656900	1.87153300
C	0.00000000	3.12765100	1.54589000	C	0.00000000	3.11797300	1.46860500
C	-1.77805400	1.39340400	1.77220900	C	-1.79073000	1.43656900	1.87153300
C	1.77805400	-1.39340400	1.77220900	C	1.79073000	-1.43656900	1.87153300
C	0.00000000	-3.12765100	1.54589000	C	0.00000000	-3.11797300	1.46860500
C	-1.77805400	-1.39340400	1.77220900	C	-1.79073000	-1.43656900	1.87153300
O	-2.89905100	1.46555200	1.54535500	O	-2.94909400	1.53497700	1.75901400
O	0.00000000	4.22479200	1.22417000	O	0.00000000	4.23672300	1.13271400
O	2.89905100	1.46555200	1.54535500	O	2.94909400	1.53497700	1.75901400
O	2.89905100	-1.46555200	1.54535500	O	2.94909400	-1.53497700	1.75901400
O	0.00000000	-4.22479200	1.22417000	O	0.00000000	-4.23672300	1.13271400
O	-2.89905100	-1.46555200	1.54535500	O	-2.94909400	-1.53497700	1.75901400
C	0.00000000	-1.52318400	3.87375600	C	0.00000000	-1.57623300	3.84179300
O	0.00000000	-1.62722100	5.01170100	O	0.00000000	-1.71690900	4.99966300
C	0.00000000	1.52318400	3.87375600	C	0.00000000	1.57623300	3.84179300
O	0.00000000	1.62722100	5.01170100	O	0.00000000	1.71690900	4.99966300
O	-1.46555200	-2.89905100	-1.54535500	O	-1.53497700	-2.94909400	-1.75901400
C	-1.39340400	-1.77805400	-1.77220900	C	-1.43656900	-1.79073000	-1.87153300
Fe	-1.43623800	0.00000000	-2.07011100	Fe	-1.44895800	0.00000000	-2.04725400
C	-3.12765100	0.00000000	-1.54589000	C	-3.11797300	0.00000000	-1.46860500
C	-1.39340400	1.77805400	-1.77220900	C	-1.43656900	1.79073000	-1.87153300
C	-1.52318400	0.00000000	-3.87375600	C	-1.57623300	0.00000000	-3.84179300
O	-4.22479200	0.00000000	-1.22417000	O	-4.23672300	0.00000000	-1.13271400
O	-1.46555200	2.89905100	-1.54535500	O	-1.53497700	2.94909400	-1.75901400
O	-1.62722100	0.00000000	-5.01170100	O	-1.71690900	0.00000000	-4.99966300
Fe	1.43623800	0.00000000	-2.07011100	Fe	1.44895800	0.00000000	-2.04725400
C	1.39340400	-1.77805400	-1.77220900	C	1.43656900	-1.79073000	-1.87153300
C	3.12765100	0.00000000	-1.54589000	C	3.11797300	0.00000000	-1.46860500
C	1.39340400	1.77805400	-1.77220900	C	1.43656900	1.79073000	-1.87153300
C	1.52318400	0.00000000	-3.87375600	C	1.57623300	0.00000000	-3.84179300
O	1.46555200	-2.89905100	-1.54535500	O	1.53497700	-2.94909400	-1.75901400
O	4.22479200	0.00000000	-1.22417000	O	4.23672300	0.00000000	-1.13271400
O	1.46555200	2.89905100	-1.54535500	O	1.53497700	2.94909400	-1.75901400
O	1.62722100	0.00000000	-5.01170100	O	1.71690900	0.00000000	-4.99966300
Sn	0.00000000	0.00000000	0.00000000	Sn	0.00000000	0.00000000	0.00000000

Table S2. Theoretical Cartesian coordinates (in Å) for the structure **16S-2** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP				BP86/DZP			
Fe	0.00000000	1.43818600	2.11445300	Fe	0.00000000	1.45167300	2.08746300
Fe	0.00000000	-1.43818600	2.11445300	Fe	0.00000000	-1.45167300	2.08746300
Fe	-1.30032300	0.00000000	-2.11140100	Fe	-1.29995000	0.00000000	-2.09074900
Fe	1.30032300	0.00000000	-2.11140100	Fe	1.29995000	0.00000000	-2.09074900
C	-2.23757100	-1.35484400	-1.38105400	C	-2.26730300	-1.35077300	-1.40752000
C	0.00000000	1.42120600	-2.67438900	C	0.00000000	1.37670200	-2.74508200
C	-2.23757100	1.35484400	-1.38105400	C	-2.26730300	1.35077300	-1.40752000
C	2.23757100	1.35484400	-1.38105400	C	2.26730300	1.35077300	-1.40752000
C	2.23757100	-1.35484400	-1.38105400	C	2.26730300	-1.35077300	-1.40752000
C	0.00000000	-1.42120600	-2.67438900	C	0.00000000	-1.37670200	-2.74508200
C	-1.80525700	-1.38593600	2.02871100	C	-1.80206300	-1.43053900	2.05897800
C	0.00000000	-2.96272200	1.20315200	C	0.00000000	-3.00769300	1.24338600
C	1.80525700	-1.38593600	2.02871100	C	1.80206300	-1.43053900	2.05897800
C	-1.80525700	1.38593600	2.02871100	C	-1.80206300	1.43053900	2.05897800
C	0.00000000	2.96272200	1.20315200	C	0.00000000	3.00769300	1.24338600
C	1.80525700	1.38593600	2.02871100	C	1.80206300	1.43053900	2.05897800
O	2.94625000	-1.43884600	1.98492400	O	2.96491000	-1.51756200	2.07483900
O	0.00000000	-3.93435700	0.59792300	O	0.00000000	-4.04688800	0.70993600
O	-2.94625000	-1.43884600	1.98492400	O	-2.96491000	-1.51756200	2.07483900
O	-2.94625000	1.43884600	1.98492400	O	-2.96491000	1.51756200	2.07483900
O	0.00000000	3.93435700	0.59792300	O	0.00000000	4.04688800	0.70993600
O	2.94625000	1.43884600	1.98492400	O	2.96491000	1.51756200	2.07483900
O	2.86177100	2.22119800	-0.96877900	O	2.95778500	2.21878800	-1.04095700
O	2.86177100	-2.22119800	-0.96877900	O	2.95778500	-2.21878800	-1.04095700
O	0.00000000	-2.51161200	-3.07750800	O	0.00000000	-2.44876200	-3.25100700
O	-2.86177100	-2.22119800	-0.96877900	O	-2.95778500	-2.21878800	-1.04095700
O	0.00000000	2.51161200	-3.07750800	O	0.00000000	2.44876200	-3.25100700
O	-2.86177100	2.22119800	-0.96877900	O	-2.95778500	2.21878800	-1.04095700
C	0.00000000	1.68596600	3.89814500	C	0.00000000	1.72436600	3.86319900
O	0.00000000	1.85881600	5.02785100	O	0.00000000	1.94311900	5.00883800
C	-2.04710600	0.00000000	-3.74334000	C	-2.08249600	0.00000000	-3.70141300
C	2.04710600	0.00000000	-3.74334000	C	2.08249600	0.00000000	-3.70141300
O	2.56907300	0.00000000	-4.75951700	O	2.65250500	0.00000000	-4.71864500
O	-2.56907300	0.00000000	-4.75951700	O	-2.65250500	0.00000000	-4.71864500
C	0.00000000	-1.68596600	3.89814500	C	0.00000000	-1.72436600	3.86319900
O	0.00000000	-1.85881600	5.02785100	O	0.00000000	-1.94311900	5.00883800
Sn	0.00000000	0.00000000	0.05916100	Sn	0.00000000	0.00000000	0.07089200

Table S3. Theoretical Cartesian coordinates (in Å) for the structure **15S-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -0.00470100 2.38071400 1.26200600	Fe 0.00872300 2.30871700 1.33303100
Fe 0.40161200 1.31357400 -1.42173000	Fe 0.39163200 1.32040500 -1.47860100
Fe -0.40161200 -1.31357400 -1.42173000	Fe -0.39163200 -1.32040500 -1.47860100
Fe 0.00470100 -2.38071400 1.26200600	Fe -0.00872300 -2.30871700 1.33303100
C 0.00000000 0.00000000 -2.82443400	C 0.00000000 0.00000000 -2.85816800
C 1.78631700 -2.09392200 1.16177800	C 1.77780300 -2.12630800 1.24086600
C 1.25868900 -2.02018300 -1.65178500	C 1.25549700 -2.03552400 -1.70587700
C 0.07825500 -2.64445100 3.02122500	C 0.04862700 -2.38265500 3.10560100
C -1.78674400 -2.15952600 1.31649200	C -1.80518300 -2.20068900 1.36856800
C -2.09181800 -0.71345900 -1.21209700	C -2.11440300 -0.81881200 -1.36569600
C 1.05007300 2.68803400 -2.32890400	C 0.98867200 2.71375700 -2.38752000
C -1.25868900 2.02018300 -1.65178500	C -1.25549700 2.03552400 -1.70587700
C -1.78631700 2.09392200 1.16177800	C -1.77780300 2.12630800 1.24086600
C 2.09181800 0.71345900 -1.21209700	C 2.11440300 0.81881200 -1.36569600
C 1.78674400 2.15952600 1.31649200	C 1.80518300 2.20068900 1.36856800
C -0.07825500 2.64445100 3.02122500	C -0.04862700 2.38265500 3.10560100
O -2.91519400 1.89422700 1.14682100	O -2.94227800 2.01810900 1.23692000
O -2.26989800 2.51179000 -1.86044600	O -2.27399500 2.55445000 -1.93990800
O 1.48056300 3.57129700 -2.91746800	O 1.39533200 3.62363500 -2.99861700
O 3.18078800 0.36872100 -1.12182700	O 3.25007300 0.54393200 -1.35294700
O 2.92002300 2.02045200 1.42329800	O 2.96962700 2.16391300 1.46550000
O -0.11792800 2.83114800 4.14891700	O -0.08035200 2.46597900 4.27052000
O 0.11792800 -2.83114800 4.14891700	O 0.08035200 -2.46597900 4.27052000
O -2.92002300 -2.02045200 1.42329800	O -2.96962700 -2.16391300 1.46550000
O -3.18078800 -0.36872100 -1.12182700	O -3.25007300 -0.54393200 -1.35294700
O 0.00000000 0.00000000 -3.99292200	O 0.00000000 0.00000000 -4.05042600
O 2.91519400 -1.89422700 1.14682100	O 2.94227800 -2.01810900 1.23692000
O 2.26989800 -2.51179000 -1.86044600	O 2.27399500 -2.55445000 -1.93990800
C 0.00633200 3.98929200 0.44656800	C 0.00782400 3.98490800 0.68454900
O 0.00000000 5.01782100 -0.05262900	O 0.00000000 5.08835100 0.30606100
C -1.05007300 -2.68803400 -2.32890400	C -0.98867200 -2.71375700 -2.38752000
C -0.00633200 -3.98929200 0.44656800	C -0.00782400 -3.98490800 0.68454900
O 0.00000000 -5.01782100 -0.05262900	O 0.00000000 -5.08835100 0.30606100
O -1.48056300 -3.57129700 -2.91746800	O -1.39533200 -3.62363500 -2.99861700
Sn 0.00000000 0.00000000 0.71779200	Sn 0.00000000 0.00000000 0.60071500

Table S4. Theoretical Cartesian coordinates (in Å) for the structure **15S-2** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -1.89631900 0.02127100 -1.04523700	Fe 1.86434200 -0.56919300 -0.88788600
Fe -3.55568200 0.09226200 0.73012900	Fe 3.60557400 0.27849600 0.62305800
Fe 2.22906300 -1.47145700 0.30771900	Fe -2.26903300 1.51148700 -0.25724000
Fe 2.62925900 1.33890800 0.08775600	Fe -2.54054300 -1.22238700 0.54674100
C 1.02327300 -2.73942900 0.59389200	C -1.29963100 2.98728400 -0.38095500
C 3.10837700 0.81316700 -1.56892200	C -3.21176900 -1.26934800 -1.12274400
C 2.19870500 -1.83253700 -1.46573200	C -2.16966500 1.26202100 -2.03834400
C 2.53476900 3.01479900 -0.48954300	C -2.16798900 -2.94957500 0.43781400
C 1.74991500 1.85074600 1.59583200	C -1.72412200 -1.15718800 2.16135900
C 2.02661200 -0.90951600 2.01536200	C -2.22123200 1.63061600 1.54187000
C -4.66298600 1.48926100 0.62847500	C 5.29068600 -0.38444700 0.62706200
C -4.82795900 -1.17689300 0.72661400	C 4.00327500 1.95961000 0.25365200
C -1.67061700 0.15864600 0.83984900	C 1.73284200 0.16840400 0.87252100
C -3.72891200 -0.05587100 -1.31711300	C 3.69029100 -0.45192900 -1.29415000
C -1.49948600 -1.45476100 -1.94144200	C 1.50141300 -0.27847600 -2.61430200
C -1.64573700 1.17153000 -2.39113500	C 1.74737500 -2.31823100 -0.93067200
O -0.70765800 0.24491500 1.61365200	O 0.82443600 0.42597300 1.68844300
O -5.61623400 -2.00462700 0.73612600	O 4.22810500 3.07838800 0.00215700
O -5.34164400 2.40779500 0.56269500	O 6.37770700 -0.80109000 0.68768600
O -4.60584900 -0.13383200 -2.08378300	O 4.51841800 -0.63083800 -2.13058300
O -1.24131800 -2.44407900 -2.46337200	O 1.27620800 -0.07178100 -3.74386100
O -1.48844400 1.93849000 -3.22790500	O 1.71502900 -3.48985700 -0.91844900
O 2.49610600 4.09364500 -0.86571700	O -1.96556300 -4.09748800 0.36982300
O 1.24077200 2.27576900 2.52487700	O -1.26382000 -1.22653600 3.22908700
O 1.88634700 -0.65493600 3.12100300	O -2.20406500 1.84018200 2.68956400
O 0.22779200 -3.53948800 0.78789000	O -0.68609800 3.97807400 -0.45559300
O 3.42518900 0.58450100 -2.64579000	O -3.68921900 -1.42569500 -2.17791800
O 2.13031300 -2.11030700 -2.57358100	O -2.09689800 1.17263300 -3.20035200
C -3.36610000 0.12162700 2.51187100	C 3.58527500 0.46124900 2.40215000
O -3.25936800 0.14684300 3.64900500	O 3.58764300 0.59421100 3.56058600
C 3.89844000 -2.09649400 0.58200800	C -4.00002000 1.99955900 -0.32030900
C 4.25294300 1.13541800 0.84691100	C -4.17597400 -1.08420500 1.28566100
O 5.28404500 1.02323100 1.32579100	O -5.23360300 -1.03852300 1.77365200
O 4.94049200 -2.52906000 0.76181100	O -5.10680700 2.36162800 -0.37797700
Sn 0.48247800 0.18330700 -0.37745500	Sn -0.45810400 -0.17529600 -0.27790600

Table S5. Theoretical Cartesian coordinates (in Å) for the structure **15T-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe 1.88768900 -0.60011800 1.04997100	Fe 1.79197500 -0.40833900 0.89167900
Fe 3.47782900 0.31616700 -0.63307700	Fe 3.68779100 0.19682400 -0.53823200
Fe -2.20760400 1.50536900 0.12000100	Fe -2.29742400 1.51777500 -0.02985100
Fe -2.48814200 -1.23854000 -0.48818900	Fe -2.53742300 -1.31108200 -0.31581800
C -1.21770100 2.97893200 0.06901600	C -1.38198200 3.01118900 -0.28628900
C -1.42567800 -1.24934700 -1.95975900	C -1.63522600 -1.48101600 -1.86669200
C -2.14323400 1.42255400 -1.68641500	C -2.42807800 1.28170100 -1.81443000
C -2.21490000 -2.97878500 -0.27765400	C -2.10266400 -2.95967300 0.15510400
C -3.10338600 -1.11225300 1.20449200	C -3.19688500 -1.00929600 1.33380000
C -1.98325500 1.38589200 1.91413700	C -2.00199900 1.59210400 1.74514000
C 4.23811200 -0.58289500 -2.02451100	C 4.63451500 -0.79430400 -1.70883600
C 4.46946500 1.84081200 -0.69067300	C 4.71097800 1.67873900 -0.60185900
C 1.91946500 1.11733000 1.62668400	C 1.94882100 1.32308600 1.38170700
C 2.01767500 0.93112500 -1.50021700	C 2.38672100 0.74502100 -1.66070000
C 1.84060200 -2.01029800 -0.07916300	C 1.90506800 -1.94900100 -0.03502600
C 1.60586300 -1.46933400 2.60798100	C 1.48579700 -1.13041400 2.49484100
O 1.86554800 2.20692800 1.98963200	O 2.00027000 2.44057800 1.73205700
O 5.09087100 2.80026200 -0.72435100	O 5.38195000 2.63367700 -0.65015800
O 4.70739500 -1.15547200 -2.89598500	O 5.25436600 -1.42858700 -2.46901600
O 1.09352500 1.33480700 -2.05890600	O 1.57264900 1.11844800 -2.41985800
O 1.74455200 -2.90078500 -0.80096200	O 1.92914600 -2.96963700 -0.61215000
O 1.42473900 -2.02561100 3.59200500	O 1.33063700 -1.61397700 3.54947800
O -2.04558000 -4.10067700 -0.13322100	O -1.84734400 -4.05567400 0.46803300
O -3.51026300 -1.13968800 2.27663300	O -3.66288900 -0.94605700 2.40426100
O -1.80184500 1.36331200 3.04597500	O -1.80541400 1.71507100 2.89122400
O -0.58385100 3.92895700 0.00610400	O -0.80915500 4.01252400 -0.46736900
O -0.73942800 -1.31690300 -2.87518100	O -1.05370600 -1.66148100 -2.86454700
O -2.11071300 1.49370800 -2.82871700	O -2.53111300 1.27490600 -2.97829800
C 4.36621800 -0.52174700 0.72367700	C 4.37413400 -0.50489300 0.99050200
O 5.01829700 -1.02249500 1.52722100	O 4.93286700 -0.93449100 1.92677200
C -3.95718700 1.95691300 0.16652100	C -4.03037700 1.98507700 0.12275400
C -4.09008800 -1.05028100 -1.30783700	C -4.16820300 -1.42145500 -1.07705100
O -5.10141600 -0.93869200 -1.82685700	O -5.21624600 -1.54333500 -1.57263500
O -5.05719300 2.26313700 0.20284500	O -5.13694600 2.33525000 0.23218400
Sn -0.38606000 -0.19665700 0.36092200	Sn -0.44968400 -0.10187100 0.22800400

