From Spiropentane to Butterfly and Tetrahedral Structures in Tetranuclear Iron Carbonyl Carbide Chemistry

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Supporting Information

Tables S1 to S22: Theoretical Cartesian coordinates for the structures of $Fe_4C(CO)_n$ (n=16-11) using the B3LYP/DZP and BP86/DZP methods.

Tables S23 to S44: Theoretical harmonic vibrational frequencies for the structures of $Fe_4C(CO)_n$ (n=16-11) using the B3LYP/DZP and BP86/DZP methods.

Tables S45 to S50: The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_n$ (n=16-11) isomers using the B3LYP/DZP and BP86/DZP methods.

Figures 1 to 6. The optimized $Fe_4C(CO)_n$ (n=16-11) structures.

Complete Gaussian03 reference (reference 37).

Table S1. Theoretical Cartesian coordinates (in Å) for the structure **16S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP

Fe	0.00000000	-1.32688600	1.65667900	0.00000000	-1.31874600	1.64755200
Fe	0.00000000	1.32688600	1.65667900	0.00000000	1.31874600	1.64755200
C	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
C	1.81973600	1.38751100	1.61057900	1.80638700	1.38654200	1.60046600
C	0.00000000	3.03339200	1.11648000	0.00000000	3.02293000	1.13123700
C	-1.81973600	1.38751100	1.61057900	-1.80638700	1.38654200	1.60046600
C	1.81973600	-1.38751100	1.61057900	1.80638700	-1.38654200	1.60046600
C	0.00000000	-3.03339200	1.11648000	0.00000000	-3.02293000	1.13123700
C	-1.81973600	-1.38751100	1.61057900	-1.80638700	-1.38654200	1.60046600
O	-2.96152300	1.54830600	1.60538800	-2.96011700	1.56773400	1.60525000
O	0.00000000	4.16407700	0.87790900	0.00000000	4.17194900	0.90927900
O	2.96152300	1.54830600	1.60538800	2.96011700	1.56773400	1.60525000
O	2.96152300	-1.54830600	1.60538800	2.96011700	-1.56773400	1.60525000
O	0.00000000	-4.16407700	0.87790900	0.00000000	-4.17194900	0.90927900
O	-2.96152300	-1.54830600	1.60538800	-2.96011700	-1.56773400	1.60525000
C	0.00000000	-1.51992100	3.47025900	0.00000000	-1.52390700	3.45067900
O	0.00000000	-1.66656400	4.61542300	0.00000000	-1.68353200	4.60821300
C	0.00000000	1.51992100	3.47025900	0.00000000	1.52390700	3.45067900
O	0.00000000	1.66656400	4.61542300	0.00000000	1.68353200	4.60821300
O	-1.54830600	-2.96152300	-1.60538800	-1.56773400	-2.96011700	-1.60525000
C	-1.38751100	-1.81973600	-1.61057900	-1.38654200	-1.80638700	-1.60046600
Fe	-1.32688600	0.00000000	-1.65667900	-1.31874600	0.00000000	-1.64755200
C	-3.03339200	0.00000000	-1.11648000	-3.02293000	0.00000000	-1.13123700
C	-1.38751100	1.81973600	-1.61057900	-1.38654200	1.80638700	-1.60046600
C	-1.51992100	0.00000000	-3.47025900	-1.52390700	0.00000000	-3.45067900
O	-4.16407700	0.00000000	-0.87790900	-4.17194900	0.00000000	-0.90927900
O	-1.54830600	2.96152300	-1.60538800	-1.56773400	2.96011700	-1.60525000
O	-1.66656400	0.00000000	-4.61542300	-1.68353200	0.00000000	-4.60821300
Fe	1.32688600	0.00000000	-1.65667900	1.31874600	0.00000000	-1.64755200
C	1.38751100	-1.81973600	-1.61057900	1.38654200	-1.80638700	-1.60046600
C	3.03339200	0.00000000	-1.11648000	3.02293000	0.00000000	-1.13123700
C	1.38751100	1.81973600	-1.61057900	1.38654200	1.80638700	-1.60046600
C	1.51992100	0.00000000	-3.47025900	1.52390700	0.00000000	-3.45067900
O	1.54830600	-2.96152300	-1.60538800	1.56773400	-2.96011700	-1.60525000
O	4.16407700	0.00000000	-0.87790900	4.17194900	0.00000000	-0.90927900
O	1.54830600	2.96152300	-1.60538800	1.56773400	2.96011700	-1.60525000
O	1.66656400	0.00000000	-4.61542300	1.68353200	0.00000000	-4.60821300