Table S6. Theoretical Cartesian coordinates (in Å) for the structure **14S-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe 2.59878200 0.01490700 -0.35281700	Fe -2.62725400 -0.04812900 -0.42123700
Fe 0.17384900 -0.21153800 1.35308000	Fe -0.17031200 0.20400500 1.37774500
Fe -1.41826000 1.46672900 -0.23415600	Fe 1.52269800 -1.41280100 -0.23098900
Fe -1.72273600 -1.19645400 -0.46588900	Fe 1.65316000 1.24393500 -0.49889400
C -0.98617200 2.21510400 1.32027700	C 1.46052300 -2.23281100 1.33703800
C -0.32282900 2.42242600 -1.29116100	C 0.47954300 -2.55875100 -1.12392500
C -0.72612700 -2.52523200 -1.11331100	C 0.62821700 2.48967400 -1.25065600
C -2.59317500 -2.19333600 0.72351400	C 2.30800500 2.35932000 0.72097600
C -2.84499000 0.41096600 0.44650200	C 2.87259300 -0.14578000 0.36866800
C 1.21098500 0.60043600 2.55707500	C -1.11981000 -0.85081900 2.44736400
C -1.15271000 -0.40988600 2.51160200	C 1.12256400 0.38224200 2.56177400
C 0.71422700 -1.89170700 1.47830600	C -0.87100500 1.77128500 1.79341900
C 2.21026300 1.71939600 0.14007100	C -2.41501400 -1.79349800 -0.01657200
C 3.69939700 0.49003600 -1.68121300	C -3.61660300 -0.37369300 -1.86617400
C 2.56894100 -1.74779900 -0.79161500	C -2.62055200 1.74125800 -0.67085300
O 1.03699200 -2.98565600 1.61685300	O -1.30152900 2.80051100 2.15115700
O -1.94511400 -0.54311000 3.32836400	O 1.89292400 0.51177100 3.43211200
O 1.85134600 1.07431000 3.38105800	O -1.71339800 -1.48145700 3.23482900
O 2.07256300 2.81312600 0.44167700	O -2.38805400 -2.92841400 0.24167100
O 4.40334100 0.80252700 -2.52268000	O -4.27647100 -0.59090400 -2.80199100
O 2.62322500 -2.85014900 -1.08115800	O -2.72477100 2.88892800 -0.83244000
O -0.22206600 -3.48150700 -1.50272800	O 0.10686000 3.41876800 -1.74093800
O -3.14601000 -2.88323100 1.44798500	O 2.74053100 3.15328500 1.45858700
O -3.86226600 0.39258200 1.00840600	O 3.93212200 -0.11737400 0.90449700
O -0.82937700 2.91126300 2.22419500	O 1.49073100 -2.91674300 2.28715000
O 0.24286300 3.19445300 -1.93510500	O -0.04140900 -3.44737100 -1.68965100
C 3.74889700 -0.23292300 1.00061600	C -3.85475900 0.12665500 0.87360400
O 4.48369600 -0.39963900 1.85683000	O -4.66656000 0.24088300 1.69998200
C -2.73420200 2.52049500 -0.78103800	C 2.91296100 -2.21858100 -0.98821200
C -2.93520700 -1.25033900 -1.76445400	C 2.88308000 1.41050100 -1.76682000
O -3.71095500 -1.28125900 -2.60389400	O 3.69181900 1.53370700 -2.60025400
O -3.57398800 3.22666100 -1.10648700	O 3.82001300 -2.77786800 -1.46587200
Sn 0.30079400 -0.05207100 -1.21526500	Sn -0.30713100 -0.05212100 -1.09281500

Table S7. Theoretical Cartesian coordinates (in Å) for the structure **14S-2** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe 1.90328100 -1.27664200 0.66096600	Fe -1.96033700 1.24215500 0.67781800
Fe 2.05679300 1.22574600 -0.62427400	Fe -1.96036800 -1.24214500 -0.67780800
Fe -2.25779000 -1.10336500 -0.36476200	Fe 2.24636200 1.10285900 -0.39274100
Fe -2.28794800 1.14875600 0.31218900	Fe 2.24636000 -1.10287200 0.39272800
C -3.07938800 0.07949300 -1.43787900	C 3.01173200 -0.12161400 -1.44502100
C -3.43081200 -2.40043600 -0.04798800	C 3.44902800 2.38388200 -0.12697900
C -1.38897900 -2.15432400 -1.48458900	C 1.47246400 2.15623300 -1.57457200
C -2.87157600 -0.05472900 1.50193500	C 3.01173400 0.12162700 1.44498300
C -1.35613600 2.27450600 1.30569300	C 1.47248600 -2.15624100 1.57457600
C -3.57106600 2.36725900 0.12414100	C 3.44903700 -2.38388800 0.12697700
C 1.42311900 0.68861300 -2.24132000	C -1.35174200 -0.68128000 -2.28198600
C 1.51015400 2.88914200 -0.93640500	C -1.32278300 -2.86956400 -0.97480500
C 2.32392600 1.62182900 1.12134300	C -2.37992000 -1.70228300 1.01758600
C 2.28071200 -1.69968600 -1.05790500	C -2.37993700 1.70230200 -1.01756200
C 1.17675000 -2.87961500 0.91617800	C -1.32275400 2.86957900 0.97479600
C 1.18328900 -0.68769800 2.22306000	C -1.35165900 0.68130900 2.28198300
O 2.50822000 1.96945100 2.19588600	O -2.68307200 -2.12172500 2.06392700
O 1.15903400 3.96063600 -1.12117300	O -0.94013000 -3.95391700 -1.17215000
O 0.99420300 0.39255500 -3.26057200	O -0.96368100 -0.38534000 -3.34251700
O 2.52465200 -2.06535900 -2.11451700	O -2.68312200 2.12174600 -2.06389300
O 0.71200200 -3.91311000 1.06417200	O -0.94010300 3.95393400 1.17212900
O 0.69801600 -0.35965000 3.20693900	O -0.96357400 0.38539100 3.34251100
O -3.27807300 -0.47475700 2.50307700	O 3.58314700 0.52689600 2.39809800
O -0.73738400 2.99474400 1.95786600	O 0.97421400 -2.86015800 2.37215000
O -4.39681300 3.15840200 0.05725900	O 4.23903300 -3.23725100 0.00543300
O -3.66843700 0.44127400 -2.36915000	O 3.58315800 -0.52689700 -2.39812100
O -4.19200100 -3.24282900 0.10626900	O 4.23901900 3.23724800 -0.00543000
O -0.80101500 -2.82515900 -2.21305100	O 0.97417400 2.86015400 -2.37213100
C 3.61881200 -1.35139400 1.22175300	C -3.67825900 1.29118900 1.21577500
O 4.70070100 -1.41156200 1.58188800	O -4.78047900 1.36499100 1.58681100
C 3.81344200 1.13855600 -1.03521500	C -3.67830400 -1.29120600 -1.21571600
O 4.92313000 1.09337900 -1.30014900	O -4.78053100 -1.36502900 -1.58672800
Sn -0.07472100 0.06819900 -0.05963800	Sn 0.07712800 -0.00001100 -0.00001700

Table S8. Theoretical Cartesian coordinates (in Å) for the structure **14S-3** using the M06-L/TZP and BP86/DZP methods.

	M06-L/TZP			BP86/DZP
Fe	-2.35599600	-0.22664900	-0.81042800	
Fe	1.17437300	1.98739200	0.91772100	
C	-4.10630200	-0.42592200	-1.09745600	
C	-2.66684000	1.16459800	0.30822400	
C	-2.26930500	-0.96974600	1.95772100	
C	2.26930500	0.96974600	1.95772100	
C	0.00000000	2.89982000	-0.11807600	
C	-1.72106000	0.67781200	-2.20979200	
O	2.87423500	0.40623800	2.75165700	
O	-0.77260800	3.49918700	-0.71229800	
O	-1.31157600	1.25330100	-3.11372900	
O	-5.22630600	-0.52206000	-1.31198900	
O	-2.89825700	2.06746400	0.97470800	
O	-2.87423500	-0.40623800	2.75165700	
C	0.25323000	2.42910600	2.34187100	
O	-0.38201200	2.65404700	3.27100600	
O	-1.99719500	-2.82600800	-2.13675800	
C	-2.04291100	-1.86542700	-1.49866500	
Fe	-1.17437300	-1.98739200	0.91772100	
C	-0.25323000	-2.42910600	2.34187100	
C	1.72106000	-0.67781200	-2.20979200	
C	2.66684000	-1.16459800	0.30822400	
C	0.00000000	-2.89982000	-0.11807600	
O	0.38201200	-2.65404700	3.27100600	
Fe	2.35599600	0.22664900	-0.81042800	
O	1.31157600	-1.25330100	-3.11372900	
O	2.89825700	-2.06746400	0.97470800	
O	0.77260800	-3.49918700	-0.71229800	
C	2.04291100	1.86542700	-1.49866500	
C	4.10630200	0.42592200	-1.09745600	
O	1.99719500	2.82600800	-2.13675800	
O	5.22630600	0.52206000	-1.31198900	
Sn	0.00000000	0.00000000	0.05306600	

Table S9. Theoretical Cartesian coordinates (in Å) for the structure **14T-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -2.28666400 1.07056600 0.60436300	Fe 2.28194600 1.05876700 -0.55471900
Fe -2.32155800 -0.95995400 -0.72376000	Fe 2.28195900 -1.05876500 0.55471200
C -3.70382100 1.75415600 1.53366200	C 3.69486800 1.85586300 -1.31708600
C -2.87683700 1.19607400 -1.10955800	C 2.85611300 0.99522900 1.13866300
C -1.20436300 2.50224600 0.75395700	C 1.28800600 2.52849000 -0.67523800
C -1.25096400 -2.28956100 -1.20534100	C 1.28802000 -2.52849100 0.67520700
C -2.55402600 -1.03372800 1.04527900	C 2.85614500 -0.99522200 -1.13866500
C -3.81470200 -1.79835100 -1.26541600	C 3.69488400 -1.85584400 1.31709300
O -0.59309800 -3.21037900 -1.42739900	O 0.70070300 -3.54506600 0.69141400
O -2.63329200 -1.46853600 2.12278300	O 3.22764700 -1.32358600 -2.21218500
O -4.75432200 -2.35670900 -1.60365100	O 4.60276400 -2.40124500 1.80904800
O -4.59192300 2.20651600 2.09054700	O 4.60274400 2.40127900 -1.80903000
O -3.22904700 1.43155600 -2.18446800	O 3.22759200 1.32358700 2.21219300
O -0.56228400 3.45391300 0.81015200	O 0.70069900 3.54507000 -0.69146100
O 0.46584300 0.73287700 3.17895600	O -1.07696900 1.50130400 -3.13550600
C 1.00314600 0.12617600 2.36839700	C -1.39708200 0.69151700 -2.35833100
Fe 1.83003200 -0.92927600 1.14500800	Fe -1.94590100 -0.64373800 -1.26955500
C 2.30222400 1.81913100 0.51448200	C -2.44348200 1.88290600 0.05041600
C 0.99786800 -2.36212700 1.78620200	C -1.16248300 -1.87809300 -2.27160600
C 1.44680100 2.30986500 -1.86451500	C -1.16247900 1.87807300 2.27163500
C 3.47457800 -0.82684200 1.87828500	C -3.63422300 -0.50693100 -1.86596600
O 2.47368800 2.52255200 1.40260500	O -2.80620100 2.78922800 -0.59234200
Fe 2.07828900 0.87938600 -1.01773400	Fe -1.94588900 0.64373000 1.26956400
O 0.47452000 -3.29973800 2.17927000	O -0.68264000 -2.70163000 -2.94625000
O 1.04126000 3.23655000 -2.39821500	O -0.68264300 2.70160200 2.94629200
O 4.50701900 -0.77893600 2.36557500	O -4.71457600 -0.44600800 -2.30091600
C 2.38322900 -1.89885900 -0.28066300	C -2.44351500 -1.88290100 -0.05040200
C 1.58899700 -0.22111300 -2.37982300	C -1.39705300 -0.69153300 2.35832200
C 3.84786300 0.76656500 -1.33475100	C -3.63421400 0.50694300 1.86597300
O 2.73867600 -2.62061700 -1.09614900	O -2.80623500 -2.78922000 0.59235900
O 1.28193400 -0.87047400 -3.27030300	O -1.07692200 -1.50132600 3.13548300
O 4.96768400 0.70706000 -1.55291300	O -4.71456700 0.44604000 2.30092400
Sn -0.08671700 0.01348700 -0.15560600	Sn 0.08185600 -0.00000200 -0.00000600

Table S10. Theoretical Cartesian coordinates (in Å) for the structure **14T-2** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe 2.36607600 -1.00838000 -0.43751900	Fe 2.39993000 -1.05254300 -0.35084000
Fe 1.33717900 1.32745500 0.60978700	Fe 1.34169100 1.41123100 0.47058200
Fe -1.28650400 1.21081100 -0.84841600	Fe -1.53048900 1.28208400 -0.44192700
Fe -2.43564500 -0.92829400 0.47302800	Fe -2.27000100 -1.21309600 0.21703000
C -0.43053400 2.62980500 -1.52535500	C -2.29813500 2.86689100 -0.65360800
C -0.95749900 0.02347300 -2.16401000	C -0.70240400 1.51539000 -2.02602300
C -2.43123300 -2.43043400 -0.54159200	C -2.37446600 -2.54700600 -0.96837700
C -2.42012000 -1.58893900 2.14174000	C -1.62586100 -2.15759600 1.58772800
C -1.74212500 1.68678100 0.84387900	C -1.91879700 1.37985500 1.32476600
C 1.01280200 3.06377700 0.91137800	C 0.78752600 3.08581100 0.25306200
C 0.76004900 0.78002100 2.24397900	C 1.05122500 1.31076000 2.22657400
C 3.08503000 1.38942100 0.98552400	C 3.06678300 1.80881200 0.60278500
C 2.09996500 0.22242700 -1.73121700	C 2.50068400 0.03800800 -1.78496400
C 1.87770400 -2.48037300 -1.32815900	C 2.12649400 -2.63042400 -1.13686600
C 2.46330100 -1.65194000 1.25608700	C 2.28121800 -1.51842500 1.38445700
O 4.17803900 1.51221000 1.31130900	O 4.18184000 2.13495100 0.74734800
O 0.45589500 0.52369000 3.32029700	O 0.91937900 1.31814800 3.39028900
O 0.81625200 4.15987500 1.17062200	O 0.55235900 4.23221300 0.18781800
O 1.99602500 0.96684900 -2.59941600	O 2.65426200 0.68495300 -2.74681500
O 1.57487900 -3.41249700 -1.91785900	O 1.98143800 -3.66996100 -1.64758100
O 2.50679800 -2.03672600 2.33299200	O 2.24008500 -1.84245200 2.50570600
O -2.41408200 -3.38507800 -1.17642500	O -2.47212800 -3.44403700 -1.71184100
O -2.41643400 -2.02614400 3.20054900	O -1.28114800 -2.83656000 2.47904200
O -2.04609300 2.05025800 1.89197800	O -2.19585800 1.54171900 2.44825600
O 0.05063400 3.53978500 -2.02858300	O -2.81888900 3.89885100 -0.81228300
O -0.78651600 -0.72332900 -3.02336600	O -0.22970800 1.73583100 -3.07240700
C 4.14346100 -0.97741000 -0.66022900	C 4.18638100 -1.06489300 -0.24715100
O 5.27511200 -0.98962000 -0.81424800	O 5.34945700 -1.11917200 -0.19607100
C -2.91586600 1.58068500 -1.47523900	C -2.99683400 0.31637700 -1.07690800
C -4.17696800 -0.54156700 0.34436700	C -3.97172100 -1.28276900 0.78723000
O -5.30296600 -0.34383300 0.27033300	O -5.06676100 -1.39973800 1.17349500
O -3.94882000 1.84547000 -1.88805700	O -3.91401700 0.32419400 -1.82789700
Sn -0.02452700 -0.78646100 0.18146400	Sn 0.03311100 -0.60631600 -0.12477300

Table S11. Theoretical Cartesian coordinates (in Å) for the structure **13S-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -0.66532700 -0.00934300 1.30189900	Fe 0.69989700 -0.00000100 1.29420700
Fe 0.34724200 2.14684200 0.00000000	Fe -0.45381800 -2.15164300 0.00000000
Fe -0.66532700 -0.00934300 -1.30189900	Fe 0.69989700 -0.00000100 -1.29420700
Fe 0.40482200 -2.12703700 0.00000000	Fe -0.45382800 2.15163700 0.00000000
C 1.28657600 -2.88114800 1.34217800	C -1.34434900 2.94838100 1.29640900
O 1.84437300 -3.35504400 2.22224000	O -1.92950000 3.49838400 2.14672100
C 1.28657600 -2.88114800 -1.34217800	C -1.34434900 2.94838100 -1.29640900
O 1.84437300 -3.35504400 -2.22224000	O -1.92950000 3.49838400 -2.14672100
C -1.00868400 -3.21189400 0.00000000	C 0.94260000 3.26249200 0.00000000
O -1.89545400 -3.93498700 0.00000000	O 1.80327100 4.05192900 0.00000000
C 1.22198900 2.92758100 -1.32982300	C -1.34434900 -2.94838300 -1.29640400
O 1.77697100 3.42425900 -2.19885800	O -1.92951300 -3.49837900 -2.14671100
C -1.07141600 3.22539200 0.00000000	C 0.94261200 -3.26249500 0.00000000
O -1.94640500 3.96229700 0.00000000	O 1.80328600 -4.05192900 0.00000000
C 1.22198900 2.92758100 1.32982300	C -1.34434900 -2.94838300 1.29640400
O 1.77697100 3.42425900 2.19885800	O -1.92951300 -3.49837900 2.14671100
C -1.42051500 -1.36910100 -2.17722700	C 1.53506400 1.34160800 -2.11953400
O -1.92596000 -2.17851700 -2.81078100	O 2.11172600 2.13296600 -2.75678200
C 0.69769700 0.07273000 -2.45562500	C -0.62068100 0.00000000 -2.48603300
O 1.47735700 0.11069300 -3.30004200	O -1.38332200 0.00000200 -3.37558600
C -1.57226100 1.31577900 -2.08231600	C 1.53507900 -1.34159300 -2.11954500
O -2.17594700 2.09811800 -2.66201600	O 2.11174400 -2.13295600 -2.75678500
C -1.57226100 1.31577900 2.08231600	C 1.53507900 -1.34159300 2.11954500
O -2.17594700 2.09811800 2.66201600	O 2.11174400 -2.13295600 2.75678500
C 0.69769700 0.07273000 2.45562500	C -0.62068100 0.00000000 2.48603300
O 1.47735700 0.11069300 3.30004200	O -1.38332200 0.00000200 3.37558600
C -1.42051500 -1.36910100 2.17722700	C 1.53506400 1.34160800 2.11953400
O -1.92596000 -2.17851700 2.81078100	O 2.11172600 2.13296600 2.75678200
C -2.16983400 -0.18954500 0.00000000	C 2.20123100 -0.00000100 0.00000000
O -3.31946000 -0.34179000 0.00000000	O 3.38472100 0.00001600 0.00000000
Sn 1.58645900 0.02321600 0.00000000	Sn -1.48144100 -0.00000600 0.00000000

Table S12. Theoretical Cartesian coordinates (in Å) for the structure **13T-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -0.02031200 -1.21071600 0.83690200	Fe 0.00000700 -1.26751100 0.81848300
Fe 2.15072200 -0.12179000 -0.52149500	Fe 2.23001300 -0.00000700 -0.54738000
Fe 0.17607500 1.33765900 0.67287100	Fe 0.00010600 1.26754000 0.81844500
Fe -2.29893200 -0.08436000 -0.40560200	Fe -2.23007600 -0.00002500 -0.54730600
C -3.28377200 -1.20425800 -1.43982300	C -2.96467700 -1.31797500 -1.47846000
O -3.92572600 -1.87195800 -2.11029400	O -3.49055600 -2.15767900 -2.10149800
C -2.69737300 1.52235100 -1.13642900	C -2.96451000 1.31818600 -1.47821800
O -2.97610000 2.52989000 -1.60579500	O -3.49028200 2.15807100 -2.10110300
C -3.41565000 0.07324300 0.97346800	C -3.41861700 -0.00005600 0.78220200
O -4.15264700 0.20548600 1.84028800	O -4.24209200 -0.00006200 1.61198000
C 3.01244500 1.01228400 -1.58950800	C 2.96463100 1.31790700 -1.47856200
O 3.56442500 1.74093700 -2.27879600	O 3.49050900 2.15760100 -2.10161300
C 3.28295100 -0.06221400 0.85187800	C 3.41851200 0.00006200 0.78216300
O 4.03389400 -0.03821100 1.71645900	O 4.24196000 0.00009700 1.61197000
C 2.70799800 -1.63677900 -1.27161000	C 2.96448000 -1.31820500 -1.47827600
O 3.06108100 -2.62068200 -1.74033300	O 3.49026200 -2.15809300 -2.10114700
C -1.14211600 2.26534700 1.44370800	C -1.32167500 2.13250600 1.64227300
O -1.95575200 2.89057600 1.94842900	O -2.13411400 2.74778300 2.20952000
C 0.24002600 2.36512000 -0.82098800	C 0.00018800 2.41977800 -0.56992600
O 0.32280400 3.17424300 -1.63373000	O 0.00018400 3.32876200 -1.30987800
C 1.53909300 2.23134400 1.39819300	C 1.32175900 2.13253700 1.64244600
O 2.37752600 2.83974900 1.88204600	O 2.13413400 2.74781100 2.20978500
C 1.32680400 -2.13639700 1.56471200	C 1.32173200 -2.13252300 1.64235300
O 2.14237200 -2.76737000 2.05919900	O 2.13414700 -2.74781500 2.20961500
C -0.27219700 -2.44174600 -0.46557700	C -0.00009000 -2.41977500 -0.56986600
O -0.42162200 -3.35436300 -1.14888500	O -0.00012200 -3.32877300 -1.30980200
C -1.29877500 -1.87199100 1.89390200	C -1.32170200 -2.13243700 1.64246700
O -2.07439500 -2.33492600 2.59545700	O -2.13410000 -2.74768600 2.20980300
C 0.22661400 0.18293700 2.24843200	C 0.00007700 0.00003600 2.31407800
O 0.35605400 0.22640500 3.40368900	O 0.00009400 0.00005100 3.50170200
Sn -0.08736000 -0.09388500 -1.52947200	Sn -0.00004300 -0.00001500 -1.41562000

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **12S-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -2.10441000 -0.30640000 0.33420900	Fe 0.00000000 2.13386100 0.35084500
Fe 2.10441000 0.30640000 0.33420900	Fe 0.00000000 -2.13386100 0.35084500
Fe 0.25219700 -1.35230700 -0.53901500	Fe -1.39781900 -0.07408700 -0.54677300
Fe -0.25219700 1.35230700 -0.53901500	Fe 1.39781900 0.07408700 -0.54677300
C 1.83866900 -1.44499900 -1.34860100	C -1.68332800 -1.59825500 -1.41430100
C 0.10372700 -3.10813800 -0.36890000	C -3.11895100 0.20026900 -0.27110000
C -0.83274900 -1.30731900 -1.92631800	C -1.33278500 1.09371900 -1.86331000
C -1.83866900 1.44499900 -1.34860100	C 1.68332800 1.59825500 -1.41430100
C 0.83274900 1.30731900 -1.92631800	C 1.33278500 -1.09371900 -1.86331000
C -0.10372700 3.10813800 -0.36890000	C 3.11895100 -0.20026900 -0.27110000
C 3.11622000 -0.78002900 1.30918400	C -1.26878400 -2.90065800 1.31500600
C 3.42641100 0.77764000 -0.76161300	C 0.18713900 -3.54085100 -0.72827100
C 2.14227600 1.79473500 1.29754400	C 1.43600800 -2.55484700 1.29222500
C -2.14227600 -1.79473500 1.29754400	C -1.43600800 2.55484700 1.29222500
C -3.42641100 -0.77764000 -0.76161300	C -0.18713900 3.54085100 -0.72827100
C -3.11622000 0.78002900 1.30918400	C 1.26878400 2.90065800 1.31500600
O 2.26044100 2.75139400 1.92123600	O 2.35989400 -2.90001600 1.92174300
O 4.30085300 1.08642700 -1.42828500	O 0.32004100 -4.50686500 -1.36698100
O 3.77254800 -1.45993200 1.95389500	O -2.08213100 -3.42792200 1.96808300
O -2.26044100 -2.75139400 1.92123600	O -2.35989400 2.90001600 1.92174300
O -4.30085300 -1.08642700 -1.42828500	O -0.32004100 4.50686500 -1.36698100
O -3.77254800 1.45993200 1.95389500	O 2.08213100 3.42792200 1.96808300
O -2.67574500 1.73661600 -2.09016700	O 2.09544400 2.38239400 -2.19135500
O 1.39186800 1.31603000 -2.93226100	O 1.39259800 -1.70756400 -2.86213300
O 0.00000000 4.23986400 -0.23133000	O 4.25708600 -0.37528300 -0.06591000
O 2.67574500 -1.73661600 -2.09016700	O -2.09544400 -2.38239400 -2.19135500
O 0.00000000 -4.23986400 -0.23133000	O -4.25708600 0.37528300 -0.06591000
O -1.39186800 -1.31603000 -2.93226100	O -1.39259800 1.70756400 -2.86213300
Sn 0.00000000 0.00000000 1.54290000	Sn 0.00000000 0.00000000 1.43540300

Table S14. Theoretical Cartesian coordinates (in Å) for the structure **12S-2** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -0.28505100 1.29931500 0.63546000	
Fe -2.11420500 -0.20400400 -0.51205400	
Fe 2.14795900 -0.05466800 -0.40791800	
Fe 0.19713800 -1.16386200 0.84915900	
C 3.24919000 -1.11204400 -1.30761000	
C 2.20244300 1.30729500 -1.56837700	
C 3.37984400 0.50136000 0.76552700	
C 1.88652300 -1.68001000 1.17904200	
C -0.69383800 -2.62211800 1.32237800	
C -0.00613000 -0.49253200 2.46286400	
C -3.54341100 0.53056700 -1.29045000	
C -2.48247400 -1.88998500 -0.95111300	
C -2.70115800 -0.18589700 1.15245400	
C -1.16027100 1.91771800 -0.78794000	
C 1.07176700 2.39147900 0.89592700	
C -1.25933100 2.33329600 1.69633400	
O -3.13204600 -0.21125800 2.21786200	
O -2.74614400 -2.96572500 -1.24452300	
O -4.47060600 0.97908900 -1.78548400	
O -1.46153000 2.71206500 -1.58388800	
O 1.86611900 3.21204400 1.03424700	
O -1.87275200 2.99482300 2.39784300	
O 2.73899900 -2.28065800 1.68767700	
O -1.26560500 -3.56485200 1.63456500	
O -0.09506600 -0.08035300 3.53345700	
O 3.95317000 -1.79972300 -1.88834800	
O 2.31700600 2.19892600 -2.27944600	
O 4.18957900 0.87283100 1.47995800	
Sn 0.03160400 -0.38657500 -1.55452800	

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **12T-1** using the M06-L/TZP and BP86/DZP methods.

M06-L/TZP	BP86/DZP
Fe -2.01710100 0.26850600 -0.19661400	Fe -2.01981800 0.20892200 -0.17970600
Fe 2.08005800 0.09978900 -0.06145200	Fe 2.07521100 0.08249800 -0.01013900
Fe 0.03759700 1.34036900 0.40679900	Fe 0.04270600 1.33597600 0.36534700
Fe -0.04938400 -1.23574400 0.88486500	Fe -0.00706200 -1.24411700 0.81491600
C 1.26352800 1.28783200 1.70457900	C 1.17953400 1.30454700 1.74548300
C -0.02435700 3.11733200 0.33288100	C -0.06488200 3.11346800 0.29650400
C -1.30980800 1.13338400 1.61922300	C -1.37228700 1.19226600 1.55064400
C -1.50068200 -1.75081200 1.82284700	C -1.33096500 -1.73797800 1.91837500
C 1.31061700 -1.68917500 1.96613000	C 1.42314700 -1.70196100 1.77689400
C 0.04733000 -2.75947000 -0.06520100	C 0.00355100 -2.79272000 -0.03967700
C 1.74950800 1.43054500 -1.26602100	C 1.58774600 1.49382700 -1.08922200
C 3.74116100 0.67834000 0.35658000	C 3.69454000 0.76191600 0.29443600
C 2.70122700 -1.29290500 -0.98462800	C 2.85732400 -1.19660800 -0.93584000
C -1.84058600 1.52224200 -1.44744400	C -2.05076200 1.42420400 -1.46549500
C -3.64276300 0.62292800 0.44403200	C -3.65567100 0.48315200 0.48445300
C -2.67598300 -1.17147500 -0.99990200	C -2.66121400 -1.24355500 -0.96367900
O 3.13271400 -2.17847400 -1.56961400	O 3.39395200 -2.01656700 -1.57691600
O 4.79583900 1.03826900 0.59928500	O 4.76643700 1.18625200 0.47596300
O 1.83644000 2.25143700 -2.07495200	O 1.83830900 2.27672400 -1.94858200
O -1.86471600 2.31212100 -2.28631800	O -2.20827600 2.20320600 -2.32792800
O -4.69219200 0.86105200 0.83108200	O -4.74131900 0.67326500 0.86645500
O -3.11260100 -2.10661300 -1.50312300	O -3.13253400 -2.18386400 -1.47832000
O -2.38362800 -2.14200500 2.43849800	O -2.13192200 -2.14628800 2.66574200
O 2.15551700 -2.03061900 2.66336900	O 2.28878700 -2.10190300 2.46057300
O 0.11342300 -3.79249700 -0.56390600	O 0.01929300 -3.86094200 -0.52238400
O 1.81155600 1.39391700 2.71857800	O 1.70996900 1.43583600 2.78840300
O -0.06254200 4.26004400 0.29082000	O -0.12491100 4.27889500 0.28530700
O -1.77738900 1.28857500 2.67088600	O -1.84945900 1.44908700 2.60383700
Sn 0.00270100 -0.56620400 -1.62977700	Sn 0.02692200 -0.52236400 -1.63050600

Table S16. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **16S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
17.6 (A2, 0.0), 19.2 (B1, 0.0), 36.2 (E, 0.2), 36.2 (E, 0.2), 43.9 (B1, 0.0), 47.8 (A1, 0.0), 49.9 (E, 0.1), 49.9 (E, 0.1), 64.7 (B2, 0.1), 73.6 (E, 0.2), 73.6 (E, 0.2), 75.6 (B1, 0.0), 79.3 (A2, 0.0), 80.3 (E, 0.1), 80.3 (E, 0.1), 81.6 (A1, 0.0), 88.2 (B2, 0.1), 92.0 (A2, 0.0), 93.3 (E, 0.0), 93.3 (E, 0.0), 94.0 (A1, 0.0), 96.6 (B1, 0.0), 99.2 (E, 0.3), 99.2 (E, 0.3), 105.6 (B1, 0.0), 107.0 (E, 0.6), 107.0 (E, 0.6), 111.8 (A2, 0.0), 112.0 (B2, 0.1), 125.2 (E, 0.4), 125.2 (E, 0.4), 140.2 (A1, 0.0), 150.2 (B2, 1.4), 160.7 (A1, 0.0), 161.5 (E, 0.0), 161.5 (E, 0.0), 167.7 (B2, 0.3), 198.1 (A1, 0.0), 203.2 (E, 2.3), 203.2 (E, 2.3), 281.3 (B2, 15.5),407.9 (A2, 0.0), 410.2 (E, 4.1), 410.2 (E, 4.1), 411.5 (B1, 0.0), 411.9 (E, 0.3), 411.9 (E, 0.3), 414.4 (B2, 2.3), 416.0 (A1, 0.0), 428.8 (B1, 0.0), 429.4 (A2, 0.0), 436.1 (E, 10.8), 436.1 (E, 10.8), 444.7 (B2, 10.6),446.2 (A1, 0.0), 450.0 (E, 0.1), 450.0 (E, 0.1), 477.5 (E, 0.6), 477.5 (E, 0.6), 482.8 (B2, 0.0), 485.0 (A1, 0.0), 487.2 (E, 0.2), 487.2 (E, 0.2), 499.0 (B2, 13.2),502.2 (A1, 0.0), 507.5 (A1, 0.0), 508.7 (E, 8.8), 508.7 (E, 8.8), 510.5 (B2, 4.2), 512.1 (A2, 0.0), 513.8 (B1, 0.0), 519.5 (E, 2.7), 519.5 (E, 2.7), 564.6 (A2, 0.0), 565.0 (B1, 0.0), 578.1 (E, 30.3), 578.1 (E, 30.3), 614.7 (E, 22.9), 614.7 (E, 22.9), 616.0 (A2, 0.0), 622.9 (B1, 0.0), 624.6 (E, 30.8), 624.6 (E, 30.8), 629.3 (B2, 661.3), 637.3 (A1, 0.0), 644.8 (E, 347.0),644.8 (E, 347.0), 658.3 (B2, 11.3),662.5 (A1, 0.0), 2029 (A2, 0), 2042 (B1, 0), 2057 (E, 1), 2057 (E, 1), 2061 (E, 260), 2061 (E, 260), 2070 (A1, 0), 2073 (E, 362), 2073 (E, 362), 2084 (B2, 1229), 2092 (B2, 28), 2097 (A1, 0), 2113 (E, 2477), 2113 (E, 2477), 2133 (B2, 1905), 2166 (A1, 0)	-13.2 (B1, 0.0), -12.7 (A2, 0.0), 21.9 (E, 0.1), 21.9 (E, 0.1), 31.4 (B1, 0.0), 42.1 (A1, 0.0), 46.1 (E, 0.1), 46.1 (E, 0.1), 54.4 (B2, 0.2), 66.6 (E, 0.2), 66.6 (E, 0.2), 68.6 (B1, 0.0), 69.2 (A2, 0.0), 71.3 (E, 0.0), 71.3 (E, 0.0), 76.9 (A1, 0.0), 84.6 (B2, 0.2), 87.2 (A1, 0.0), 87.3 (E, 0.0), 87.3 (E, 0.0), 88.0 (A2, 0.0), 91.5 (B1, 0.0), 97.3 (E, 0.1), 97.3 (E, 0.1), 101.3 (B2, 0.1), 101.5 (E, 0.6), 101.5 (E, 0.6), 106.2 (B1, 0.0), 106.5 (A2, 0.0), 126.2 (E, 0.8), 126.2 (E, 0.8), 127.2 (A1, 0.0), 127.8 (B2, 1.9), 136.3 (E, 0.1), 136.3 (E, 0.1), 141.2 (A1, 0.0), 152.5 (B2, 1.2), 182.5 (E, 4.6), 182.5 (E, 4.6), 186.7 (A1, 0.0), 250.4 (B2, 27.0), 391.7 (E, 3.4), 391.7 (E, 3.4), 392.8 (A1, 0.0), 393.3 (B2, 0.0), 394.6 (A2, 0.0), 396.0 (B1, 0.0), 397.3 (E, 0.6), 397.3 (E, 0.6), 417.9 (A2, 0.0), 419.5 (B1, 0.0), 432.1 (E, 0.0), 432.1 (E, 0.0), 447.3 (E, 8.5), 447.3 (E, 8.5), 454.0 (B2, 7.2), 454.8 (A1, 0.0), 468.0 (E, 3.2), 468.0 (E, 3.2), 471.9 (B2, 0.3), 473.8 (A1, 0.0), 491.8 (A1, 0.0), 494.8 (E, 1.9), 494.8 (E, 1.9), 494.8 (B2, 1.2), 504.5 (E, 0.6), 504.5 (E, 0.6), 509.2 (B2, 7.2), 510.2 (A1, 0.0), 525.1 (A2, 0.0), 525.7 (B1, 0.0), 528.6 (E, 0.5), 528.6 (E, 0.5), 553.7 (A2, 0.0), 555.6 (B1, 0.0), 563.2 (E, 13.2), 563.2 (E, 13.2), 606.7 (A2, 0.0), 608.7 (E, 78.9), 608.7 (E, 78.9), 613.6 (B1, 0.0), 622.2 (E, 0.1), 622.2 (E, 0.1), 625.8 (B2, 583.7), 635.9 (A1, 0.0), 640.7 (E, 307.1), 640.7 (E, 307.1), 645.5 (B2, 3.8), 648.1 (A1, 0.0), 1960.1 (A2, 0.0), 1968.7 (B1, 0.0), 1979.4 (E, 47.6), 1979.4 (E, 47.6), 1988.9 (E, 34.4), 1988.9 (E, 34.4), 1989.2 (A1, 0.0), 1996.5 (E, 716.4), 1996.5 (E, 716.4), 1999.8 (B2, 1044.2), 2014.1 (A1, 0.0), 2014.9 (B2, 483.2), 2033.4 (E, 2182.5), 2033.4 (E, 2182.5), 2053.2 (B2, 1474.2), 2084.0 (A1, 0.0)