Table S2. Theoretical Cartesian coordinates (in Å) for the structure **16S-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.00000000	1.31583600	1.69457100	0.00000000	1.30929800	1.68069700
Fe	0.00000000	-1.31583600	1.69457100	0.00000000	-1.30929800	1.68069700
Fe	-1.25567400	0.00000000	-1.68175800	-1.25220800	0.00000000	-1.66858000
Fe	1.25567400	0.00000000	-1.68175800	1.25220800	0.00000000	-1.66858000
C	0.00000000	0.00000000	0.06524700	0.00000000	0.00000000	0.06372700
C	-2.28951500	-1.38023800	-1.12242900	-2.29226300	-1.37004600	-1.11925800
C	0.00000000	1.40411800	-2.32943500	0.00000000	1.40242200	-2.32811600
C	-2.28951500	1.38023800	-1.12242900	-2.29226300	1.37004600	-1.11925800
C	2.28951500	1.38023800	-1.12242900	2.29226300	1.37004600	-1.11925800
C	2.28951500	-1.38023800	-1.12242900	2.29226300	-1.37004600	-1.11925800
C	0.00000000	-1.40411800	-2.32943500	0.00000000	-1.40242200	-2.32811600
C	-1.82182700	-1.36098100	1.83321400	-1.80630100	-1.35712400	1.83500400
C	0.00000000	-2.86718300	0.80116300	0.00000000	-2.85663300	0.79511700
C	1.82182700	-1.36098100	1.83321400	1.80630100	-1.35712400	1.83500400
C	-1.82182700	1.36098100	1.83321400	-1.80630100	1.35712400	1.83500400
C	0.00000000	2.86718300	0.80116300	0.00000000	2.85663300	0.79511700
C	1.82182700	1.36098100	1.83321400	1.80630100	1.35712400	1.83500400
O	2.95033500	-1.50223900	2.01769700	2.94354100	-1.51895200	2.04215600
O	0.00000000	-3.88602000	0.25868100	0.00000000	-3.89504900	0.25914000
O	-2.95033500	-1.50223900	2.01769700	-2.94354100	-1.51895200	2.04215600
O	-2.95033500	1.50223900	2.01769700	-2.94354100	1.51895200	2.04215600
O	0.00000000	3.88602000	0.25868100	0.00000000	3.89504900	0.25914000
O	2.95033500	1.50223900	2.01769700	2.94354100	1.51895200	2.04215600
O	2.99992300	2.25792400	-0.88854900	3.02980400	2.24902600	-0.90138000
O	2.99992300	-2.25792400	-0.88854900	3.02980400	-2.24902600	-0.90138000
O	0.00000000	-2.46339600	-2.84013600	0.00000000	-2.46348100	-2.86014800
O	-2.99992300	-2.25792400	-0.88854900	-3.02980400	-2.24902600	-0.90138000
O	0.00000000	2.46339600	-2.84013600	0.00000000	2.46348100	-2.86014800
O	-2.99992300	2.25792400	-0.88854900	-3.02980400	2.24902600	-0.90138000
C	0.00000000	1.69581500	3.48340400	0.00000000	1.72568500	3.44867500
O	0.00000000	1.94362800	4.61078400	0.00000000	2.00549200	4.58312400
C	-2.01627500	0.00000000	-3.34278900	-2.02204500	0.00000000	-3.31262400
C	2.01627500	0.00000000	-3.34278900	2.02204500	0.00000000	-3.31262400
O	2.51951000	0.00000000	-4.37917100	2.55130200	0.00000000	-4.35285400
O	-2.51951000	0.00000000	-4.37917100	-2.55130200	0.00000000	-4.35285400
C	0.00000000	-1.69581500	3.48340400	0.00000000	-1.72568500	3.44867500
O	0.00000000	-1.94362800	4.61078400	0.00000000	-2.00549200	4.58312400

Table S3. Theoretical Cartesian coordinates (in Å) for the structure **16S-3** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.00000000	-1.25861000	1.72220000	0.00000000	-1.25436000	1.70534400
Fe	0.00000000	1.25861000	1.72220000	0.00000000	1.25436000	1.70534400
C	-1.28331900	-2.45201200	1.23738500	-1.26777700	-2.45386500	1.22526600
C	1.45357300	0.00000000	2.22942800	1.45648700	0.00000000	2.22189400
C	1.28331900	-2.45201200	1.23738500	1.26777700	-2.45386500	1.22526600
C	1.28331900	2.45201200	1.23738500	1.26777700	2.45386500	1.22526600
C	-1.28331900	2.45201200	1.23738500	-1.26777700	2.45386500	1.22526600
C	-1.45357300	0.00000000	2.22942800	-1.45648700	0.00000000	2.22189400
O	2.00829800	3.33196000	1.07356900	1.98626200	3.35966600	1.06819000
O	-2.00829800	3.33196000	1.07356900	-1.98626200	3.35966600	1.06819000
O	-2.56871100	0.00000000	2.60309400	-2.57490200	0.00000000	2.61930200
O	-2.00829800	-3.33196000	1.07356900	-1.98626200	-3.35966600	1.06819000
O	2.56871100	0.00000000	2.60309400	2.57490200	0.00000000	2.61930200
O	2.00829800	-3.33196000	1.07356900	1.98626200	-3.35966600	1.06819000
C	0.00000000	-1.86981800	3.44950900	0.00000000	-1.87241000	3.41748500
C	0.00000000	1.86981800	3.44950900	0.00000000	1.87241000	3.41748500
O	0.00000000	2.25544100	4.53477400	0.00000000	2.28130800	4.51017600
O	0.00000000	-2.25544100	4.53477400	0.00000000	-2.28130800	4.51017600
O	3.33196000	-2.00829800	-1.07356900	3.35966600	-1.98626200	-1.06819000
C	2.45201200	-1.28331900	-1.23738500	2.45386500	-1.26777700	-1.22526600
Fe	1.25861000	0.00000000	-1.72220000	1.25436000	0.00000000	-1.70534400
C	2.45201200	1.28331900	-1.23738500	2.45386500	1.26777700	-1.22526600
C	0.00000000	-1.45357300	-2.22942800	0.00000000	-1.45648700	-2.22189400
C	0.00000000	1.45357300	-2.22942800	0.00000000	1.45648700	-2.22189400
C	1.86981800	0.00000000	-3.44950900	1.87241000	0.00000000	-3.41748500
O	3.33196000	2.00829800	-1.07356900	3.35966600	1.98626200	-1.06819000
Fe	-1.25861000	0.00000000	-1.72220000	-1.25436000	0.00000000	-1.70534400
O	0.00000000	-2.56871100	-2.60309400	0.00000000	-2.57490200	-2.61930200
O	0.00000000	2.56871100	-2.60309400	0.00000000	2.57490200	-2.61930200
O	2.25544100	0.00000000	-4.53477400	2.28130800	0.00000000	-4.51017600
C	-2.45201200	-1.28331900	-1.23738500	-2.45386500	-1.26777700	-1.22526600
C	-2.45201200	1.28331900	-1.23738500	-2.45386500	1.26777700	-1.22526600
C	-1.86981800	0.00000000	-3.44950900	-1.87241000	0.00000000	-3.41748500
O	-3.33196000	-2.00829800	-1.07356900	-3.35966600	-1.98626200	-1.06819000
O	-3.33196000	2.00829800	-1.07356900	-3.35966600	1.98626200	-1.06819000
O	-2.25544100	0.00000000	-4.53477400	-2.28130800	0.00000000	-4.51017600
C	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000