Table S17. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **16S-2** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
-40.9 (A2, 0.0),-14.7 (A2, 0.0), 21.4 (B2, 0.0), 33.4 (B2, 0.1), 34.3 (A2, 0.0), 42.0 (A1, 0.0), 51.8 (B2, 0.1), 52.5 (B1, 0.1), 53.1 (A1, 0.3), 55.3 (B1, 0.0), 55.7 (A2, 0.0), 63.2 (B2, 0.1), 71.5 (A1, 0.0), 71.9 (B2, 0.6), 72.2 (A2, 0.0), 82.4 (A1, 0.4), 83.9 (A2, 0.0), 85.3 (B1, 0.0), 85.6 (B2, 0.0), 88.7 (B1, 0.1), 90.8 (A1, 0.0), 93.3 (A1, 0.0), 97.1 (B2, 0.1),102.9 (B1, 0.1),106.0 (A2, 0.0),109.6 (B2, 0.1), 111.5 (B1, 0.2),121.6 (A1, 0.1),126.1 (A2, 0.0),136.5 (B2, 0.7),137.9 (B1, 0.0), 144.2 (A1, 0.7),166.2 (A2, 0.0),169.9 (B1, 0.0),170.9 (A1, 0.2),182.9 (A1, 1.7),186.9 (B1, 1.1),205.2 (B2, 2.9),238.0 (A1, 4.9),240.5 (B1, 2.3), 280.1 (A1, 10.2),317.6 (A2, 0.0),379.9 (A1, 0.7), 380.4 (B2, 0.5),404.7 (B2, 1.3), 406.1 (B2, 0.5), 408.5 (A2, 0.0),409.3 (A1, 1.8), 411.2 (B1, 0.2),420.6 (A2, 0.0), 423.5 (A1, 24.6),425.7 (A2, 0.0),436.0 (B2, 8.6), 436.4 (B1, 1.4),443.7 (A1, 1.3),445.7 (B1, 0.4), 459.9 (B2, 1.2), 470.3 (B1, 19), 471.0 (A1, 12.9), 471.1 (B2, 2.3), 474.5 (A1, 6.5), 478.1 (A2, 0.0), 480.4 (A1, 1.1), 482.7 (B2, 0.9), 485.1 (A1, 1.6), 490.9 (B2, 14.0), 495.2 (B1, 5.7), 497.4 (B2, 2.4), 501.0 (A2, 0.0), 501.6 (A1, 0.3), 513.7 (A2, 0.0), 520.5 (B1, 1.1), 531.7 (B1, 33.4), 545.7 (B2, 0.0), 550.8 (A1, 1.4), 570.0 (A2, 0.0), 577.1 (B1, 10.4), 600.2 (B2, 98.5), 606.2 (B1, 23.7), 608.1 (A1, 194.6), 613.2 (A2, 0.0), 616.0 (B1, 0.1), 623.3 (B2, 7.0), 629.1 (B1, 614.5), 632.8 (A2, 0.0), 634.5 (A1, 300.4), 642.7 (A1, 6.3), 651.1 (B2, 348.1), 665.6 (A1, 27.2), 1931 (B2, 572), 1954 (A1, 198), 2048 (A2, 0), 2061 (B2, 133), 2067 (B1, 42), 2070 (B2, 447), 2073 (A1, 1188), 2073 (A2, 0), 2077 (B2, 16), 2082 (A1, 138), 2091 (B1, 151), 2098 (A1, 295), 2111 (B1, 2830), 2113 (B2, 2044), 2129 (A1, 1794), 2167 (A1, 83)	-15.7 (A2, 0.0), 14.8 (B2, 0.0), 30.3 (A2, 0.0), 31.4 (A1, 0.0), 37.7 (B2, 0.0), 51.0 (B1, 0.0), 55.2 (B2, 0.3), 56.1 (A1, 0.2), 57.0 (A2, 0.0), 59.9 (B1, 0.1), 63.7 (B2, 0.0), 67.7 (A1, 0.0), 67.8 (A2, 0.0), 72.6 (A2, 0.0), 74.3 (B2, 0.3), 83.9 (A1, 0.2), 84.8 (B1, 0.0), 87.1 (A1, 0.0), 87.8 (A2, 0.0), 87.9 (B2, 0.0), 90.5 (B1, 0.2), 97.1 (B2, 0.1), 99.4 (A1, 0.0),102.1 (B1, 0.1), 105.2 (A2, 0.0),106.8 (A1, 0.0), 107.1 (B1, 0.2),107.8 (A2, 0.0), 108.3 (B2, 0.2),124.9 (A1, 1.2), 126.1 (B2, 0.8),132.8 (B1, 0.0), 139.1 (B1, 0.0),145.7 (A1, 0.0), 162.1 (B1, 0.4),169.1 (A1, 2.8), 171.6 (A2, 0.0),188.8 (B2, 5.3), 235.7 (A1, 10.1),239.7 (B1, 3.7), 260.5 (A1, 17.0),319.8 (A2, 0.0), 380.3 (B2, 0.4), 390.9 (A1, 0.1), 391.7 (A1, 1.0),393.1 (B2, 0.9), 395.5 (A2, 0.0),396.9 (B2, 1.0), 397.5 (B1, 0.0),412.3 (A2, 0.0), 418.7 (A2, 0.0),419.8 (A1, 17.3), 425.9 (B1, 4.5), 431.6 (B1, 0.7), 444.6 (B2, 2.5), 446.1 (B2, 3.1), 450.2 (A1, 0.1), 471.0 (A1, 5.7), 472.6 (A2, 0.0), 473.3 (B2, 6.2), 477.9 (A1, 4.6), 484.6 (A1, 0.2), 487.1 (B2, 1.0), 488.4 (B1, 6.0), 494.7 (B2, 4.4), 497.3 (B2, 0.9), 501.6 (A1, 0.7), 503.7 (B1, 2.2), 504.0 (A1, 2.1), 505.1 (A2, 0.0), 515.8 (B1, 28.1), 527.7 (A2, 0.0), 533.1 (B1, 13.1), 537.9 (A1, 4.7), 539.6 (B2, 0.0), 555.5 (A2, 0.0), 559.3 (B1, 6.4), 597.8 (B1, 56.0), 599.0 (B2, 97.0), 606.4 (A2, 0.0), 607.6 (B1, 51.1), 607.6 (A1, 145.1), 622.9 (B2, 0.0), 624.6 (A2, 0.0), 628.9 (A1, 314.9), 634.4 (B1, 531.6), 636.3 (A1, 17.0), 642.0 (B2, 325.3), 646.5 (A1, 7.7), 1858.6 (B2, 534.9), 1875.7 (A1, 219.6), 1968.0 (A2, 0.0), 1981.6 (B2, 241.3), 1986.4 (B1, 69.2), 1991.1 (B2, 500.3), 1991.6 (A2, 0.0), 1993.7 (A1, 1323.4), 1998.0 (B2, 8.7), 2001.3 (A1, 0.9), 2008.0 (B1, 330.7), 2015.3 (A1, 264.1), 2028.9 (B1, 2574.2), 2037.0 (B2, 1773.7), 2046.5 (A1, 1473.3), 2083.3 (A1, 92.7)

Table S18. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
25.9 (A, 0.1), 28.6 (A, 0.0), 31.4 (B, 0.0), 37.8 (A, 0.1), 46.3 (B, 0.2), 51.8 (B, 0.2), 56.5 (A, 0.0), 60.7 (B, 0.1), 71.6 (B, 0.0), 72.1 (A, 0.0), 72.7 (B, 0.1), 74.1 (A, 0.4), 75.9 (A, 0.3), 77.3 (B, 0.0), 81.9 (B, 0.3), 84.7 (A, 0.0), 87.6 (A, 0.0), 89.4 (A, 0.0), 90.8 (B, 0.1), 93.6 (B, 0.2), 97.9 (B, 0.8), 98.7 (A, 0.1), 100.3 (B, 1.1), 107.5 (A, 0.5), 113.1 (B, 0.1), 114.7 (A, 0.0), 121.9 (A, 0.6), 124.5 (B, 0.2), 127.0 (B, 0.3), 133.5 (B, 0.1), 134.3 (A, 2.2), 140.0 (A, 0.5), 143.7 (B, 0.0), 158.0 (B, 0.3), 178.7 (A, 3.0), 200.3 (A, 1.8), 223.7 (A, 2.3), 262.5 (B, 3.0), 288.2 (B, 3.5), 393.4 (A, 2.8), 393.5 (B, 7.1), 396.9 (A, 0.7), 404.8 (A, 3.5), 405.0 (B, 4.4), 422.3 (B, 4.3), 423.2 (A, 2.4), 431.1 (B, 47.0), 432.6 (A, 6.1), 434.5 (B, 33.2), 438.2 (B, 0.7), 440.3 (A, 7.7), 441.4 (B, 1.4), 443.9 (A, 0.1), 448.7 (B, 5.0), 471.2 (A, 1.5), 475.4 (B, 44.6), 477.2 (A, 3.0), 482.1 (A, 0.1), 482.4 (B, 1.8), 483.6 (B, 0.0), 486.4 (B, 15.7), 488.0 (A, 5.0), 493.8 (B, 18.1), 496.8 (A, 4.4), 500.2 (A, 0.0), 500.2 (B, 18.5), 505.4 (A, 0.0), 511.4 (A, 0.3), 514.7 (B, 12.8), 570.3 (A, 2.6), 570.6 (B, 4.6), 578.7 (B, 1.4), 608.5 (A, 0.1), 608.7 (B, 24.5), 610.9 (A, 12.7), 614.7 (B, 59.5), 622.6 (A, 167.9), 622.7 (B, 132.4), 625.3 (B, 173.5), 631.1 (A, 28.6), 643.0 (A, 261.5), 643.5 (B, 265.8), 653.8 (A, 4.2), 666.1 (B, 161.4), 1916 (A, 407), 2031 (A, 4), 2038 (B, 125), 2047 (A, 30), 2058 (B, 25), 2065 (B, 48), 2067 (A, 34), 2070 (A, 1), 2073 (B, 305), 2087 (B, 1840), 2088 (A, 529), 2090 (B, 1228), 2104 (A, 2319), 2120 (B, 2958), 2161 (A, 0)	15.6 (B, 0.0), 21.1 (A, 0.0), 21.8 (A, 0.1), 31.0 (A, 0.1), 37.8 (B, 0.1), 41.2 (B, 0.4), 48.4 (A, 0.0), 55.4 (B, 0.2), 55.9 (A, 0.6), 63.8 (B, 0.1), 66.1 (B, 0.0), 69.1 (B, 0.0), 69.2 (A, 0.1), 70.0 (A, 0.0), 73.6 (B, 0.3), 81.5 (A, 0.1), 83.4 (B, 0.2), 87.3 (A, 0.0), 91.3 (A, 0.0), 91.5 (B, 0.0), 93.8 (B, 0.3), 95.6 (A, 0.0), 99.5 (A, 0.4), 102.0 (B, 0.7), 104.0 (A, 0.2), 105.3 (B, 0.1), 111.3 (A, 0.0), 112.4 (B, 0.1), 114.4 (B, 0.3), 115.8 (A, 0.0), 123.1 (B, 0.1), 128.1 (B, 0.0), 128.6 (A, 2.7), 153.2 (B, 0.6), 163.4 (A, 2.6), 193.3 (A, 3.5), 221.8 (A, 4.1), 258.6 (B, 7.8), 272.5 (B, 4.1), 379.2 (B, 3.5), 381.0 (A, 3.3), 388.1 (A, 2.4), 389.4 (B, 1.6), 394.6 (A, 0.0), 413.0 (B, 0.3), 417.9 (A, 0.1), 421.3 (A, 1.1), 422.1 (B, 5.6), 422.9 (B, 1.3), 424.2 (B, 3.9), 442.4 (A, 12.9), 449.7 (B, 1.4), 452.8 (B, 17.9), 454.8 (A, 4.5), 456.8 (A, 0.1), 457.9 (A, 0.2), 462.0 (B, 54.2), 474.2 (B, 50.5), 478.8 (A, 0.2), 484.7 (B, 8.4), 486.6 (A, 0.0), 495.3 (B, 4.8), 496.3 (A, 0.9), 498.4 (B, 4.4), 507.0 (A, 4.6), 508.4 (B, 12.1), 521.6 (A, 0.0), 523.9 (B, 1.7), 523.9 (A, 0.4), 554.4 (A, 1.8), 555.6 (B, 1.3), 562.4 (B, 1.5), 593.8 (A, 1.3), 602.4 (A, 52.5), 604.1 (B, 32.7), 606.7 (A, 2.1), 608.7 (B, 47.0), 612.9 (B, 117.9), 621.2 (B, 69.4), 630.3 (A, 87.1), 630.5 (B, 328.6), 636.1 (A, 293.7), 641.8 (A, 0.6), 658.8 (B, 149.3), 1834.3 (A, 372.2), 1954.6 (A, 4.7), 1963.2 (B, 96.8), 1971.0 (A, 28.0), 1983.5 (B, 85.1), 1985.9 (B, 25.7), 1991.0 (A, 181.7), 1991.6 (A, 29.4), 1996.8 (B, 488.4), 2003.8 (B, 2690.3), 2007.0 (A, 321.8), 2012.8 (B, 420.4), 2025.5 (A, 2159.3), 2039.8 (B, 2599.9), 2078.1 (A, 0.7)

Table S19. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15S-2** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
7.0 (A, 0.0), 11.4 (A, 0.0), 18.6 (A, 0.0), 25.6 (A, 0.2), 29.1 (A, 0.1), 31.9 (A, 0.0), 41.5 (A, 0.3), 44.5 (A, 0.0), 56.1 (A, 0.2), 62.0 (A, 0.1), 69.7 (A, 0.1), 71.3 (A, 0.1), 72.9 (A, 0.0), 74.1 (A, 0.1), 78.7 (A, 0.1), 82.4 (A, 0.1), 83.5 (A, 0.1), 86.5 (A, 0.3), 90.0 (A, 0.0), 93.1 (A, 0.0), 94.8 (A, 0.2), 97.4 (A, 0.6), 98.5 (A, 0.3), 106.2 (A, 0.0), 108.8 (A, 0.2), 114.1 (A, 0.3), 116.4 (A, 0.1), 127.6 (A, 0.1), 134.8 (A, 0.4), 137.0 (A, 3.4), 150.9 (A, 0.3), 152.2 (A, 0.1), 162.4 (A, 1.1), 174.0 (A, 0.7), 206.4 (A, 4.1), 235.9 (A, 1.6), 252.7 (A, 1.4), 282.9 (A, 10.0), 345.5 (A, 55.6), 383.3 (A, 0.4), 392.4 (A, 1.2), 399.4 (A, 4.5), 401.5 (A, 30.8), 406.5 (A, 2.0), 408.2 (A, 1.5), 409.9 (A, 1.6), 414.0 (A, 5.6), 427.2 (A, 1.1), 432.7 (A, 11.5), 439.1 (A, 4.1), 440.8 (A, 6.7), 443.3 (A, 2.3), 449.3 (A, 0.8), 458.5 (A, 4.7), 461.4 (A, 1.2), 465.1 (A, 7.5), 472.2 (A, 4.7), 476.7 (A, 1.0), 478.3 (A, 27.4), 484.3 (A, 2.3), 486.9 (A, 1.3), 495.5 (A, 2.9), 502.4 (A, 1.7), 504.9 (A, 3.6), 509.6 (A, 9.0), 514.5 (A, 6.2), 521.6 (A, 11.1), 530.7 (A, 7.9), 535.8 (A, 10.5), 566.8 (A, 19.7), 567.4 (A, 35.5), 574.6 (A, 15.9), 576.5 (A, 28.7), 591.6 (A, 68.5), 614.8 (A, 10.7), 616.1 (A, 93.2), 619.4 (A, 0.2), 626.0 (A, 289.5), 631.3 (A, 49.6), 633.9 (A, 103.5), 637.3 (A, 32.4), 643.6 (A, 393.0), 660.0 (A, 54.4), 681.4 (A, 230.8), 1543 (A, 588), 1931 (A, 366), 2043 (A, 250), 2053 (A, 35), 2068 (A, 58), 2073 (A, 508), 2075 (A, 461), 2078 (A, 97), 2080 (A, 473), 2082 (A, 218), 2093 (A, 2565), 2098 (A, 691), 2113 (A, 1996), 2129 (A, 1878), 2161 (A, 231)	10.4 (A, 0.0), 14.6 (A, 0.0), 20.4 (A, 0.1), 23.5 (A, 0.2), 26.2 (A, 0.0), 27.6 (A, 0.1), 37.0 (A, 0.1), 39.2 (A, 0.1), 51.8 (A, 0.3), 65.3 (A, 0.0), 66.8 (A, 0.0), 68.1 (A, 0.0), 72.6 (A, 0.1), 73.8 (A, 0.1), 77.3 (A, 0.2), 78.8 (A, 0.2), 81.8 (A, 0.3), 85.9 (A, 0.2), 88.0 (A, 0.1), 89.6 (A, 0.3), 93.4 (A, 0.1), 94.1 (A, 0.1), 99.5 (A, 0.1), 103.5 (A, 0.8), 103.9 (A, 0.3), 111.1 (A, 0.1), 115.8 (A, 0.9), 118.4 (A, 0.4), 121.2 (A, 0.5), 127.0 (A, 0.1), 130.9 (A, 1.6), 136.7 (A, 2.5), 138.4 (A, 1.8), 163.6 (A, 0.6), 186.5 (A, 7.4), 228.4 (A, 1.4), 242.5 (A, 4.5), 254.9 (A, 2.5), 306.1 (A, 49.8), 371.8 (A, 0.4), 382.7 (A, 1.6), 384.1 (A, 0.7), 393.1 (A, 2.7), 395.0 (A, 0.2), 395.8 (A, 0.0), 397.3 (A, 6.8), 407.5 (A, 5.6), 414.4 (A, 0.9), 423.9 (A, 5.4), 427.3 (A, 1.3), 436.6 (A, 1.9), 445.4 (A, 6.1), 447.8 (A, 4.0), 450.8 (A, 9.3), 453.1 (A, 2.2), 457.7 (A, 3.0), 466.9 (A, 2.0), 472.0 (A, 4.4), 484.1 (A, 0.3), 490.0 (A, 14.0), 490.8 (A, 1.1), 496.3 (A, 2.1), 500.8 (A, 1.9), 502.6 (A, 3.3), 505.2 (A, 13.6), 522.0 (A, 14.1), 525.0 (A, 3.4), 529.9 (A, 4.2), 538.9 (A, 12.7), 553.0 (A, 0.6), 556.5 (A, 1.4), 557.4 (A, 10.4), 577.6 (A, 117.0), 584.4 (A, 39.7), 603.9 (A, 47.3), 607.2 (A, 55.4), 616.1 (A, 80.5), 618.9 (A, 18.9), 626.8 (A, 60.7), 629.8 (A, 216.7), 632.9 (A, 339.7), 634.4 (A, 33.3), 643.2 (A, 25.5), 669.7 (A, 281.9), 1540.3 (A, 510.5), 1848.6 (A, 335.9), 1964.9 (A, 235.7), 1972.3 (A, 55.6), 1988.2 (A, 75.2), 1990.6 (A, 172.5), 1993.7 (A, 715.1), 2000.2 (A, 612.2), 2000.7 (A, 161.0), 2002.4 (A, 109.0), 2009.0 (A, 2476.2), 2014.7 (A, 583.3), 2035.3 (A, 1756.9), 2044.8 (A, 1810.2), 2077.7 (A, 234.4)