Table S4. Theoretical Cartesian coordinates (in Å) for the structure **15S-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	1.97805500	-0.93224800	-0.50175100	1.31928100	-1.35178300	-1.03136200
Fe	1.05928800	1.19040100	0.74710700	-0.00888000	-1.34590300	1.07568000
Fe	-1.34571800	1.13539200	-0.70781800	0.00888000	1.34590300	1.07568000
Fe	-1.62719300	-1.25645200	0.46255700	-1.31928100	1.35178300	-1.03136200
C	0.09794800	-0.26084400	0.17394600	0.00000000	0.00000000	-0.34957600
C	-0.70662300	2.81368100	-0.81057500	0.00000000	0.00000000	2.58626900
C	-1.83634200	-1.69679800	-1.29974100	0.00000000	2.72959700	-0.27704000
C	-0.62454700	0.63653800	-2.31975600	1.80096500	1.62140400	1.19713800
C	-1.13974400	-2.95351400	0.79449300	-0.45437700	1.54445800	-2.61986000
C	-1.31306700	-0.80921400	2.21635100	-2.43095800	0.01518000	-1.52744200
C	-2.27364900	1.47261900	0.83444600	-2.00477400	1.30182500	0.82762500
C	2.07220700	2.63515600	0.19454200	0.32076200	-2.59841700	2.35630000
C	0.26352400	1.97252400	2.14114900	-1.80096500	-1.62140400	1.19713800
C	2.33732500	0.57540800	1.81555800	0.00000000	-2.72959700	-0.27704000
C	2.23660800	0.42995500	-1.67301700	2.00477400	-1.30182500	0.82762500
C	1.43708600	-2.12790500	-1.71893600	2.43095800	-0.01518000	-1.52744200
C	1.89120000	-2.06363900	0.93096400	0.45437700	-1.54445800	-2.61986000
O	3.13755100	0.28071100	2.60401400	-0.44431400	-3.78722600	-0.57496400
O	-0.14761100	2.50060400	3.08702900	-2.91060700	-1.94947400	1.34780800
O	2.70502800	3.54391700	-0.13042200	0.51282000	-3.39667800	3.18325000
O	2.50309800	1.21076100	-2.48707500	3.00238900	-1.29824200	1.46816900
O	1.13645300	-2.91646300	-2.51102600	3.14829300	0.82282200	-1.90726400
O	1.85787800	-2.78972000	1.82685000	-0.04276800	-1.69608500	-3.66395800
O	-0.88980600	-4.06492500	0.97091700	0.04276800	1.69608500	-3.66395800
O	-1.10918100	-0.63300600	3.33383600	-3.14829300	-0.82282200	-1.90726400
O	-2.93931200	1.81725800	1.71327000	-3.00238900	1.29824200	1.46816900
O	-0.48287200	3.93928700	-0.95576100	0.00000000	0.00000000	3.76959300
O	-2.02563000	-2.07457600	-2.37227800	0.44431400	3.78722600	-0.57496400
O	-0.27856400	0.38971700	-3.38825600	2.91060700	1.94947400	1.34780800
C	3.78587900	-1.11629900	-0.46711900	2.51156700	-2.68427300	-1.39013800
O	4.93156300	-1.26530900	-0.45858300	3.29450300	-3.50911500	-1.64557000
C	-2.92388400	1.31442300	-1.56941200	-0.32076200	2.59841700	2.35630000
C	-3.44656300	-1.36676900	0.72644300	-2.51156700	2.68427300	-1.39013800
O	-4.58015100	-1.42256000	0.92407200	-3.29450300	3.50911500	-1.64557000
O	-3.92086700	1.44725800	-2.13390000	-0.51282000	3.39667800	3.18325000

Table S5. Theoretical Cartesian coordinates (in Å) for the structure **15S-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.72072600	0.62434100	0.13267300	0.74530900	0.65627100	0.15748000
Fe	3.39109100	-0.00474500	-0.06231400	3.34168500	-0.02492800	-0.06785700
Fe	-1.39549000	-1.46390800	-0.08554100	-1.37010800	-1.44078800	-0.11265500
Fe	-2.84131100	0.87066200	0.02053300	-2.82497600	0.85796600	0.04242700
C	-0.95296700	0.53703400	0.05243500	-0.93949100	0.54415500	0.10714700
C	-0.05642500	-2.63604200	-0.34485900	-0.02295100	-2.54210000	-0.52587200
C	-2.99323200	0.54287200	1.81525800	-3.09415900	0.29748400	1.74773900
C	-1.08009100	-1.58805900	1.72042400	-0.95101000	-1.62274200	1.65474400
C	-2.89776100	2.63217600	0.38040900	-2.93662900	2.54724800	0.61668000
C	-2.62466100	1.28743200	-1.75747500	-2.49544700	1.47475900	-1.64004500
C	-1.46909300	-1.30726500	-1.91755600	-1.61610900	-1.22669500	-1.90441200
C	4.21467000	0.65900100	1.41878200	4.27533800	0.55262000	1.36965700
C	4.53376100	-0.94525800	-1.07409400	4.40573600	-1.08060200	-1.04113100
C	1.79896600	-0.09309600	-1.32211700	1.79218700	0.02852400	-1.35950200
C	2.91663200	-1.46667900	0.91186700	2.72445400	-1.38196900	0.95094100
C	1.16032300	0.89515200	1.87515100	1.18331400	0.95594400	1.88980200
C	0.70947700	2.26438900	-0.49852100	0.71251900	2.29361800	-0.45806100
O	1.62295800	-0.46204500	-2.43179900	1.60939300	-0.23365500	-2.51105600
O	5.29897600	-1.54959800	-1.69585900	5.12832600	-1.77270700	-1.64836400
O	4.79109400	1.06728600	2.33454900	4.92779700	0.91492500	2.27115600
O	2.67652400	-2.38564300	1.57071600	2.43385300	-2.27588500	1.65200000
O	1.32252200	1.18133000	2.98724700	1.37383100	1.28047900	3.00109500
O	0.61260800	3.36003200	-0.86977400	0.61117900	3.40896000	-0.81477600
O	-2.92761900	3.75684000	0.62720900	-3.01067900	3.64320500	1.00920300
O	-2.50494700	1.63462300	-2.84555700	-2.30726600	1.94941200	-2.68510600
O	-1.48508200	-1.29315600	-3.06632600	-1.74494600	-1.20265700	-3.06231800
O	0.73238700	-3.45110400	-0.55403400	0.77780000	-3.33057400	-0.84352700
O	-3.13213800	0.40783500	2.94909100	-3.33384800	0.02181400	2.85486000
O	-0.85682300	-1.74707600	2.83782200	-0.68598400	-1.83897100	2.76837100
C	3.77500100	1.55746700	-0.92831100	3.83347100	1.49109200	-0.93273000
O	4.04105600	2.53996900	-1.47047900	4.18704300	2.45914700	-1.48297900
C	-2.88590800	-2.50040000	-0.01256000	-2.79305500	-2.54740100	0.02952000
C	-4.57471700	0.29791300	-0.27139100	-4.52051400	0.34005600	-0.43184400
O	-5.64880100	-0.06810000	-0.46707500	-5.59139600	0.01163900	-0.75464900
O	-3.81699900	-3.17930600	0.04129700	-3.69205300	-3.28582100	0.12858400