Table S20. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15T-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
9.3 (A, 0.1), 21.4 (A, 0.1), 23.1 (A, 0.0), 25.5 (A, 0.1), 30.5 (A, 0.2), 33.4 (A, 0.2), 41.8 (A, 0.1), 43.0 (A, 0.3), 46.5 (A, 0.2), 54.3 (A, 0.2), 63.6 (A, 0.3), 68.8 (A, 0.2), 68.9 (A, 1.3), 70.8 (A, 0.1), 71.3 (A, 0.3), 76.1 (A, 0.3), 78.3 (A, 0.1), 80.7 (A, 0.0), 82.7 (A, 0.1), 85.9 (A, 0.1), 88.4 (A, 0.2), 89.8 (A, 0.1), 93.4 (A, 0.1), 94.2 (A, 0.1), 95.9 (A, 1.1), 97.8 (A, 1.1), 101.2 (A, 0.2), 106.1 (A, 0.6), 112.3 (A, 1.7), 119.6 (A, 2.0), 123.2 (A, 0.9), 133.0 (A, 0.7), 134.4 (A, 0.2), 147.4 (A, 0.3), 150.3 (A, 1.0), 173.2 (A, 0.1), 204.2 (A, 3.6), 220.6 (A, 0.2), 295.5 (A, 29.5), 341.2 (A, 0.4), 368.3 (A, 13.5), 371.8 (A, 3.6), 392.8 (A, 0.0), 395.0 (A, 1.2), 403.4 (A, 15.6), 406.9 (A, 5.0), 408.8 (A, 0.8), 412.1 (A, 0.6), 415.8 (A, 8.3), 425.5 (A, 2.2), 428.6 (A, 14.3), 437.9 (A, 3.5), 440.7 (A, 15.9), 442.4 (A, 1.0), 452.5 (A, 0.9), 454.9 (A, 4.8), 458.0 (A, 3.0), 468.7 (A, 10.7), 473.0 (A, 20.1), 473.3 (A, 22.4), 478.2 (A, 7.9), 482.6 (A, 1.1), 487.0 (A, 0.7), 494.7 (A, 1.7), 496.1 (A, 0.3), 499.7 (A, 2.9), 515.3 (A, 20.9), 517.9 (A, 98.3), 521.0 (A, 1.8), 525.4 (A, 14.2), 553.4 (A, 50.8), 562.0 (A, 81.4), 563.7 (A, 14.0), 567.6 (A, 314.2), 568.8 (A, 52.2), 577.9 (A, 28.6), 581.9 (A, 22.1), 600.3 (A, 29.6), 611.4 (A, 72.3), 613.1 (A, 100.9), 617.0 (A, 10.5), 634.1 (A, 197.8), 639.8 (A, 331.9), 655.8 (A, 57.3), 1998 (A, 769), 2018 (A, 321), 2032 (A, 205), 2037 (A, 66), 2048 (A, 21), 2058 (A, 58), 2063 (A, 244), 2068 (A, 932), 2074 (A, 314), 2078 (A, 994), 2083 (A, 1148), 2088 (A, 865), 2108 (A, 2088), 2115 (A, 1863), 2154 (A, 286)	10.2 (A, 0.0), 14.6 (A, 0.1), 18.6 (A, 0.1), 20.3 (A, 0.1), 29.5 (A, 0.0), 32.8 (A, 0.0), 37.2 (A, 0.1), 40.3 (A, 0.1), 42.8 (A, 0.2), 51.9 (A, 0.9), 53.0 (A, 0.2), 68.7 (A, 0.1), 70.5 (A, 0.1), 73.6 (A, 0.1), 75.0 (A, 0.2), 76.1 (A, 1.7), 78.3 (A, 0.3), 79.5 (A, 0.3), 80.5 (A, 0.1), 81.6 (A, 0.5), 85.7 (A, 0.5), 86.1 (A, 0.0), 90.3 (A, 0.1), 93.6 (A, 0.0), 94.9 (A, 0.0), 96.8 (A, 0.2), 98.5 (A, 0.6), 100.4 (A, 0.3), 102.5 (A, 0.5), 107.9 (A, 3.7), 117.3 (A, 0.7), 122.3 (A, 1.4), 125.9 (A, 4.1), 128.6 (A, 0.7), 142.7 (A, 0.8), 175.1 (A, 0.3), 186.0 (A, 6.0), 222.4 (A, 2.8), 296.0 (A, 44.9), 345.7 (A, 0.0), 359.8 (A, 8.6), 364.4 (A, 0.1), 380.5 (A, 0.5), 381.2 (A, 0.9), 392.3 (A, 2.2), 393.6 (A, 0.4), 395.8 (A, 0.1), 412.2 (A, 0.7), 422.5 (A, 8.6), 424.4 (A, 3.3), 427.9 (A, 27.1), 435.7 (A, 0.3), 449.8 (A, 6.8), 450.3 (A, 3.7), 454.0 (A, 6.4), 461.5 (A, 2.4), 468.0 (A, 3.3), 470.0 (A, 43.6), 471.8 (A, 2.1), 475.1 (A, 1.5), 484.4 (A, 74.4), 485.3 (A, 18.7), 490.1 (A, 1.8), 495.7 (A, 1.9), 501.1 (A, 0.1), 502.8 (A, 0.8), 505.9 (A, 0.9), 512.1 (A, 67.5), 525.6 (A, 2.4), 528.9 (A, 0.6), 551.0 (A, 31.2), 552.8 (A, 70.6), 553.7 (A, 15.9), 558.1 (A, 34.9), 572.9 (A, 240.3), 579.0 (A, 39.6), 585.3 (A, 48.3), 597.3 (A, 83.3), 604.8 (A, 74.3), 606.6 (A, 48.8), 616.8 (A, 53.0), 628.9 (A, 226.5), 631.1 (A, 322.5), 640.8 (A, 6.8), 1937.4 (A, 620.7), 1942.7 (A, 302.4), 1960.8 (A, 119.3), 1964.4 (A, 62.9), 1969.4 (A, 105.1), 1981.8 (A, 456.1), 1983.7 (A, 41.5), 1987.3 (A, 566.3), 1991.4 (A, 1603.5), 1999.8 (A, 538.5), 2001.5 (A, 762.8), 2005.6 (A, 524.9), 2029.9 (A, 1729.7), 2030.7 (A, 1918.8), 2071.3 (A, 282.9)

Table S21. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
24.4 (A, 0.1), 26.9 (A, 0.2), 36.8 (A, 0.2), 41.2 (A, 0.2), 46.4 (A, 0.0), 61.0 (A, 0.0), 68.1 (A, 0.1), 72.4 (A, 0.0), 79.1 (A, 0.1), 80.7 (A, 0.3), 81.0 (A, 0.1), 83.0 (A, 1.7), 85.5 (A, 0.1), 88.1 (A, 0.1), 90.4 (A, 0.1), 92.2 (A, 0.2), 93.6 (A, 1.0), 99.2 (A, 0.5), 101.0 (A, 0.2), 106.9 (A, 1.3), 108.5 (A, 0.2), 113.6 (A, 0.5), 118.8 (A, 0.0), 119.4 (A, 1.6), 124.3 (A, 0.1), 129.9 (A, 0.3), 131.6 (A, 0.3), 138.8 (A, 0.6), 145.5 (A, 0.3), 148.0 (A, 1.4), 156.0 (A, 1.6), 166.3 (A, 2.0), 183.9 (A, 3.3), 203.8 (A, 1.2), 216.4 (A, 1.6), 230.0 (A, 1.5), 275.8 (A, 0.2), 359.9 (A, 4.2), 388.7 (A, 20.3), 401.6 (A, 3.3), 407.4 (A, 0.7), 408.5 (A, 0.7), 414.7 (A, 0.3), 419.9 (A, 5.5), 420.2 (A, 0.3), 426.7 (A, 0.5), 433.0 (A, 9.6), 434.2 (A, 4.4), 445.4 (A, 1.3), 453.8 (A, 0.8), 456.6 (A, 8.9), 474.6 (A, 12.3), 478.2 (A, 0.9), 480.0 (A, 4.1), 483.8 (A, 1.3), 490.5 (A, 4.7), 498.3 (A, 2.8), 501.3 (A, 1.8), 503.2 (A, 3.9), 506.5 (A, 10.4), 510.0 (A, 8.1), 511.2 (A, 3.1), 518.4 (A, 10.2), 520.2 (A, 4.0), 527.2 (A, 3.6), 555.1 (A, 2.0), 566.0 (A, 24.3), 566.2 (A, 33.3), 584.3 (A, 57.7), 593.4 (A, 48.4), 594.3 (A, 99.4), 605.7 (A, 14.8), 611.0 (A, 31.3), 618.1 (A, 59.5), 621.7 (A, 67.6), 629.2 (A, 108.1), 633.1 (A, 253.7), 638.4 (A, 281.1), 656.2 (A, 29.5), 1942 (A, 350), 2014 (A, 298), 2026 (A, 77), 2036 (A, 61), 2047 (A, 152), 2050 (A, 191), 2068 (A, 45), 2082 (A, 98), 2087 (A, 751), 2096 (A, 1934), 2100 (A, 1439), 2102 (A, 1145), 2122 (A, 2644), 2160 (A, 250)	10.5 (A, 0.3), 25.0 (A, 0.2), 30.6 (A, 0.0), 37.3 (A, 0.0), 43.3 (A, 0.1), 47.5 (A, 0.0), 56.3 (A, 0.2), 61.6 (A, 0.0), 70.6 (A, 0.4), 75.2 (A, 0.4), 75.2 (A, 0.7), 77.8 (A, 0.1), 80.4 (A, 0.2), 82.4 (A, 0.7), 88.1 (A, 0.1), 88.8 (A, 0.3), 91.7 (A, 0.3), 92.4 (A, 1.6), 93.3 (A, 0.7), 98.4 (A, 0.1), 100.2 (A, 0.5), 103.1 (A, 0.2), 107.6 (A, 0.3), 109.0 (A, 0.2), 118.2 (A, 0.0), 119.5 (A, 0.2), 123.1 (A, 0.5), 126.1 (A, 0.1), 126.8 (A, 0.5), 136.2 (A, 0.5), 140.5 (A, 0.6), 158.8 (A, 1.4), 194.5 (A, 0.7), 200.9 (A, 0.3), 230.4 (A, 2.7), 237.3 (A, 5.4), 281.2 (A, 1.3), 367.6 (A, 2.4), 386.6 (A, 13.6), 389.5 (A, 1.0), 392.9 (A, 0.8), 397.1 (A, 4.4), 400.6 (A, 0.1), 403.1 (A, 1.5), 410.9 (A, 0.6), 411.4 (A, 1.3), 417.1 (A, 0.8), 429.1 (A, 10.3), 437.4 (A, 3.2), 441.5 (A, 4.3), 447.0 (A, 3.8), 461.7 (A, 26.6), 475.5 (A, 3.1), 485.8 (A, 17.6), 487.5 (A, 1.6), 493.5 (A, 0.3), 496.4 (A, 3.8), 503.1 (A, 9.6), 506.1 (A, 0.4), 514.3 (A, 3.3), 521.0 (A, 1.1), 522.8 (A, 2.8), 524.6 (A, 1.5), 527.6 (A, 4.3), 539.3 (A, 4.4), 546.8 (A, 0.5), 551.6 (A, 0.4), 567.4 (A, 31.0), 582.3 (A, 13.5), 586.2 (A, 55.8), 590.2 (A, 66.1), 598.9 (A, 32.0), 603.4 (A, 2.9), 607.4 (A, 123.9), 614.4 (A, 86.1), 620.9 (A, 102.8), 629.1 (A, 205.9), 636.1 (A, 215.7), 640.5 (A, 92.6), 1849.3 (A, 342.8), 1948.9 (A, 296.5), 1956.0 (A, 1.3), 1963.8 (A, 169.7), 1968.0 (A, 195.6), 1975.8 (A, 98.8), 1987.7 (A, 28.9), 2005.2 (A, 248.1), 2007.6 (A, 87.4), 2015.3 (A, 2251.3), 2020.0 (A, 1936.7), 2022.3 (A, 824.1), 2041.4 (A, 2012.5), 2078.6 (A, 282.7)

Table S22. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-2** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
10.6 (A, 0.1), 23.6 (A, 0.0), 32.7 (A, 0.1), 37.2 (A, 0.1), 42.3 (A, 0.1), 44.3 (A, 0.1), 46.5 (A, 0.0), 50.8 (A, 0.0), 56.6 (A, 0.9), 65.5 (A, 0.1), 70.3 (A, 0.4), 71.7 (A, 0.2), 73.2 (A, 0.1), 75.5 (A, 0.1), 81.9 (A, 0.2), 86.2 (A, 0.3), 89.8 (A, 0.4), 93.0 (A, 0.0), 94.3 (A, 0.3), 99.8 (A, 0.5), 101.2 (A, 0.0), 103.7 (A, 0.3), 104.1 (A, 0.4), 107.8 (A, 0.1), 110.0 (A, 0.0), 117.6 (A, 0.2), 133.1 (A, 0.1), 134.5 (A, 0.1), 137.1 (A, 0.4), 139.8 (A, 0.6), 168.6 (A, 0.5), 173.8 (A, 0.1), 177.4 (A, 1.1), 184.6 (A, 2.0), 215.5 (A, 1.8), 221.1 (A, 1.8), 291.3 (A, 5.2), 324.6 (A, 10.2), 329.7 (A, 2.6), 396.0 (A, 0.4), 402.9 (A, 1.9), 404.7 (A, 0.9), 406.5 (A, 1.2), 408.8 (A, 0.5), 409.9 (A, 0.5), 423.2 (A, 1.3), 424.1 (A, 14.0), 439.1 (A, 3.8), 448.6 (A, 1.0), 450.6 (A, 0.8), 453.4 (A, 1.0), 471.1 (A, 0.7), 473.1 (A, 1.2), 475.1 (A, 3.1), 478.4 (A, 1.3), 485.4 (A, 1.3), 489.6 (A, 0.1), 489.9 (A, 0.2), 491.9 (A, 3.0), 494.9 (A, 5.4), 501.3 (A, 2.4), 506.5 (A, 10.4), 509.6 (A, 10.6), 514.5 (A, 1.4), 519.1 (A, 16.1), 556.3 (A, 9.8), 563.7 (A, 0.0), 568.0 (A, 11.3), 573.2 (A, 36.9), 590.3 (A, 18.2), 607.0 (A, 57.2), 608.4 (A, 10.8), 609.5 (A, 49.7), 616.1 (A, 22.4), 630.3 (A, 255.6), 632.1 (A, 167.2), 639.2 (A, 352.6), 651.5 (A, 102.4), 659.9 (A, 2.5), 1975 (A, 301), 1981 (A, 514), 2025 (A, 325), 2029 (A, 205), 2048 (A, 147), 2066 (A, 194), 2070 (A, 874), 2074 (A, 469), 2086 (A, 20), 2087 (A, 1882), 2089 (A, 12), 2100 (A, 2844), 2113 (A, 2035), 2157 (A, 409)	14.3 (A, 0.1), 18.7 (A, 0.0), 28.4 (A, 0.1), 30.7 (A, 0.0), 32.9 (A, 0.0), 38.4 (A, 0.2), 42.6 (A, 0.1), 49.2 (A, 0.1), 53.0 (A, 1.0), 60.7 (A, 0.0), 63.1 (A, 0.1), 70.5 (A, 0.2), 72.7 (A, 0.2), 74.7 (A, 0.1), 82.8 (A, 0.1), 84.4 (A, 0.4), 88.6 (A, 0.3), 89.1 (A, 0.6), 91.0 (A, 0.1), 92.7 (A, 0.1), 96.2 (A, 0.0), 99.0 (A, 0.1), 102.3 (A, 0.0), 102.7 (A, 0.4), 107.9 (A, 0.8), 114.6 (A, 0.3), 116.0 (A, 0.3), 123.8 (A, 0.6), 129.6 (A, 0.1), 134.6 (A, 0.8), 158.6 (A, 0.5), 160.4 (A, 1.1), 163.9 (A, 3.8), 167.3 (A, 0.0), 191.6 (A, 3.3), 219.6 (A, 2.2), 274.0 (A, 10.6), 314.6 (A, 10.3), 322.4 (A, 1.1), 382.1 (A, 0.3), 391.1 (A, 0.8), 391.7 (A, 2.3), 392.7 (A, 2.1), 394.8 (A, 0.2), 396.0 (A, 0.7), 413.5 (A, 0.5), 421.5 (A, 7.6), 443.5 (A, 2.3), 444.9 (A, 1.8), 447.4 (A, 5.7), 452.0 (A, 2.2), 452.1 (A, 1.2), 470.5 (A, 3.1), 471.4 (A, 2.5), 479.2 (A, 0.9), 488.0 (A, 0.2), 491.5 (A, 1.2), 491.9 (A, 4.4), 497.2 (A, 0.2), 499.9 (A, 0.9), 508.4 (A, 1.6), 520.6 (A, 2.9), 521.3 (A, 7.9), 522.7 (A, 0.0), 526.3 (A, 8.5), 550.9 (A, 0.9), 553.4 (A, 9.6), 567.5 (A, 1.6), 577.5 (A, 27.7), 590.1 (A, 16.4), 601.7 (A, 61.9), 602.2 (A, 4.4), 604.0 (A, 45.3), 614.5 (A, 22.0), 616.6 (A, 152.7), 626.6 (A, 290.7), 630.7 (A, 321.1), 639.0 (A, 24.7), 643.8 (A, 1.7), 1898.6 (A, 228.9), 1902.6 (A, 504.8), 1956.1 (A, 243.0), 1958.5 (A, 213.1), 1971.4 (A, 134.5), 1988.8 (A, 304.5), 1992.8 (A, 457.6), 1997.3 (A, 834.8), 2004.4 (A, 46.1), 2006.9 (A, 1856.4), 2010.3 (A, 94.6), 2018.1 (A, 2412.1), 2035.4 (A, 1805.3), 2074.7 (A, 376.8)

Table S23. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-3** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
21.5 (B, 2.1), 23.1 (A, 0.3), 28.3 (A, 0.0), 42.1 (B, 0.2), 44.3 (A, 0.3), 51.4 (A, 0.0), 56.5 (B, 0.0), 63.6 (A, 0.0), 64.4 (B, 0.4), 71.6 (B, 0.6), 74.2 (B, 0.2), 74.9 (A, 0.1), 77.6 (A, 0.0), 82.8 (A, 0.2), 87.6 (B, 1.0), 88.2 (A, 0.1), 89.9 (B, 0.4), 95.5 (B, 0.1), 96.3 (A, 0.3), 98.7 (A, 0.0), 104.1 (B, 0.4), 110.6 (B, 0.0), 114.9 (B, 0.3), 116.5 (A, 0.8), 121.7 (A, 0.2), 127.0 (A, 0.9), 140.9 (B, 1.3), 141.4 (A, 0.1), 145.9 (B, 2.1), 153.9 (A, 1.0), 160.1 (B, 4.8), 163.1 (A, 0.0), 163.6 (B, 0.9), 195.7 (A, 0.9), 210.9 (B, 2.3), 218.2 (A, 0.1), 295.4 (B, 11.1), 374.8 (B, 5.8), 376.3 (A, 5.6), 394.1 (A, 3.8), 397.3 (B, 1.9), 404.1 (B, 1.2), 404.7 (A, 0.2), 413.1 (A, 8.6), 415.3 (B, 7.5), 418.6 (A, 3.3), 419.6 (B, 5.5), 438.9 (B, 3.6), 439.8 (A, 0.4), 449.5 (B, 8.6), 450.3 (A, 0.2), 458.7 (B, 2.4), 460.6 (A, 3.2), 482.5 (A, 0.6), 483.1 (B, 9.3), 487.1 (A, 1.1), 491.0 (B, 6.6), 495.2 (B, 11.9), 496.6 (A, 3.6), 500.6 (B, 8.0), 504.0 (A, 4.8), 511.0 (B, 7.9), 511.6 (A, 1.2), 530.1 (A, 2.8), 536.4 (B, 16.5), 556.7 (B, 17.2), 560.2 (A, 1.9), 586.8 (A, 26.5), 588.6 (B, 19.1), 593.1 (B, 16.5), 600.9 (A, 221.3), 611.0 (B, 55.2), 612.8 (A, 12.4), 621.6 (A, 22.1), 624.4 (B, 92.4), 628.9 (B, 361.6), 630.8 (A, 13.2), 652.3 (B, 63.3), 655.1 (A, 130.5), 2001 (B, 391), 2004 (A, 116), 2035 (B, 292), 2037 (A, 108), 2047 (B, 272), 2054 (A, 116), 2057 (A, 172), 2060 (B, 354), 2072 (A, 1156), 2073 (B, 446), 2089 (A, 1769), 2096 (B, 2489), 2115 (B, 1560), 2149 (A, 4)	

Table S24. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14T-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
12.1 (A, 0.1), 27.2 (A, 0.0), 28.3 (A, 0.1), 31.2 (A, 0.0), 44.0 (A, 0.1), 44.9 (A, 0.1), 47.7 (A, 0.1), 52.6 (A, 0.2), 52.9 (A, 0.0), 56.9 (A, 0.2), 58.7 (A, 0.3), 68.0 (A, 0.0), 70.2 (A, 0.1), 75.7 (A, 0.1), 77.8 (A, 1.0), 84.9 (A, 0.2), 87.0 (A, 0.1), 89.1 (A, 0.4), 92.6 (A, 0.0), 94.3 (A, 0.7), 97.4 (A, 0.1), 100.1 (A, 0.3), 102.7 (A, 0.2), 107.5 (A, 0.4), 112.7 (A, 0.4), 119.4 (A, 0.7), 125.7 (A, 0.3), 131.0 (A, 0.1), 136.5 (A, 0.2), 140.9 (A, 0.8), 143.9 (A, 0.8), 157.4 (A, 4.9), 173.2 (A, 2.6), 185.2 (A, 0.9), 207.8 (A, 2.0), 226.1 (A, 2.4), 284.4 (A, 8.3), 307.8 (A, 21.0), 316.0 (A, 9.3), 368.8 (A, 14.5), 378.2 (A, 14.7), 388.7 (A, 1.3), 393.0 (A, 10.5), 398.6 (A, 2.1), 406.6 (A, 1.5), 409.7 (A, 1.0), 411.1 (A, 1.8), 421.7 (A, 8.2), 423.8 (A, 1.6), 424.1 (A, 13.5), 441.8 (A, 3.9), 448.6 (A, 4.7), 449.3 (A, 0.1), 458.5 (A, 12.9), 472.7 (A, 3.6), 474.7 (A, 1.5), 476.1 (A, 12.6), 482.2 (A, 1.6), 484.8 (A, 20.3), 486.0 (A, 8.4), 491.5 (A, 1.4), 499.4 (A, 2.2), 502.4 (A, 1.1), 507.3 (A, 6.4), 512.9 (A, 5.2), 519.8 (A, 6.0), 536.2 (A, 48.4), 549.5 (A, 26.6), 566.4 (A, 14.0), 568.3 (A, 59.5), 570.0 (A, 51.2), 591.3 (A, 20.9), 607.8 (A, 104.8), 609.6 (A, 21.6), 613.3 (A, 67.2), 616.6 (A, 69.8), 632.2 (A, 208.7), 637.5 (A, 360.0), 656.5 (A, 53.0) , 1947 (A, 441), 1973 (A, 483), 2016 (A, 332), 2034 (A, 359), 2043 (A, 246), 2061 (A, 47), 2066 (A, 86), 2073 (A, 1165), 2081 (A, 773), 2082 (A, 861), 2086 (A, 876), 2101 (A, 2514), 2108 (A, 1870), 2154 (A, 340)	17.3 (A, 0.2), 21.5 (A, 0.2), 27.9 (A, 0.0), 31.0 (A, 0.0), 36.8 (A, 0.0), 41.3 (A, 0.2), 43.0 (A, 0.0), 51.2 (A, 0.3), 56.4 (A, 0.4), 57.8 (A, 0.0), 64.6 (A, 0.3), 67.7 (A, 0.1), 73.0 (A, 0.4), 73.9 (A, 0.0), 76.4 (A, 0.4), 83.6 (A, 0.4), 83.8 (A, 0.1), 85.0 (A, 0.3), 90.1 (A, 0.3), 94.3 (A, 0.0), 94.7 (A, 0.7), 96.7 (A, 0.1), 101.0 (A, 0.1), 102.9 (A, 0.3), 103.5 (A, 0.1), 113.5 (A, 0.4), 118.4 (A, 0.3), 119.7 (A, 0.1), 130.7 (A, 1.5), 135.8 (A, 0.2), 145.0 (A, 0.3), 150.4 (A, 1.3), 153.4 (A, 0.1), 174.2 (A, 0.2), 184.1 (A, 3.7), 233.4 (A, 5.0), 264.1 (A, 7.0), 282.1 (A, 34.9), 316.8 (A, 1.5), 374.3 (A, 0.7), 375.0 (A, 3.7), 382.8 (A, 0.4), 392.3 (A, 0.2), 393.4 (A, 6.1), 394.5 (A, 0.5), 396.1 (A, 2.3), 410.1 (A, 5.2), 414.8 (A, 1.2), 414.9 (A, 8.8), 421.7 (A, 21.2), 445.0 (A, 6.1), 448.4 (A, 0.7), 467.3 (A, 5.2), 471.6 (A, 0.9), 474.5 (A, 9.2), 478.1 (A, 3.3), 479.7 (A, 5.3), 480.6 (A, 13.4), 485.1 (A, 0.0), 487.0 (A, 6.0), 497.8 (A, 0.7), 500.7 (A, 0.2), 514.9 (A, 1.2), 519.1 (A, 3.2), 524.8 (A, 1.8), 528.7 (A, 22.2), 550.1 (A, 2.2), 550.4 (A, 7.7), 551.9 (A, 26.7), 552.1 (A, 14.9), 579.0 (A, 107.4), 580.6 (A, 49.5), 599.4 (A, 1.5), 600.0 (A, 113.2), 607.0 (A, 53.8), 613.1 (A, 62.9), 626.7 (A, 207.9), 627.7 (A, 330.4), 642.7 (A, 24.3), 1885.0 (A, 684.4), 1896.5 (A, 87.6), 1943.8 (A, 426.3), 1956.9 (A, 340.8), 1966.9 (A, 123.9), 1982.5 (A, 318.4), 1984.9 (A, 441.4), 1996.7 (A, 177.5), 1999.6 (A, 176.6), 2000.8 (A, 2513.1), 2005.0 (A, 120.1), 2013.7 (A, 2420.4), 2030.2 (A, 1707.6), 2070.8 (A, 379.1)

Table S25. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14T-2** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
18.1 (A, 0.0), 27.8 (A, 0.3), 35.5 (A, 0.1), 39.1 (A, 0.1), 44.4 (A, 0.1), 51.9 (A, 0.1), 54.9 (A, 0.1), 60.4 (A, 0.1), 66.2 (A, 0.3), 70.3 (A, 0.2), 75.9 (A, 0.1), 77.3 (A, 0.4), 81.1 (A, 0.3), 82.6 (A, 0.3), 85.5 (A, 0.2), 88.0 (A, 0.4), 88.6 (A, 0.2), 90.0 (A, 0.1), 92.5 (A, 0.4), 97.2 (A, 0.0), 98.8 (A, 0.9), 102.9 (A, 0.3), 105.3 (A, 0.3), 109.7 (A, 0.0), 111.9 (A, 0.1), 116.3 (A, 0.1), 119.3 (A, 1.6), 120.8 (A, 0.3), 122.4 (A, 0.4), 128.2 (A, 0.6), 136.9 (A, 0.6), 142.9 (A, 0.3), 153.5 (A, 4.4), 179.2 (A, 0.7), 193.9 (A, 0.5), 210.4 (A, 1.9), 284.7 (A, 1.9), 363.9 (A, 0.5), 375.0 (A, 0.9), 386.7 (A, 5.2), 391.1 (A, 12.3), 393.2 (A, 3.0), 399.1 (A, 4.9), 399.9 (A, 6.3), 404.2 (A, 0.8), 410.0 (A, 18.0), 411.3 (A, 5.3), 422.8 (A, 10.9), 427.3 (A, 5.6), 436.0 (A, 3.1), 440.2 (A, 4.3), 441.8 (A, 1.3), 446.4 (A, 4.0), 470.5 (A, 4.9), 473.0 (A, 7.5), 478.4 (A, 19.1), 482.3 (A, 0.6), 485.6 (A, 8.3), 489.4 (A, 6.2), 493.5 (A, 0.9), 494.0 (A, 3.7), 497.5 (A, 5.2), 507.2 (A, 6.4), 511.4 (A, 4.5), 519.7 (A, 13.0), 540.3 (A, 4.1), 547.1 (A, 28.4), 550.3 (A, 14.3), 555.7 (A, 11.3), 564.3 (A, 27.7), 568.9 (A, 23.3), 594.2 (A, 113.0), 601.1 (A, 176.2), 608.5 (A, 57.9), 616.5 (A, 31.2), 617.9 (A, 152.5), 623.5 (A, 88.0), 632.0 (A, 242.2), 640.7 (A, 88.8), 2012 (A, 128), 2026 (A, 108), 2040 (A, 122), 2043 (A, 94), 2045 (A, 156), 2050 (A, 453), 2053 (A, 466), 2065 (A, 237), 2077 (A, 272), 2084 (A, 534), 2088 (A, 1425), 2098 (A, 2416), 2116 (A, 2809), 2148 (A, 78)	14.5 (A, 0.0), 20.1 (A, 0.4), 25.7 (A, 0.1), 36.4 (A, 0.1), 36.7 (A, 0.0), 40.3 (A, 0.1), 45.2 (A, 0.7), 50.2 (A, 0.3), 54.6 (A, 0.2), 59.5 (A, 0.4), 68.1 (A, 0.2), 72.1 (A, 0.3), 73.4 (A, 0.5), 76.6 (A, 0.1), 77.8 (A, 0.4), 83.5 (A, 0.1), 85.2 (A, 0.0), 86.3 (A, 0.4), 88.9 (A, 1.4), 89.9 (A, 0.3), 92.6 (A, 0.8), 94.8 (A, 0.6), 96.8 (A, 0.3), 99.2 (A, 0.1), 101.4 (A, 0.0), 105.8 (A, 0.1), 109.0 (A, 0.4), 115.0 (A, 0.2), 118.0 (A, 0.3), 122.6 (A, 0.0), 134.7 (A, 1.3), 156.5 (A, 3.6), 161.3 (A, 0.8), 198.3 (A, 3.3), 200.9 (A, 1.7), 219.2 (A, 3.3), 278.6 (A, 4.8), 333.1 (A, 20.5), 367.0 (A, 5.5), 371.8 (A, 0.6), 378.6 (A, 12.2), 383.6 (A, 22.3), 389.2 (A, 0.7), 391.1 (A, 0.4), 392.5 (A, 10.1), 398.8 (A, 4.1), 402.3 (A, 3.0), 407.9 (A, 0.3), 421.0 (A, 3.8), 433.0 (A, 5.0), 446.2 (A, 7.3), 449.1 (A, 6.3), 466.0 (A, 1.0), 469.9 (A, 17.2), 478.9 (A, 23.1), 480.2 (A, 21.1), 485.5 (A, 1.8), 488.8 (A, 1.9), 494.0 (A, 0.8), 496.0 (A, 3.6), 497.4 (A, 2.5), 503.5 (A, 4.1), 509.1 (A, 0.2), 511.6 (A, 5.6), 514.8 (A, 10.2), 524.7 (A, 4.5), 542.8 (A, 0.6), 553.1 (A, 12.6), 556.4 (A, 25.1), 558.2 (A, 37.5), 577.0 (A, 62.7), 582.6 (A, 15.7), 592.8 (A, 93.0), 595.5 (A, 115.2), 602.0 (A, 87.4), 612.1 (A, 79.8), 616.7 (A, 45.2), 621.9 (A, 321.8), 628.3 (A, 49.2), 1868.8 (A, 412.3), 1949.8 (A, 54.3), 1956.5 (A, 96.6), 1961.0 (A, 198.2), 1962.7 (A, 27.0), 1980.2 (A, 332.7), 1988.5 (A, 513.8), 1990.3 (A, 735.1), 1994.0 (A, 672.9), 2003.9 (A, 25.8), 2004.9 (A, 1183.5), 2016.7 (A, 2325.2), 2035.1 (A, 2519.0), 2065.9 (A, 101.7)

Table S26. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **13S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
18.1 (A', 0.2), 32.1 (A", 0.0), 39.4 (A', 0.0), 45.1 (A", 0.1), 47.9 (A', 0.0), 49.0 (A", 0.0), 51.7 (A", 0.0), 53.3 (A", 0.0), 73.5 (A', 0.4), 76.1 (A', 0.0), 80.4 (A", 0.3), 81.3 (A', 0.1), 85.0 (A', 0.0), 86.4 (A", 0.0), 87.0 (A', 0.3), 92.3 (A', 0.1), 92.3 (A", 0.0), 97.4 (A", 0.1), 97.8 (A', 0.2), 99.8 (A", 0.0), 104.5 (A', 0.0), 112.9 (A', 0.0), 113.1 (A", 0.1), 119.2 (A', 0.0), 122.6 (A", 0.4), 132.9 (A', 0.0), 149.5 (A", 1.5), 158.8 (A', 0.1), 169.7 (A", 0.0), 177.5 (A', 3.2), 183.5 (A", 2.1), 205.4 (A', 0.2), 223.8 (A", 8.7), 246.2 (A', 0.9), 260.5 (A', 5.4), 351.7 (A", 24.0), 389.9 (A', 0.6), 393.5 (A", 0.0), 396.6 (A', 0.0), 418.5 (A", 0.2), 419.2 (A", 0.0), 426.9 (A', 0.6), 430.5 (A", 0.0), 432.5 (A', 1.0), 435.3 (A", 13.9), 443.1 (A', 4.8), 457.4 (A", 0.2), 462.4 (A', 0.4), 468.7 (A", 16.4), 479.8 (A", 0.0), 481.3 (A', 4.4), 487.0 (A', 0.6), 488.2 (A', 5.1), 495.1 (A', 0.5), 495.9 (A", 1.0), 499.7 (A', 1.8), 507.3 (A", 22.8), 510.0 (A', 3.6), 513.3 (A", 0.6), 519.1 (A', 4.7), 525.5 (A", 0.0), 555.6 (A', 0.0), 569.4 (A', 1.5), 573.5 (A", 0.3), 579.0 (A', 84.5), 586.4 (A", 0.0), 586.6 (A', 72.4), 589.5 (A', 59.9), 595.4 (A", 77.7), 619.7 (A", 5.0), 630.3 (A', 57.1), 633.6 (A", 277.1), 634.0 (A', 298.2), 653.7 (A', 4.4), 1954 (A', 347), 2033 (A", 13), 2037 (A', 107), 2048 (A', 25), 2054 (A", 1), 2062 (A', 174), 2064 (A", 160), 2071 (A", 3), 2072 (A', 21), 2086 (A', 1817), 2097 (A", 2746), 2109 (A', 3362), 2148 (A', 118)	24.2 (A', 0.0), 29.5 (A", 0.0), 44.7 (A", 0.1), 45.2 (A", 0.0), 47.4 (A', 0.0), 48.5 (A', 0.2), 52.8 (A", 0.1), 66.0 (A", 0.0), 77.6 (A', 0.1), 81.3 (A', 0.1), 83.9 (A", 0.3), 84.9 (A', 0.1), 86.8 (A", 0.0), 87.2 (A', 0.1), 89.6 (A', 0.2), 91.0 (A", 0.0), 94.9 (A', 0.0), 98.9 (A', 0.2), 101.1 (A", 0.1), 102.4 (A", 0.0), 104.7 (A', 0.0), 104.8 (A', 0.0), 105.8 (A", 0.0), 114.8 (A", 0.2), 118.1 (A', 0.1), 131.1 (A', 0.1), 137.9 (A", 0.4), 157.5 (A', 0.4), 158.6 (A", 0.0), 160.6 (A', 3.6), 189.4 (A", 0.1), 204.5 (A', 0.1), 239.0 (A", 6.1), 257.4 (A', 0.1), 274.4 (A', 1.3), 370.6 (A", 19.1), 382.8 (A", 0.0), 384.0 (A', 0.1), 404.1 (A', 0.3), 404.2 (A", 0.0), 404.2 (A", 0.0), 417.0 (A', 2.0), 421.1 (A", 0.0), 427.9 (A', 1.7), 428.8 (A', 1.7), 430.3 (A", 9.1), 443.1 (A', 1.1), 445.5 (A", 0.0), 461.6 (A", 29.5), 484.5 (A", 0.0), 490.6 (A', 3.3), 497.1 (A', 7.9), 505.4 (A', 0.1), 506.7 (A", 1.8), 508.8 (A', 6.8), 509.2 (A', 1.6), 515.5 (A", 1.2), 516.0 (A', 0.1), 524.7 (A", 9.3), 526.6 (A', 1.7), 530.7 (A", 0.0), 550.4 (A', 2.1), 570.8 (A", 0.0), 576.0 (A', 0.6), 583.1 (A', 68.9), 584.8 (A', 63.4), 585.9 (A", 0.0), 589.1 (A", 49.5), 591.0 (A', 74.0), 614.8 (A", 102.7), 625.5 (A', 49.0), 626.1 (A", 197.5), 629.5 (A', 230.8), 637.2 (A', 0.1), 1873.5 (A', 324.1), 1961.8 (A", 24.5), 1966.3 (A', 10.8), 1968.7 (A', 29.1), 1972.4 (A", 0.0), 1983.8 (A", 325.0), 1984.6 (A', 606.1), 1990.4 (A", 0.0), 1991.4 (A', 0.4), 2008.1 (A', 1408.0), 2019.4 (A", 2416.1), 2028.1 (A', 2995.0), 2063.8 (A', 99.2)