Table S6. Theoretical Cartesian coordinates (in Å) for the structure **15S-3** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	-1.05273100	1.12479900	0.00000000	-0.96124600	1.08865000	0.00000000
Fe	0.67523800	3.13677300	0.00000000	0.50925500	3.20953700	0.00000000
Fe	0.26175200	-2.03163100	1.24223400	0.24967700	-2.04208400	1.24425600
Fe	0.26175200	-2.03163100	-1.24223400	0.24967700	-2.04208400	-1.24425600
C	-0.30453000	-0.53951200	0.00000000	-0.29084600	-0.56397200	0.00000000
C	1.30997000	-0.86028500	2.16183900	1.33051800	-0.92019300	2.18223600
C	-0.75924600	-3.22193700	0.00000000	-0.80226500	-3.20476700	0.00000000
C	-1.29908600	-1.86052500	2.16814000	-1.27777800	-1.83106900	2.20338600
C	-1.29908600	-1.86052500	-2.16814000	-1.27777800	-1.83106900	-2.20338600
C	1.30997000	-0.86028500	-2.16183900	1.33051800	-0.92019300	-2.18223600
C	1.81519100	-2.23838900	0.00000000	1.79658100	-2.29493300	0.00000000
C	1.08612500	3.09542100	1.78923700	1.12361900	3.13873300	1.70906400
C	1.19180900	4.82738900	0.00000000	1.04015200	4.89050500	0.00000000
C	1.08612500	3.09542100	-1.78923700	1.12361900	3.13873300	-1.70906400
C	-0.97698300	1.19504700	1.81743800	-0.85144400	1.28247300	1.80438500
C	-2.82824900	0.84542200	0.00000000	-2.68602400	0.59987000	0.00000000
C	-0.97698300	1.19504700	-1.81743800	-0.85144400	1.28247300	-1.80438500
O	1.47237500	3.12849100	-2.87532200	1.61344800	3.21008500	-2.77069800
O	1.47478400	5.95058100	0.00000000	1.36917900	6.01608100	0.00000000
O	1.47237500	3.12849100	2.87532200	1.61344800	3.21008500	2.77069800
O	-1.02102100	1.21200300	2.97169300	-0.91104600	1.33431300	2.97175000
O	-3.95488900	0.59341200	0.00000000	-3.79704400	0.23893400	0.00000000
O	-1.02102100	1.21200300	-2.97169300	-0.91104600	1.33431300	-2.97175000
O	-2.27373100	-1.78731100	-2.77629200	-2.23604200	-1.73540200	-2.85964300
O	1.98921900	-0.15044700	-2.76221700	2.03874900	-0.25261800	-2.82209600
O	2.97850500	-2.40088500	0.00000000	2.96424200	-2.49783000	0.00000000
O	1.98921900	-0.15044700	2.76221700	2.03874900	-0.25261800	2.82209600
O	-1.51687200	-4.11913500	0.00000000	-1.59125200	-4.08932800	0.00000000
O	-2.27373100	-1.78731100	2.77629200	-2.23604200	-1.73540200	2.85964300
C	-1.16354100	3.30283100	0.00000000	-1.25420900	3.52140900	0.00000000
O	-2.03486600	4.08700200	0.00000000	-2.30098600	4.06520800	0.00000000
C	0.82929100	-3.51861500	2.16318700	0.77293400	-3.53972600	2.15472100
C	0.82929100	-3.51861500	-2.16318700	0.77293400	-3.53972600	-2.15472100
O	1.17878400	-4.43468500	-2.76576100	1.09619700	-4.47389800	-2.77161400
O	1.17878400	-4.43468500	2.76576100	1.09619700	-4.47389800	2.77161400

Table S7. Theoretical Cartesian coordinates (in Å) for the structure **15T-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	-1.22924000	1.79648100	0.00000000	-1.16581900	1.85056700	0.00000000
Fe	1.39178100	1.34722500	0.00000000	1.39410800	1.24287900	0.00000000
Fe	-0.04527600	-1.54751900	1.25686600	-0.07953900	-1.52423700	1.25575100
Fe	-0.04527600	-1.54751900	-1.25686600	-0.07953900	-1.52423700	-1.25575100
C	-0.19608000	0.12100200	0.00000000	-0.21678500	0.12920700	0.00000000
C	1.19545900	-0.76362300	2.34602200	1.18094800	-0.79372000	2.35546100
C	-1.35638700	-2.37600800	0.00000000	-1.41229300	-2.32274300	0.00000000
C	-1.51829200	-1.06587300	2.20751600	-1.52413900	-1.00273000	2.21120500
C	-1.51829200	-1.06587300	-2.20751600	-1.52413900	-1.00273000	-2.21120500
C	1.19545900	-0.76362300	-2.34602200	1.18094800	-0.79372000	-2.35546100
C	1.40187900	-2.13290700	0.00000000	1.34401500	-2.17986000	0.00000000
C	1.73871200	2.58575400	1.37499400	1.78740100	2.41216800	1.34492600
C	3.05761200	0.54338700	0.00000000	3.01696200	0.44507300	0.00000000
C	1.73871200	2.58575400	-1.37499400	1.78740100	2.41216800	-1.34492600
C	-1.06541700	1.86516500	1.81785400	-1.01546500	1.92904600	1.80532300
C	-2.91486800	1.18406700	0.00000000	-2.87508400	1.32662200	0.00000000
C	-1.06541700	1.86516500	-1.81785400	-1.01546500	1.92904600	-1.80532300
O	1.98638900	3.37540000	-2.18171600	2.10486200	3.19005700	-2.16180600
O	4.14073900	0.14250500	0.00000000	4.12194300	0.05436600	0.00000000
O	1.98638900	3.37540000	2.18171600	2.10486200	3.19005700	2.16180600
O	-0.99028500	1.94827600	2.96480100	-0.96204200	2.03588400	2.96597300
O	-3.99440900	0.77584500	0.00000000	-3.99225800	0.98425800	0.00000000
O	-0.99028500	1.94827600	-2.96480100	-0.96204200	2.03588400	-2.96597300
O	-2.45178700	-0.84477800	-2.84531700	-2.45660600	-0.76688100	-2.87148600
O	1.92959200	-0.36242700	-3.13881800	1.92510600	-0.44744200	-3.18518200
O	2.47280400	-2.61350200	0.00000000	2.39588500	-2.72427700	0.00000000
O	1.92959200	-0.36242700	3.13881800	1.92510600	-0.44744200	3.18518200
O	-2.34461200	-3.01189000	0.00000000	-2.42493700	-2.94062700	0.00000000
O	-2.45178700	-0.84477800	2.84531700	-2.45660600	-0.76688100	2.87148600
C	-1.41547600	3.62459700	0.00000000	-1.26888600	3.67009500	0.00000000
O	-1.51235400	4.77329600	0.00000000	-1.32514700	4.83597200	0.00000000
C	0.11391900	-3.17042700	2.09119200	0.02238500	-3.13374800	2.09770700
C	0.11391900	-3.17042700	-2.09119200	0.02238500	-3.13374800	-2.09770700
O	0.21348400	-4.17848000	-2.63836900	0.07964800	-4.14845300	-2.66962000
O	0.21348400	-4.17848000	2.63836900	0.07964800	-4.14845300	2.66962000