Table S27. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **13T-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
20.8 (A, 0.0), 26.0 (A, 0.0), 31.0 (A, 0.0), 41.5 (A, 0.0), 45.6 (A, 0.2), 48.5 (A, 0.0), 49.8 (A, 0.1), 57.7 (A, 0.2), 63.4 (A, 0.0), 69.2 (A, 0.1), 76.2 (A, 0.2), 77.2 (A, 0.2), 80.8 (A, 0.1), 82.1 (A, 0.1), 84.4 (A, 0.2), 86.4 (A, 0.2), 88.8 (A, 0.2), 90.3 (A, 0.1), 94.4 (A, 0.0), 98.0 (A, 0.0), 100.6 (A, 0.1), 103.4 (A, 0.0), 107.5 (A, 0.0), 111.3 (A, 0.1), 112.3 (A, 0.1), 125.4 (A, 0.0), 138.3 (A, 0.2), 150.1 (A, 0.3), 154.3 (A, 0.2), 157.4 (A, 0.5), 180.5 (A, 0.2), 188.5 (A, 0.2), 232.5 (A, 0.7), 243.7 (A, 1.3), 250.0 (A, 1.7), 362.3 (A, 1.0), 375.4 (A, 6.6), 387.0 (A, 0.7), 388.4 (A, 0.4), 397.5 (A, 2.6), 399.3 (A, 2.0), 404.0 (A, 0.9), 408.8 (A, 3.7), 416.1 (A, 7.2), 424.5 (A, 7.2), 425.1 (A, 0.9), 431.9 (A, 3.2), 436.6 (A, 0.8), 444.0 (A, 2.1), 452.2 (A, 1.0), 456.9 (A, 11.2), 466.9 (A, 8.0), 477.8 (A, 0.6), 479.4 (A, 3.8), 481.8 (A, 6.9), 487.8 (A, 1.4), 488.1 (A, 1.2), 488.6 (A, 1.2), 494.1 (A, 4.1), 499.8 (A, 1.8), 513.1 (A, 0.2), 533.3 (A, 17.6), 535.4 (A, 7.7), 559.1 (A, 27.1), 565.8 (A, 34.3), 571.7 (A, 5.3), 578.0 (A, 51.0), 582.2 (A, 30.2), 585.5 (A, 29.2), 590.6 (A, 75.4), 606.6 (A, 73.1), 619.7 (A, 176.6), 625.4 (A, 242.7), 637.9 (A, 45.1), 1935 (A, 411), 2025 (A, 11), 2031 (A, 30), 2046 (A, 19), 2048 (A, 96), 2058 (A, 611), 2059 (A, 568), 2069 (A, 397), 2073 (A, 10), 2084 (A, 1442), 2097 (A, 2310), 2101 (A, 3324), 2145 (A, 187)	6.6 (A, 0.0), 19.7 (A, 0.6), 25.3 (A, 0.1), 28.6 (A, 0.1), 32.5 (A, 0.0), 41.8 (A, 0.1), 43.5 (A, 0.5), 45.5 (A, 0.0), 50.9 (A, 1.0), 62.9 (A, 0.0), 66.1 (A, 0.1), 74.0 (A, 0.3), 77.7 (A, 0.1), 81.2 (A, 0.0), 84.7 (A, 0.0), 86.4 (A, 0.4), 87.2 (A, 0.0), 88.8 (A, 0.3), 92.2 (A, 0.0), 95.1 (A, 0.1), 97.2 (A, 0.1), 97.3 (A, 0.0), 103.0 (A, 0.0), 105.9 (A, 0.6), 108.1 (A, 0.0), 116.3 (A, 0.1), 131.3 (A, 0.3), 138.3 (A, 0.0), 147.7 (A, 0.1), 153.1 (A, 0.5), 178.9 (A, 0.0), 190.5 (A, 0.2), 245.7 (A, 0.3), 254.9 (A, 0.8), 263.4 (A, 0.0), 363.8 (A, 0.0), 367.4 (A, 0.0), 372.6 (A, 2.9), 374.5 (A, 0.0), 393.3 (A, 1.1), 395.2 (A, 0.0), 398.0 (A, 0.8), 410.7 (A, 0.2), 413.9 (A, 0.0), 415.3 (A, 2.1), 421.4 (A, 1.9), 432.7 (A, 0.0), 439.0 (A, 0.0), 450.4 (A, 1.3), 454.4 (A, 2.9), 477.4 (A, 20.3), 486.1 (A, 0.5), 492.6 (A, 10.3), 493.3 (A, 0.6), 495.8 (A, 0.2), 496.0 (A, 3.9), 497.3 (A, 0.0), 497.4 (A, 1.3), 502.4 (A, 0.6), 504.4 (A, 3.4), 516.7 (A, 0.7), 517.5 (A, 0.0), 562.3 (A, 1.3), 563.8 (A, 0.0), 565.4 (A, 20.6), 568.1 (A, 22.7), 571.3 (A, 0.0), 578.6 (A, 96.7), 582.9 (A, 9.5), 593.8 (A, 135.7), 606.7 (A, 254.5), 607.2 (A, 27.8), 628.4 (A, 28.3), 633.6 (A, 200.1), 1857.7 (A, 406.6), 1950.6 (A, 22.6), 1958.3 (A, 0.7), 1963.6 (A, 2.5), 1964.7 (A, 0.0), 1977.3 (A, 844.2), 1977.8 (A, 1066.2), 1990.0 (A, 71.2), 1994.3 (A, 0.0), 2007.9 (A, 1053.1), 2019.8 (A, 1872.2), 2020.0 (A, 3113.6), 2059.9 (A, 209.2)

Table S28. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12S-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
26.0 (A, 0.1), 26.8 (A, 0.0), 39.8 (A, 0.0), 40.8 (A, 0.1), 43.1 (A, 0.0), 53.8 (A, 0.0), 60.2 (A, 0.1), 61.4 (A, 0.1), 75.4 (A, 0.1), 76.6 (A, 0.0), 78.9 (A, 0.1), 82.2 (A, 0.3), 87.6 (A, 0.0), 89.3 (A, 0.1), 91.3 (A, 0.0), 95.7 (A, 0.0), 96.3 (A, 0.2), 99.7 (A, 0.0), 100.4 (A, 0.2), 108.5 (A, 0.1), 109.4 (A, 0.6), 114.1 (A, 0.2), 124.6 (A, 0.7), 127.0 (A, 0.0), 140.1 (A, 0.0), 148.0 (A, 0.3), 154.9 (A, 3.8), 157.1 (A, 0.1), 162.1 (A, 0.0), 197.2 (A, 0.3), 203.9 (A, 0.8), 251.8 (A, 3.7), 264.6 (A, 4.6), 363.0 (A, 0.4), 382.6 (A, 8.6), 397.7 (A, 2.7), 406.1 (A, 0.5), 407.4 (A, 0.1), 411.0 (A, 1.0), 413.6 (A, 5.7), 419.2 (A, 2.9), 421.0 (A, 0.2), 435.1 (A, 4.9), 437.1 (A, 0.1), 444.9 (A, 1.4), 479.3 (A, 4.3), 483.8 (A, 3.7), 485.7 (A, 3.1), 488.3 (A, 0.0), 490.4 (A, 2.4), 497.4 (A, 1.1), 500.5 (A, 1.1), 507.9 (A, 1.0), 514.7 (A, 3.9), 524.8 (A, 1.9), 536.5 (A, 1.6), 544.3 (A, 30.3), 546.6 (A, 3.3), 548.2 (A, 46.3), 561.4 (A, 11.8), 563.7 (A, 28.9), 595.3 (A, 0.9), 596.1 (A, 84.3), 602.3 (A, 9.5), 609.4 (A, 1.4), 624.5 (A, 73.7), 630.3 (A, 329.7), 632.5 (A, 121.5), 640.1 (A, 1.3), 1993 (A, 78), 1994 (A, 308), 2022 (A, 23), 2040 (A, 213), 2047 (A, 53), 2053 (A, 409), 2074 (A, 69), 2080 (A, 778), 2083 (A, 679), 2087 (A, 3067), 2111 (A, 3212), 2142 (A, 66)	21.9 (A, 0.0), 29.3 (B, 0.1), 33.9 (A, 0.0), 35.3 (B, 0.1), 42.2 (B, 0.1), 45.7 (A, 0.0), 51.0 (B, 0.0), 54.5 (A, 0.1), 66.8 (B, 0.2), 69.1 (A, 0.1), 72.2 (A, 0.1), 80.9 (A, 0.2), 81.6 (B, 0.2), 87.2 (A, 0.0), 87.4 (A, 0.0), 88.1 (B, 0.1), 93.3 (A, 0.1), 93.4 (B, 0.4), 94.2 (B, 0.1), 104.4 (A, 0.0), 104.7 (B, 0.2), 109.7 (B, 1.0), 118.0 (B, 1.2), 124.1 (A, 0.0), 129.8 (B, 0.0), 137.5 (A, 0.9), 138.5 (B, 3.9), 144.4 (A, 0.0), 150.0 (A, 0.0), 195.7 (A, 0.1), 211.7 (B, 0.4), 264.4 (A, 1.4), 270.7 (B, 1.7), 349.5 (A, 0.4), 368.5 (B, 9.1), 384.8 (B, 3.3), 394.0 (A, 0.1), 396.0 (B, 0.5), 397.1 (A, 1.1), 400.0 (B, 0.8), 406.8 (B, 3.6), 407.0 (A, 0.0), 420.3 (B, 1.3), 423.9 (A, 0.4), 429.7 (A, 2.2), 473.0 (A, 0.3), 486.1 (B, 0.0), 492.6 (B, 2.6), 497.5 (A, 0.1), 498.1 (B, 0.2), 503.6 (A, 5.1), 505.1 (B, 3.7), 509.7 (A, 6.8), 516.0 (A, 2.4), 522.2 (B, 1.3), 532.2 (A, 44.8), 536.7 (B, 5.0), 554.2 (A, 0.0), 559.8 (B, 1.2), 569.4 (B, 23.1), 571.9 (A, 29.3), 594.7 (A, 1.1), 595.9 (B, 12.3), 598.5 (B, 38.8), 604.0 (A, 3.2), 616.3 (B, 284.1), 618.2 (A, 51.3), 624.6 (B, 116.8), 625.6 (A, 0.0), 1918.1 (A, 89.4), 1919.5 (B, 218.1), 1947.4 (B, 36.2), 1958.7 (A, 279.5), 1973.8 (B, 5.6), 1979.5 (A, 95.4), 1991.5 (B, 11.9), 1995.8 (A, 322.0), 1999.3 (A, 1263.0), 2003.4 (B, 2969.4), 2029.9 (B, 2916.6), 2057.4 (A, 21.9)

Table S29. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12S-2** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
24.2 (A, 0.0), 29.0 (A, 0.2), 39.9 (A, 0.3), 44.8 (A, 0.1), 52.8 (A, 0.1), 58.0 (A, 0.8), 63.9 (A, 0.0), 66.1 (A, 0.4), 71.1 (A, 0.6), 75.1 (A, 0.3), 80.0 (A, 0.1), 83.7 (A, 0.1), 85.3 (A, 0.0), 89.6 (A, 0.2), 95.8 (A, 0.4), 97.2 (A, 0.1), 99.7 (A, 0.4), 100.9 (A, 0.1), 103.7 (A, 0.3), 106.9 (A, 0.2), 109.6 (A, 0.3), 112.1 (A, 0.4), 119.9 (A, 2.3), 122.8 (A, 0.8), 127.6 (A, 0.0), 146.8 (A, 0.8), 160.2 (A, 0.6), 166.5 (A, 2.3), 174.8 (A, 1.8), 190.3 (A, 2.2), 192.7 (A, 1.7), 246.3 (A, 1.5), 271.9 (A, 2.4), 341.4 (A, 8.9), 360.8 (A, 5.5), 400.8 (A, 0.4), 406.3 (A, 1.5), 411.6 (A, 5.8), 414.1 (A, 0.7), 421.0 (A, 1.4), 426.5 (A, 1.3), 429.6 (A, 2.5), 439.9 (A, 2.9), 440.7 (A, 5.6), 450.0 (A, 5.4), 469.0 (A, 1.2), 473.3 (A, 7.8), 479.6 (A, 1.5), 486.0 (A, 1.0), 487.7 (A, 2.9), 491.7 (A, 8.1), 497.0 (A, 10.1), 511.9 (A, 6.3), 516.6 (A, 3.4), 531.4 (A, 1.3), 534.5 (A, 30.2), 538.6 (A, 14.4), 544.1 (A, 17.6), 554.3 (A, 9.8), 565.2 (A, 16.6), 582.0 (A, 38.3), 585.0 (A, 61.2), 592.4 (A, 5.0), 598.2 (A, 36.3), 599.4 (A, 42.1), 622.4 (A, 125.0), 630.9 (A, 164.9), 635.6 (A, 122.6), 647.2 (A, 26.1), 1946 (A, 268), 1968 (A, 386), 2023 (A, 41), 2030 (A, 190), 2041 (A, 149), 2053 (A, 149), 2066 (A, 491), 2081 (A, 258), 2083 (A, 1560), 2093 (A, 2022), 2108 (A, 3174), 2140 (A, 91)	

Table S30. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12T-1** using the M06-L/TZP and BP86/DZP methods

M06-L/TZP	BP86/DZP
28 (A, 0), 36 (A, 0), 37 (A, 0), 44 (A, 0), 54 (A, 0), 56 (A, 1), 59 (A, 0), 66 (A, 2), 73 (A, 0), 75 (A, 1), 82 (A, 0), 87 (A, 0), 89 (A, 0), 95 (A, 0), 95 (A, 1), 98 (A, 0), 100 (A, 0), 104 (A, 0), 105 (A, 0), 108 (A, 1), 114 (A, 0), 118 (A, 0), 125 (A, 0), 133 (A, 0), 135 (A, 0), 152 (A, 1), 155 (A, 1), 167 (A, 1), 175 (A, 0), 188 (A, 0), 206 (A, 0), 229 (A, 1), 240 (A, 1), 308 (A, 27), 324 (A, 12), 362 (A, 5), 374 (A, 4), 380 (A, 9), 385 (A, 29), 392 (A, 1), 400 (A, 2), 408 (A, 3), 411 (A, 4), 430 (A, 2), 436 (A, 20), 445 (A, 9), 454 (A, 1), 459 (A, 5), 467 (A, 4), 476 (A, 6), 484 (A, 18), 485 (A, 6), 489 (A, 4), 496 (A, 6), 499 (A, 15), 504 (A, 20), 514 (A, 1), 521 (A, 34), 539 (A, 6), 541 (A, 26), 548 (A, 31), 555 (A, 19), 559 (A, 8), 567 (A, 30), 594 (A, 140), 596 (A, 114), 611 (A, 57), 618 (A, 95), 638 (A, 67), 1948 (A, 398), 1975 (A, 390), 1991 (A, 190), 2023 (A, 307), 2031 (A, 114), 2043 (A, 85), 2053 (A, 850), 2065 (A, 622), 2075 (A, 717), 2083 (A, 1995), 2098 (A, 3438), 2132 (A, 106)	17.2 (A, 0), 25.2 (A, 0), 30.0 (A, 0), 41.5 (A, 0), 48.6 (A, 0), 49.3 (A, 0), 61.0 (A, 0), 66.6 (A, 1), 67.8 (A, 0), 76.4 (A, 0), 78.6 (A, 0), 83.6 (A, 0), 87.2 (A, 0), 90.4 (A, 0), 91.9 (A, 0), 93.4 (A, 0), 99.0 (A, 0), 100.5 (A, 0), 102.7 (A, 0), 104.0 (A, 0), 110.9 (A, 0), 118.7 (A, 0), 122.9 (A, 0), 125.0 (A, 0), 129.9 (A, 2), 138.5 (A, 0), 155.6 (A, 0), 165.5 (A, 1), 172.3 (A, 0), 183.1 (A, 0), 208.0 (A, 0), 235.8 (A, 1), 241.1 (A, 2), 304.4 (A, 9), 317.2 (A, 6), 355.0 (A, 1), 360.5 (A, 4), 366.9 (A, 0), 384.1 (A, 2), 390.1 (A, 3), 393.4 (A, 2), 394.8 (A, 5), 408.4 (A, 3), 425.1 (A, 0), 436.8 (A, 1), 448.4 (A, 5), 461.8 (A, 2), 469.9 (A, 1), 476.2 (A, 10), 478.2 (A, 6), 490.3 (A, 2), 494.4 (A, 3), 497.1 (A, 5), 502.8 (A, 3), 506.9 (A, 8), 509.9 (A, 5), 516.3 (A, 2), 524.0 (A, 23), 540.4 (A, 18), 548.0 (A, 10), 549.6 (A, 29), 561.0 (A, 40), 562.4 (A, 5), 564.9 (A, 25), 585.5 (A, 116), 596.3 (A, 59), 601.4 (A, 81), 612.8 (A, 145), 620.7 (A, 3), 1840.6 (A, 454), 1867.3 (A, 196), 1923.5 (A, 127), 1948.5 (A, 396), 1958.6 (A, 11), 1963.2 (A, 120), 1976.0 (A, 261), 1979.9 (A, 1093), 1991.0 (A, 550), 2003.8 (A, 1969), 2011.6 (A, 3094), 2045.1 (A, 142)

Table S31. Metal- Metal Distances, Natural Population Analysis Natural Charges, Metal Electron Configuration, Formal Metal-Metal Bond Orders, and WBIs for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures Using the M06-L/TZP and BP86/DZP Methods.

		16S-1		16S-2		15S-1		15S-2	
		M06-X	BP86	M06-X	BP86	M06-X	BP86	M06-X	BP86
Metal-metal distanc	Fe1-Fe2	2.872	2.898	2.876	2.903	2.917	3.005	2.431	2.456
	Fe3-Fe4	2.872	2.898	2.601	2.600	2.917	3.005	2.847	2.863
	Fe1-Fe3	/	/	/	/	/	/	/	/
	Fe1-Fe4	/	/	/	/	/	/	/	/
	Fe2-Fe3	/	/	/	/	2.747	2.755	/	/
	Fe2-Fe4	/	/	/	/	/	/	/	/
	Sn- Fe1	2.520	2.508	2.509	2.485	2.442	2.422	2.476	2.456
	Sn- Fe2	2.520	2.508	2.509	2.485	2.543	2.494	/	/
	Sn- Fe3	2.520	2.508	2.530	2.522	2.543	2.494	2.502	2.475
	Sn- Fe4	2.520	2.508	2.530	2.522	2.442	2.422	2.482	2.472
Metal natural charge	Fe1	-0.91	-1.48	-0.93	-1.50	-0.96	-1.59	-0.69	-1.23
	Fe2	-0.91	-1.48	-0.93	-1.50	-0.78	-1.23	-0.69	-1.05
	Fe3	-0.91	-1.48	-1.01	-1.53	-0.78	-1.23	-0.96	-1.54
	Fe4	-0.91	-1.48	-1.01	-1.53	-0.96	-1.59	-0.95	-1.55
	Sn	0.41	1.10	0.52	1.22	0.7	1.40	0.86	1.45
Metal electron configuration	Fe1	18	18	18	18	18	18	18	18
	Fe2	18	18	18	18	18	18	18	18
	Fe3	18	18	18	18	18	18	18	18
	Fe4	18	18	18	18	18	18	18	18
Formal bond order	Fe1-Fe2	1	1	1	1	1	1	2	2
	Fe3-Fe4	1	1	1	1	1	1	1	1
	Fe1-Fe3	/	/	/	/	/	/	/	/
	Fe1-Fe4	/	/	/	/	/	/	/	/
	Fe2-Fe3	/	/	/	/	1	1	/	/
	Fe2-Fe4	/	/	/	/	/	/	/	/
	Sn- Fe1	1	1	1	1	1	1	2	2
	Sn- Fe2	1	1	1	1	1	1	/	/
	Sn- Fe3	1	1	1	1	1	1	1	1
	Sn- Fe4	1	1	1	1	1	1	1	1
Wiberg bond index	Fe1-Fe2	0.19	0.40	0.18	0.39	0.14	0.31	0.37	0.62
	Fe3-Fe4	0.19	0.40	0.14	0.32	0.14	0.31	0.19	0.40
	Fe1-Fe3	0.03	0.04	0.03	0.05	0.05	0.10	0.04	0.08
	Fe1-Fe4	0.03	0.04	0.03	0.05	0.07	0.09	0.06	0.08
	Fe2-Fe3	0.03	0.04	0.03	0.05	0.19	0.40	0.01	0.01
	Fe2-Fe4	0.03	0.04	0.03	0.05	0.05	0.10	0.01	0.01
	Sn- Fe1	0.37	0.56	0.40	0.59	0.44	0.64	0.39	0.65
	Sn- Fe2	0.37	0.56	0.40	0.59	0.31	0.44	0.03	0.03
	Sn- Fe3	0.37	0.56	0.37	0.53	0.31	0.44	0.39	0.56
	Sn- Fe4	0.37	0.56	0.37	0.53	0.44	0.64	0.43	0.58

Values for global minimum structures are shown in bold type.