Table S8. Theoretical Cartesian coordinates (in Å) for the structure **15T-2** using the B3LYP/DZP and BP86/DZP methods.

B3LYP/DZP				BP86/DZP		
Fe	0.91016200	-0.84275700	0.36766800	-1.01735300	0.26642000	0.78163300
Fe	3.30198900	0.27941800	-0.17002700	-3.34708400	-0.15493100	-0.37019900
Fe	-1.80981700	1.52173700	0.00821300	2.05023300	-1.31547000	-0.03456500
Fe	-2.36678700	-1.10331000	-0.19232500	2.26128800	1.16475500	-0.27569200
C	-0.65483900	-0.01900700	0.09861900	0.63048400	0.16664200	0.21805700
C	-0.69388200	2.93121800	-0.10999200	0.92887000	-2.25784600	-1.12186100
C	-1.76659100	-1.30318900	-1.91641100	1.32604500	2.11464800	-1.50528600
C	-1.90498100	1.50060700	-1.81904300	2.53526800	-0.23935500	-1.66428700
C	-2.00820300	-2.84874500	0.08667200	1.97751100	2.27926400	1.13045900
C	-2.84922900	-0.96834300	1.56600700	3.17855600	-0.10713500	1.03232300
C	-1.60659900	1.56325600	1.83580300	1.54323900	-2.13571000	1.50831900
C	4.12652300	-0.77876000	-1.40402300	-4.08707500	1.39528500	-0.95914800
C	4.37304800	1.67349500	0.21169000	-4.51618100	-1.43092300	-0.84975000
C	1.80726700	0.78875100	1.04628800	-2.06350700	-1.37055700	0.48537000
C	2.42051500	1.13585600	-1.51403400	-2.36063100	-0.21735000	-1.89388900
C	1.42651500	-2.20960300	-0.82980200	-1.46252700	2.01682900	0.59950800
C	0.69794400	-1.61351700	2.05269000	-0.69439500	0.21411300	2.55036200
O	1.53751600	1.67371800	1.78393300	-1.86619400	-2.51816200	0.74994000
O	5.07950900	2.55998100	0.43594400	-5.28463100	-2.25021000	-1.17012600
O	4.68743500	-1.42019400	-2.18600400	-4.60706700	2.36381800	-1.35454700
O	1.87538500	1.68205300	-2.37455300	-1.77112100	-0.24402600	-2.90196600
O	1.66386400	-3.05279600	-1.58357700	-1.65593400	3.16816200	0.48181900
O	0.51420200	-2.04846900	3.10699000	-0.43003100	0.21836000	3.69187000
O	-1.82732400	-3.97417900	0.26862200	1.80573700	3.03689600	1.99904400
O	-3.19280400	-0.97020000	2.66610500	3.96163700	-0.06461300	1.92095700
O	-1.46598600	1.65557600	2.97158700	1.25583300	-2.72450300	2.47134200
O	0.00149300	3.84391200	-0.21202400	0.25862000	-2.91801600	-1.80892000
O	-1.38765400	-1.51378100	-2.98203900	0.74540700	2.76272200	-2.28070100
O	-1.96194600	1.59149100	-2.96608100	2.83385100	-0.38238500	-2.80237100
C	3.96637300	-0.77569200	1.16002900	-4.06658100	0.16292200	1.26588700
O	4.40392700	-1.44010400	1.99715600	-4.56315200	0.37059200	2.30220800
C	-3.51604100	2.21634300	0.12472400	3.48358000	-2.39739000	-0.32443400
C	-4.12508600	-1.01206300	-0.72793100	3.89274200	1.88073600	-0.69719600
O	-5.22244200	-0.95092900	-1.07692600	4.91823100	2.36789700	-0.96112100
O	-4.59025500	2.62442900	0.21093200	4.38674200	-3.11468000	-0.49707900

Table S9. Theoretical Cartesian coordinates (in Å) for the structure **14S-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	2.12960700	-0.16704700	-0.58816900	2.12675800	-0.11438900	-0.57205800
Fe	0.32101300	0.27828200	1.34859600	0.28364200	0.27465700	1.33975900
Fe	-1.28831300	1.24120700	-0.59857900	-1.33444500	1.18380800	-0.60253800
Fe	-1.32517300	-1.31264500	-0.16753300	-1.25749100	-1.32640700	-0.18374700
C	0.15505700	0.06556700	-0.50496900	0.15769700	0.00169300	-0.53340200
C	-2.21496900	2.49234200	0.36029500	-2.12094400	2.51527000	0.33826300
C	-0.32743800	2.42217300	-1.53153400	-0.35606600	2.26057500	-1.63829600
C	-0.50683700	-2.10294000	-1.58871600	-0.48400300	-2.17380900	-1.57583000
C	-0.93904000	-2.31316200	1.25768500	-0.84470700	-2.33134100	1.22312800
C	-2.60213600	-0.13172700	0.52542700	-2.55343900	-0.05651900	0.50837900
C	0.93988500	1.91927700	1.70059900	0.67911100	1.96688600	1.73377900
C	-0.92371100	0.45355200	2.65656600	-0.88207700	0.20657700	2.70778900
C	1.47242900	-0.66592500	2.37837600	1.57363500	-0.54550000	2.27519200
C	2.46581500	1.63341600	-0.72372200	2.36969100	1.68600600	-0.55562800
C	2.28046700	-0.39405500	-2.36737900	2.26130400	-0.23585600	-2.35250200
C	2.02304600	-1.96943600	-0.23191300	2.10266700	-1.91744300	-0.28341600
O	2.19890800	-1.21496600	3.09062700	2.38494300	-1.00219900	2.98889600
O	-1.64960400	0.58191800	3.54296000	-1.57055200	0.18063900	3.65075600
O	1.31124200	2.97741300	1.98355800	0.91290500	3.05831100	2.09074000
O	2.81147500	2.72660200	-0.80850800	2.66634700	2.81254000	-0.55578900
O	2.36951400	-0.52371800	-3.50881700	2.33935700	-0.30164200	-3.51404700
O	2.07308100	-3.09536500	-0.00465500	2.21574600	-3.06151500	-0.10131900
O	-0.09666700	-2.64572900	-2.52377700	-0.08296200	-2.76013300	-2.50670500
O	-0.79028800	-3.07360100	2.12104000	-0.64772200	-3.11932300	2.07101300
O	-3.61361300	0.05218900	1.09355400	-3.56778500	0.03900400	1.12261800
O	-2.74561200	3.32115900	0.96105600	-2.60013300	3.40124000	0.92791900
O	0.20780700	3.19820200	-2.19972500	0.18561200	2.98168100	-2.38412000
C	3.82423900	-0.27157400	0.11151100	3.84886400	-0.19267300	0.01804600
O	4.88941600	-0.33945800	0.54626800	4.95648700	-0.24859000	0.37901700
C	-2.39167700	1.03256300	-1.99529100	-2.50637400	1.00874000	-1.93267500
C	-2.78210000	-2.26895600	-0.63537100	-2.75090300	-2.25435800	-0.56617300
O	-3.70430700	-2.89648200	-0.92877600	-3.70735300	-2.87530300	-0.81946700
O	-3.08680900	0.87665900	-2.90500100	-3.26574000	0.88418000	-2.81410300

Table S10. Theoretical Cartesian coordinates (in Å) for the structure **14S-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.88901400	-1.05193200	-1.28502000	-1.33494300	-0.32581200	-1.27098400
Fe	-0.88901400	1.05193200	-1.28502000	1.33494300	0.32581200	-1.27098400
Fe	0.00000000	-1.41087500	1.36159400	-1.27108600	0.60902800	1.30826400
Fe	0.00000000	1.41087500	1.36159400	1.27108600	-0.60902800	1.30826400
C	0.00000000	0.00000000	0.19968600	0.00000000	0.00000000	0.17276000
C	-1.69106000	-1.35784600	1.91163600	-0.44784200	1.40098700	2.66133800
C	1.18432600	-1.48705800	2.74167700	-2.52531600	-0.29248100	2.30798900
C	-0.18683700	-3.19606900	1.25182700	-1.86831600	2.22982600	0.85215100
C	1.69106000	1.35784600	1.91163600	0.44784200	-1.40098700	2.66133800
C	0.18683700	3.19606900	1.25182700	1.86831600	-2.22982600	0.85215100
C	-1.18432600	1.48705800	2.74167700	2.52531600	0.29248100	2.30798900
C	-2.38340000	0.03805500	-0.90142800	1.31794000	2.04046800	-0.62155000
C	-1.81892900	2.48983300	-0.70080900	2.96542300	-0.03992000	-0.55874300
C	0.59432000	2.09035900	-1.62525000	1.16217500	-1.32317900	-2.04209200
C	-0.59432000	-2.09035900	-1.62525000	-1.16217500	1.32317900	-2.04209200
C	1.81892900	-2.48983300	-0.70080900	-2.96542300	0.03992000	-0.55874300
C	2.38340000	-0.03805500	-0.90142800	-1.31794000	-2.04046800	-0.62155000
O	1.46684200	2.78934900	-1.89687200	1.23681800	-2.34737100	-2.59962200
O	-2.48039000	3.40744500	-0.47146700	4.12153700	-0.18695500	-0.42700000
O	-3.36571500	-0.51664800	-0.69472300	1.37863400	3.13340800	-0.22979700
O	-1.46684200	-2.78934900	-1.89687200	-1.23681800	2.34737100	-2.59962200
O	2.48039000	-3.40744500	-0.47146700	-4.12153700	0.18695500	-0.42700000
O	3.36571500	0.51664800	-0.69472300	-1.37863400	-3.13340800	-0.22979700
O	2.77341800	1.33742700	2.33223300	0.00000000	-2.00935700	3.56032300
O	0.33490200	4.34288300	1.17100800	2.27404800	-3.31347400	0.64658000
O	-1.82599500	1.54285700	3.70393900	3.33938400	0.81191500	2.96898600
O	-2.77341800	-1.33742700	2.33223300	0.00000000	2.00935700	3.56032300
O	1.82599500	-1.54285700	3.70393900	-3.33938400	-0.81191500	2.96898600
O	-0.33490200	-4.34288300	1.17100800	-2.27404800	3.31347400	0.64658000
C	1.28465800	-1.00545600	-3.05934400	-1.84898000	-0.96812600	-2.87447900
O	1.54422700	-0.97549800	-4.18159800	-2.19288300	-1.40836600	-3.89887500
C	-1.28465800	1.00545600	-3.05934400	1.84898000	0.96812600	-2.87447900
O	-1.54422700	0.97549800	-4.18159800	2.19288300	1.40836600	-3.89887500