Table S32. Metal- Metal Distances, Natural Population Analysis Natural Charges, Metal Electron Configuration, Formal Metal-Metal Bond Orders, and WBIs for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures Using the M06-L/TZP and BP86/DZP Methods.

		15T-1		14S-1		14S-2	
		M06-X	BP86	M06-X	BP86	M06-X	BP86
Metal-metal distanc	Fe1-Fe2	2.490	2.451	2.973	3.056	2.817	2.830
	Fe3-Fe4	2.824	2.853	2.691	2.673	2.352	2.341
	Fe1-Fe3	/	/	/	/	/	/
	Fe1-Fe4	/	/	/	/	/	/
	Fe2-Fe3	/	/	2.805	2.840	/	/
	Fe2-Fe4	/	/	2.806	2.816	/	/
	Sn- Fe1	2.410	2.358	2.455	2.415	2.498	2.481
	Sn- Fe2	/	/	2.576	2.488	2.490	2.481
	Sn- Fe3	2.505	2.471	2.495	2.438	2.496	2.465
	Sn- Fe4	2.495	2.473	2.443	2.424	2.491	2.465
Metal natural charge	Fe1	-0.53	-1.19	-0.92	-1.56	-0.92	-1.50
	Fe2	-0.53	-1.02	-0.56	-1.00	-0.92	-1.50
	Fe3	-0.95	-1.54	-0.83	-1.30	-0.61	-1.07
	Fe4	-0.95	-1.54	-0.72	-1.30	-0.63	-1.07
	Sn	0.67	1.32	0.53	1.23	0.53	1.28
Metal electron configuration	Fe1	18	18	18	18	18	18
	Fe2	18	18	18	18	18	18
	Fe3	18	18	18	18	18	18
	Fe4	18	18	18	18	18	18
Formal bond order	Fe1-Fe2	2	2	1	1	1	1
	Fe3-Fe4	1	1	1	1	3	3
	Fe1-Fe3	/	/	/	/	/	/
	Fe1-Fe4	/	/	/	/	/	/
	Fe2-Fe3	/	/	1	1	/	/
	Fe2-Fe4	/	/	1	1	/	/
	Sn- Fe1	2	2	1	1	1	1
	Sn- Fe2	/	/	1	1	1	1
	Sn- Fe3	1	1	1	1	1	1
	Sn- Fe4	1	1	1	1	1	1
Wiberg bond index	Fe1-Fe2	0.21	0.44	0.20	0.39	0.19	0.39
	Fe3-Fe4	0.19	0.40	0.15	0.34	0.32	0.69
	Fe1-Fe3	0.05	0.09	0.04	0.08	0.03	0.05
	Fe1-Fe4	0.05	0.08	0.08	0.10	0.08	0.13
	Fe2-Fe3	0.00	0.00	0.21	0.44	0.07	0.13
	Fe2-Fe4	0.00	0.01	0.23	0.46	0.03	0.05
	Sn- Fe1	0.57	0.90	0.53	0.76	0.39	0.55
	Sn- Fe2	0.04	0.03	0.30	0.40	0.40	0.55
	Sn- Fe3	0.39	0.54	0.38	0.55	0.43	0.01
	Sn- Fe4	0.39	0.53	0.48	0.61	0.44	0.01

Values for global minimum structures are shown in bold type.

Table S33. Metal- Metal Distances, Natural Population Analysis Natural Charges, Metal Electron Configuration, Formal Metal-Metal Bond Orders, and WBIs for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures Using the M06-L/TZP and BP86/DZP Methods.

		14S-3		14T-1		14T-2		13S-1	
		M06-X	BP86	M06-X	BP86	M06-X	BP86	M06-X	BP86
Metal-metal distanc	Fe1-Fe2	/		2.427	2.391	2.759	2.804	2.715	2.763
	Fe3-Fe4	/		2.830	2.847	2.765	2.685	2.706	2.763
	Fe1-Fe3	2.736		/	/	/	/	2.604	2.588
	Fe1-Fe4	/		/	/	/	/	2.706	2.763
	Fe2-Fe3	/		/	/	/	/	2.715	2.763
	Fe2-Fe4	2.736		/	/	/	/	/	/
	Sn- Fe1	2.519		2.556	2.504	2.479	2.419	2.601	2.536
	Sn- Fe2	2.465		2.503	2.504	2.551	2.477	2.459	2.384
	Sn- Fe3	2.465		2.501	2.477	2.577	2.472	2.601	2.536
	Sn- Fe4	2.519		2.486	2.477	2.433	2.406	2.454	2.384
Metal natural charge	Fe1	-0.95		-0.78	-0.95	-0.97	-1.62	-0.84	-1.28
	Fe2	-0.47		-0.54	-0.95	-0.32	-0.89	-0.55	-1.11
	Fe3	-0.47		-0.49	-1.50	-0.94	-1.37	-0.84	-1.28
	Fe4	-0.95		-0.47	-1.50	-0.40	-1.20	-0.56	-1.11
	Sn	0.57		0.18	1.20	0.48	1.31	0.42	1.12
Metal electron configuration	Fe1	18		17	17	18	18	19	19
	Fe2	16		17	17	16	16	17	17
	Fe3	16		18	18	18	17	19	19
	Fe4	18		18	18	16	17	17	17
Formal bond order	Fe1-Fe2	/		2	2	1	1	1	1
	Fe3-Fe4	/		1	1	1	1	1	1
	Fe1-Fe3	1		/	/	/	/	1	1
	Fe1-Fe4	/		/	/	/	/	1	1
	Fe2-Fe3	/		/	/	/	/	1	1
	Fe2-Fe4	1		/	/	/	/	/	/
	Sn- Fe1	1		1	1	1	1	1	1
	Sn- Fe2	1		1	1	1	1	1	1
	Sn- Fe3	1		1	1	1	1	1	1
	Sn- Fe4	1		1	1	1	1	1	1
Wiberg bond index	Fe1-Fe2	0.05		0.22	0.52	0.05	0.38	0.22	0.43
	Fe3-Fe4	0.05		0.18	0.37	0.04	0.33	0.22	0.43
	Fe1-Fe3	0.20		0.03	0.06	0.01	0.08	0.16	0.34
	Fe1-Fe4	0.05		0.03	0.05	0.02	0.09	0.22	0.43
	Fe2-Fe3	0.07		0.03	0.05	0.04	0.33	0.22	0.43
	Fe2-Fe4	0.20		0.05	0.06	0.01	0.07	0.15	0.23
	Sn- Fe1	0.37		0.32	0.51	0.10	0.66	0.34	0.39
	Sn- Fe2	0.54		0.38	0.51	0.07	0.46	0.50	0.71
	Sn- Fe3	0.54		0.38	0.56	0.08	0.49	0.34	0.39
	Sn- Fe4	0.37		0.40	0.56	0.13	0.66	0.51	0.71

Values for global minimum structures are shown in bold type.

Table S34. Metal- Metal Distances, Natural Population Analysis Natural Charges, Metal Electron Configuration, Formal Metal-Metal Bond Orders, and WBIs for the $SnFe_4(CO)_n$ (n = 16 to 12) Structures Using the M06-L/TZP and BP86/DZP Methods.

		13T-1		12S-1		12S-2		12T-1	
		M06-X	BP86	M06-X	BP86	M06-X	BP86	M06-X	BP86
Metal-metal distanc	Fe1-Fe2	2.783	2.906	/	/	2.631		/	/
	Fe3-Fe4	/	2.906	2.751	2.800	2.572		2.622	2.619
	Fe1-Fe3	2.561	2.535	2.722	2.763	2.973		2.395	2.413
	Fe1-Fe4	2.829	2.906	2.635	2.646	2.519		2.703	2.674
	Fe2-Fe3	2.731	2.906	2.635	2.646	/		2.435	2.417
	Fe2-Fe4	/	/	2.722	2.763	2.849		2.686	2.603
	Sn- Fe1	2.618	2.569	2.446	2.394	2.782		2.613	2.613
	Sn- Fe2	2.455	2.393	2.446	2.394	2.393		2.687	2.681
	Sn- Fe3	2.640	2.569	2.495	2.427	2.430		2.790	2.727
	Sn- Fe4	2.481	2.393	2.495	2.427	2.532		2.603	2.550
Metal natural charge	Fe1	-0.56	-1.20	-0.67	-1.22	-0.45		-0.36	-1.18
	Fe2	-0.45	-1.04	-0.67	-1.22	-0.70		-0.56	-0.79
	Fe3	-0.53	-1.20	-0.59	-0.99	-0.70		-0.35	-0.96
	Fe4	-0.65	-1.04	-0.59	-0.99	-0.57		-0.67	-0.95
	Sn	0.24	1.09	0.44	1.14	0.44		0.19	0.95
Metal electron configuration	Fe1	19	19	17	17	17		18	18
	Fe2	17	17	17	17	18		18	18
	Fe3	18	19	18	18	18		18	18
	Fe4	16	17	18	18	17		18	18
Formal bond order	Fe1-Fe2	1	1	/	/	1		/	/
	Fe3-Fe4	/	/	1	1	1		1	1
	Fe1-Fe3	1	1	1	1	1		1	1
	Fe1-Fe4	1	1	1	1	1		1	1
	Fe2-Fe3	1	1	1	1	/		2	2
	Fe2-Fe4	/	/	1	1	1		1	1
	Sn- Fe1	1	1	1	1	1		1	1
	Sn- Fe2	1	1	1	1	1		1	1
	Sn- Fe3	1	1	1	1	1		1	1
	Sn- Fe4	1	1	1	1	1		1	1
Wiberg bond index	Fe1-Fe2	0.05	0.28	0.15	0.25	0.22		0.07	0.09
	Fe3-Fe4	0.02	0.28	0.19	0.39	0.28		0.18	0.37
	Fe1-Fe3	0.04	0.44	0.23	0.44	0.15		0.30	0.55
	Fe1-Fe4	0.03	0.28	0.21	0.46	0.22		0.16	0.37
	Fe2-Fe3	0.06	0.28	0.21	0.46	0.11		0.27	0.47
	Fe2-Fe4	0.03	0.22	0.23	0.44	0.20		0.18	0.42
	Sn- Fe1	0.08	0.38	0.51	0.69	0.22		0.33	0.41
	Sn- Fe2	0.13	0.72	0.51	0.69	0.60		0.24	0.29
	Sn- Fe3	0.08	0.38	0.48	0.58	0.53		0.24	0.30
	Sn- Fe4	0.12	0.72	0.48	0.58	0.45		0.29	0.37

Values for global minimum structures are shown in bold type.

Table S35. ν(CO) Frequencies (in cm^{-1}) and IR Intensities (in km/mol) in Parentheses for the SnFe$_4$(CO)$_n$ (*n* = 16 to 12) Structures are calculated by using the BP86/DZP Method except for **14S-3** and **12S-2** which are calculated by M06-L/TZP because the corresponding isomers are not optimized by BP86/DZP. Bridging ν(CO) frequencies are given in bold type, whereas weakly semibridging ν(CO) frequencies are given in italic type.

16S-1(D_{2d})	1960.1 (A2, 0.0), 1968.7 (B1, 0.0), 1979.4 (E, 47.6), 1979.4 (E, 47.6), 1988.9 (E, 34.4), 1988.9 (E, 34.4), 1989.2 (A1, 0.0), 1996.5 (E, 716.4), 1996.5 (E, 716.4), 1999.8 (B2, 1044.2), 2014.1 (A1, 0.0), 2014.9 (B2, 483.2), 2033.4 (E, 2182.5), 2033.4 (E, 2182.5), 2053.2 (B2, 1474.2), 2084.0 (A1, 0.0)
16S-2(C_{2v})	**1858.6 (B2, 534.9), 1875.7 (A1, 219.6),** 1968.0 (A2, 0.0), 1981.6 (B2, 241.3), 1986.4 (B1, 69.2), 1991.1 (B2, 500.3), 1991.6 (A2, 0.0), 1993.7 (A1, 1323.4), 1998.0 (B2, 8.7), 2001.3 (A1, 0.9), 2008.0 (B1, 330.7), 2015.3 (A1, 264.1), 2028.9 (B1, 2574.2), 2037.0 (B2, 1773.7), 2046.5 (A1, 1473.3), 2083.3 (A1, 92.7)
15S-1(C_2)	**1834.3 (A, 372.2),** 1954.6 (A, 4.7), 1963.2 (B, 96.8), 1971.0 (A, 28.0), 1983.5 (B, 85.1), 1985.9 (B, 25.7), 1991.0 (A, 181.7), 1991.6 (A, 29.4), 1996.8 (B, 488.4), 2003.8 (B, 2690.3), 2007.0 (A, 321.8), 2012.8 (B, 420.4), 2025.5 (A, 2159.3), 2039.8 (B, 2599.9), 2078.1 (A, 0.7)
15S-2(C_1)	**1540.3 (A, 510.5), 1848.6 (A, 335.9)**, 1964.9 (A, 235.7), 1972.3 (A, 55.6), 1988.2 (A, 75.2), 1990.6 (A, 172.5), 1993.7 (A, 715.1), 2000.2 (A, 612.2), 2000.7 (A, 161.0), 2002.4 (A, 109.0), 2009.0 (A, 2476.2), 2014.7 (A, 583.3), 2035.3 (A, 1756.9), 2044.8 (A, 1810.2), 2077.7 (A, 234.4)
15T-1(C_1)	1937.4 (A, 620.7), 1942.7 (A, 302.4), 1960.8 (A, 119.3), 1964.4 (A, 62.9), 1969.4 (A, 105.1), 1981.8 (A, 456.1), 1983.7 (A, 41.5), 1987.3 (A, 566.3), 1991.4 (A, 1603.5), 1999.8 (A, 538.5), 2001.5 (A, 762.8), 2005.6 (A, 524.9), 2029.9 (A, 1729.7), 2030.7 (A, 1918.8), 2071.3 (A, 282.9)
14S-1(C_1)	**1849.3 (A, 342.8)**, 1948.9 (A, 296.5), 1956.0 (A, 1.3), 1963.8 (A, 169.7), 1968.0 (A, 195.6), 1975.8 (A, 98.8), 1987.7 (A, 28.9), 2005.2 (A, 248.1), 2007.6 (A, 87.4), 2015.3 (A, 2251.3), 2020.0 (A, 1936.7), 2022.3 (A, 824.1), 2041.4 (A, 2012.5), 2078.6 (A, 282.7)
14S-2(C_1)	*1898.6 (A, 228.9), 1902.6 (A, 504.8)*, 1956.1 (A, 243.0), 1958.5 (A, 213.1), 1971.4 (A, 134.5), 1988.8 (A, 304.5), 1992.8 (A, 457.6), 1997.3 (A, 834.8), 2004.4 (A, 46.1), 2006.9 (A, 1856.4), 2010.3 (A, 94.6), 2018.1 (A, 2412.1), 2035.4 (A, 1805.3), 2074.7 (A, 376.8)
14S-3(C_2)	2001 (B, 391), 2004 (A, 116), 2035 (B, 292), 2037 (A, 108), 2047 (B, 272), 2054 (A, 116), 2057 (A, 172), 2060 (B, 354), 2072 (A, 1156), 2073 (B, 446), 2089 (A, 1769), 2096 (B, 2489), 2115 (B, 1560), 2149 (A, 4)
14T-1(C_1)	*1885.0 (A, 684.4), 1896.5 (A, 87.6)*, 1943.8 (A, 426.3), 1956.9 (A, 340.8), 1966.9 (A, 123.9), 1982.5 (A, 318.4), 1984.9 (A, 441.4), 1996.7 (A, 177.5), 1999.6 (A, 176.6), 2000.8 (A, 2513.1), 2005.0 (A, 120.1), 2013.7 (A, 2420.4), 2030.2 (A, 1707.6), 2070.8 (A, 379.1)
14T-2(C_1)	**1868.8 (A, 412.3)**, 1949.8 (A, 54.3), 1956.5 (A, 96.6), 1961.0 (A, 198.2), 1962.7 (A, 27.0), 1980.2 (A, 332.7), 1988.5 (A, 513.8), 1990.3 (A, 735.1), 1994.0 (A, 672.9), 2003.9 (A, 25.8), 2004.9 (A, 1183.5), 2016.7 (A, 2325.2), 2035.1 (A, 2519.0), 2065.9 (A, 101.7)
13S-1(C_s)	**1873.5 (A', 324.1),** 1961.8 (A", 24.5), 1966.3 (A', 10.8), 1968.7 (A', 29.1), 1972.4

(A", 0.0), 1983.8 (A", 325.0), 1984.6 (A', 606.1), 1990.4 (A", 0.0), 1991.4 (A', 0.4), 2008.1 (A', 1408.0), 2019.4 (A", 2416.1), 2028.1 (A', 2995.0), 2063.8 (A', 99.2)

13T-1(C_1) **1857.7 (A, 406.6),** 1950.6 (A, 22.6), 1958.3 (A, 0.7), 1963.6 (A, 2.5), 1964.7 (A, 0.0), 1977.3 (A, 844.2), 1977.8 (A, 1066.2), 1990.0 (A, 71.2), 1994.3 (A, 0.0), 2007.9 (A, 1053.1), 2019.8 (A, 1872.2), 2020.0 (A, 3113.6), 2059.9 (A, 209.2)

12T-1(C_1) **1840.6 (A, 454.4), 1867.3 (A, 196.0)**, *1923.5 (A, 127.2)*, 1948.5 (A, 396.0), 1958.6 (A, 11.1), 1963.2 (A, 120.2), 1976.0 (A, 261.0), 1979.9 (A, 1092.8), 1991.0 (A, 550.2), 2003.8 (A, 1969.1), 2011.6 (A, 3093.8), 2045.1 (A, 141.7)

12S-1(C_2) 1918.1 (A, 89.4), 1919.5 (B, 218.1), 1947.4 (B, 36.2), 1958.7 (A, 279.5), 1973.8 (B, 5.6), 1979.5 (A, 95.4), 1991.5 (B, 11.9), 1995.8 (A, 322.0), 1999.3 (A, 1263.0), 2003.4 (B, 2969.4), 2029.9 (B, 2916.6), 2057.4 (A, 21.9)

12S-2(C_1) *1946 (A, 268), 1968 (A, 386),* 2023 (A, 41), 2030 (A, 190), 2041 (A, 149), 2053 (A, 149), 2066 (A, 491), 2081 (A, 258), 2083 (A, 1560), 2093 (A, 2022), 2108 (A, 3174), 2140 (A, 91)

Complete Gaussian 09 reference   (Reference 15)

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