Table S11. Theoretical Cartesian coordinates (in Å) for the structure **14S-3** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.97698700	-0.14219400	-1.01613500	-1.00654800	0.02460800	0.96222800
Fe	3.16793900	0.02757200	0.18206000	-3.17833400	0.03756200	-0.19938200
C	1.77061900	-1.47346800	-0.08819900	-1.87140100	-1.43827200	0.31518600
C	2.38377100	1.34406000	-0.79677800	-2.29333300	1.47680200	0.57577900
C	0.48001800	-1.08695200	-2.43535000	-0.55931500	-0.62571000	2.55687800
C	4.49392700	1.20025800	0.47680100	-4.37576200	1.27101800	-0.69250100
C	2.93427600	-0.21269400	1.95541300	-3.08168200	-0.56996200	-1.88350500
C	4.30258900	-1.22241500	-0.47453700	-4.40306700	-0.98123800	0.63680700
O	5.35009200	1.95318700	0.66330800	-5.16920100	2.06845700	-1.01351400
O	2.78489700	-0.35696500	3.09402000	-3.02973500	-0.95094300	-2.98984500
O	5.06102600	-1.99281600	-0.88581300	-5.22589800	-1.61880400	1.17209900
O	1.62031500	-2.58625900	0.28549600	-1.75696700	-2.62032900	0.16635800
O	2.12784300	2.35469200	-1.35404400	-2.08938600	2.60438900	0.92153600
O	0.16421500	-1.74465300	-3.33465300	-0.29118800	-1.09959100	3.59500800
O	-0.29232300	4.05876000	-0.45622900	0.48114300	4.07465900	-0.09996100
C	-0.77826800	3.02647300	-0.29721300	0.94148400	3.00287500	-0.07470800
Fe	-1.65622100	1.47884600	0.00247800	1.77644200	1.41713500	-0.09744800
C	-0.98276400	1.53403700	1.70350000	1.34381600	1.30354000	-1.85607700
C	-2.07061900	1.48600300	-1.78408500	2.00261900	1.59749700	1.70050300
C	-1.11328500	-1.31139200	1.91962100	0.97764700	-1.53081200	-1.76236400
C	-3.33459900	1.98096700	0.53225200	3.51369000	1.82486800	-0.46164400
O	-0.54415200	1.65277100	2.76111000	1.06779800	1.33932900	-2.98924800
Fe	-2.09094200	-1.16397400	0.36919900	2.02167700	-1.24925500	-0.29637900
O	-2.28994100	1.56556000	-2.91079100	2.13071800	1.80332700	2.84038800
O	-0.51940300	-1.48440500	2.88679500	0.32240900	-1.79718200	-2.68574400
O	-4.39245500	2.30165200	0.86069500	4.62625200	2.09475100	-0.68839800
C	-3.04955200	-1.12231900	-1.18836600	3.02065400	-1.04424200	1.20317000
C	-1.64309900	-2.87102900	-0.01026400	1.56848000	-2.88251900	0.28825800
C	-3.65985900	-1.17549300	1.34354700	3.53713500	-1.44209400	-1.30804800
O	-3.67825700	-1.17538100	-2.15107000	3.68939100	-1.01364200	2.15860900
O	-1.39388100	-3.96506100	-0.26531100	1.32402900	-3.95323300	0.67872800
O	-4.63376300	-1.17406200	1.95861000	4.49317300	-1.56236000	-1.96486700
C	-0.60907600	-0.17314800	-0.38878400	0.59162400	-0.11708000	0.36164800

Table S12. Theoretical Cartesian coordinates (in Å) for the structure **14T-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	1.94608100	-0.86340400	-0.48761800	1.93735100	-0.86390300	-0.45340200
Fe	0.86953500	1.07623100	0.90631500	0.91018200	1.09118800	0.83846900
Fe	-1.24341500	1.02872200	-0.78833500	-1.24744200	1.04769100	-0.73300100
Fe	-1.65381400	-1.20351300	0.28456300	-1.65239400	-1.20025600	0.28133700
C	0.04625100	-0.28570800	-0.26808600	0.03353900	-0.32453700	-0.19633900
C	-1.61029800	2.75793600	-0.34915500	-1.66802000	2.75983600	-0.31948900
C	-0.23614800	1.40478700	-2.22983600	-0.22253600	1.48030500	-2.13560800
C	-1.02819300	-2.79894000	-0.37078900	-1.06696000	-2.75826200	-0.43281300
C	-1.40583100	-1.58730900	2.07412700	-1.41054300	-1.66019400	2.00589400
C	-2.55847400	0.50152000	0.69003700	-2.56058600	0.50388500	0.70942300
C	1.34110400	2.80239700	0.41719600	1.27646900	2.83974900	0.50300000
C	-0.15823200	1.53091700	2.34222500	-0.08498400	1.43021500	2.28772000
C	2.34773100	0.79020700	1.87883300	2.38232300	0.75978900	1.78727300
C	2.52391300	0.65279600	-1.32461500	2.51922200	0.71598400	-1.15000300
C	1.57578600	-1.80216500	-1.97225600	1.52372500	-1.66098900	-2.00064300
C	1.64384900	-2.10122500	0.82948900	1.67152300	-2.18735300	0.77574800
O	3.28930200	0.67275100	2.54534200	3.32181600	0.63511800	2.48062300
O	-0.77557100	1.84317800	3.26800300	-0.67965200	1.68908700	3.26283100
O	1.64230100	3.88500100	0.15077700	1.52495800	3.97006100	0.33426100
O	3.04293700	1.52149000	-1.88211900	3.09959000	1.57968600	-1.69071500
O	1.33395800	-2.37505100	-2.94420000	1.25980600	-2.15685100	-3.02448800
O	1.52411200	-2.88530000	1.66575700	1.58355100	-3.04145800	1.56480300
O	-0.68692000	-3.82709400	-0.76427500	-0.74580300	-3.79854100	-0.85624300
O	-1.25222700	-1.83914800	3.18810100	-1.26909400	-1.97917300	3.12112500
O	-3.41166800	0.97996000	1.33168200	-3.43123100	0.95745700	1.37239800
O	-1.84781000	3.85654600	-0.09339800	-1.95290100	3.86503100	-0.07652400
O	0.33717100	1.65340300	-3.19893300	0.36035400	1.78816000	-3.10028700
C	3.72502700	-1.22217400	-0.23968300	3.70166400	-1.27903800	-0.32842700
O	4.84081900	-1.47407500	-0.09568300	4.82821000	-1.58088800	-0.27631300
C	-2.62217300	0.70369700	-1.90728600	-2.56675800	0.68010900	-1.88297500
C	-3.37174500	-1.84857400	0.10538900	-3.36333800	-1.81957300	0.09524400
O	-4.44525300	-2.25575800	-0.00496800	-4.44611200	-2.24272600	-0.01553600
O	-3.48533600	0.49685700	-2.64628900	-3.40706300	0.46225300	-2.66799700

Table S13. Theoretical Cartesian coordinates (in Å) for the structure **14T-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.74299200	0.67532300	0.15326100	0.80073500	-0.50415700	-0.60040400
Fe	3.32970100	0.10436100	0.02216600	3.16827400	-0.13167600	0.20793000
C	1.62747500	0.59030400	-1.46614500	1.61870000	-1.47558200	0.70777100
C	1.67497200	0.26584900	1.69629800	2.21159600	0.54532400	-1.43457700
C	0.74416200	2.42889700	0.33706800	0.65628600	-1.68997400	-1.89430900
C	4.48992700	-0.34041900	1.37610500	4.43528300	1.07736200	-0.19730800
C	3.91664400	-1.22421900	-1.12195200	3.37942200	0.13483000	1.98465800
C	4.32742000	1.52883900	-0.61843600	4.27358600	-1.52663700	-0.09296300
O	5.26106500	-0.62555900	2.19098000	5.28529700	1.84478800	-0.43801100
O	4.32164200	-2.05086600	-1.82432700	3.54748300	0.32248400	3.12820400
O	4.97382300	2.40628500	-1.00871000	5.00937600	-2.41923000	-0.27215000
O	1.75732600	0.65928900	-2.62515700	1.54449300	-2.36856500	1.49484300
O	1.82947700	0.09233300	2.84119900	2.38789200	1.26004400	-2.37097400
O	0.67263100	3.57866000	0.45511200	0.52394400	-2.51240100	-2.72107700
O	1.32784700	-3.07438100	-0.13275600	1.21307000	3.17180700	0.45020600
C	0.41612900	-2.36755700	-0.09052900	0.33912900	2.41682900	0.27046700
Fe	-1.11817900	-1.42905400	-0.03863900	-1.13539700	1.42204500	0.06249200
C	-1.05019100	-1.32132700	-1.87300400	-1.20027800	1.21476700	1.87208300
C	-1.03328800	-1.52148000	1.79864300	-0.95570100	1.52325000	-1.75704200
C	-2.55673200	1.10470000	-1.79083200	-2.03421400	-1.55096000	1.70681700
C	-2.44500800	-2.66466900	-0.10746500	-2.45343800	2.65526100	0.09386800
O	-0.96830600	-1.33595500	-3.01929700	-1.20504300	1.19393600	3.03867200
Fe	-2.82239900	0.76541100	-0.00517900	-2.69389500	-0.83845900	0.16319400
O	-0.93140000	-1.65242900	2.93529300	-0.85837900	1.69614700	-2.90572400
O	-2.40864800	1.40419000	-2.88953500	-1.63853000	-2.07137000	2.66791200
O	-3.27114100	-3.46825000	-0.14846000	-3.28570100	3.47405600	0.10362300
C	-2.99678100	0.53852800	1.80599500	-3.27329200	-0.14173700	-1.41228300
C	-3.13122800	2.52196800	0.23352200	-3.01267800	-2.48694400	-0.45646500
C	-4.46185000	-0.03208400	-0.32121500	-4.23441900	-0.29153700	0.99848400
O	-3.15198600	0.47729000	2.94328300	-3.72599600	0.21348600	-2.42667000
O	-3.31554700	3.64735200	0.39330200	-3.21933900	-3.55685900	-0.87197300
O	-5.46988800	-0.54823800	-0.52731400	-5.20102000	0.06150200	1.54592500
C	-0.93001500	0.64352900	0.12682500	-0.85881600	-0.59094500	-0.23019100

Table S14. Theoretical Cartesian coordinates (in Å) for the structure **13S-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.00000000	1.30462500	0.71546400	0.00000000	1.28413200	0.70650800
Fe	-1.80079000	0.00000000	-0.74906700	-1.80994100	0.00000000	-0.74323100
Fe	0.00000000	-1.30462500	0.71546400	0.00000000	-1.28413200	0.70650800
Fe	1.80079000	0.00000000	-0.74906700	1.80994100	0.00000000	-0.74323100
C	2.25570600	1.27817000	-1.90711000	2.28394900	1.25876400	-1.89261400
O	2.53878700	2.08852300	-2.68072800	2.59972100	2.06552200	-2.68094700
C	2.25570600	-1.27817000	-1.90711000	2.28394900	-1.25876400	-1.89261400
O	2.53878700	-2.08852300	-2.68072800	2.59972100	-2.06552200	-2.68094700
C	3.34354600	0.00000000	0.26585800	3.33840900	0.00000000	0.26723000
O	4.30999300	0.00000000	0.89557800	4.32650500	0.00000000	0.89117600
C	-2.25570600	-1.27817000	-1.90711000	-2.28394900	-1.25876400	-1.89261400
O	-2.53878700	-2.08852300	-2.68072800	-2.59972100	-2.06552200	-2.68094700
C	-3.34354600	0.00000000	0.26585800	-3.33840900	0.00000000	0.26723000
O	-4.30999300	0.00000000	0.89557800	-4.32650500	0.00000000	0.89117600
C	-2.25570600	1.27817000	-1.90711000	-2.28394900	1.25876400	-1.89261400
O	-2.53878700	2.08852300	-2.68072800	-2.59972100	2.06552200	-2.68094700
C	1.44522500	-2.01152200	1.54019500	1.43018700	-2.00172600	1.53088900
O	2.31498700	-2.53563800	2.09132400	2.30248000	-2.54363800	2.08932400
C	0.00000000	-2.67100900	-0.45582500	0.00000000	-2.65028800	-0.45229300
O	0.00000000	-3.58038100	-1.16271600	0.00000000	-3.58781100	-1.14482600
C	-1.44522500	-2.01152200	1.54019500	-1.43018700	-2.00172600	1.53088900
O	-2.31498700	-2.53563800	2.09132400	-2.30248000	-2.54363800	2.08932400
C	-1.44522500	2.01152200	1.54019500	-1.43018700	2.00172600	1.53088900
O	-2.31498700	2.53563800	2.09132400	-2.30248000	2.54363800	2.08932400
C	0.00000000	2.67100900	-0.45582500	0.00000000	2.65028800	-0.45229300
O	0.00000000	3.58038100	-1.16271600	0.00000000	3.58781100	-1.14482600
C	1.44522500	2.01152200	1.54019500	1.43018700	2.00172600	1.53088900
O	2.31498700	2.53563800	2.09132400	2.30248000	2.54363800	2.08932400
C	0.00000000	0.00000000	2.25047600	0.00000000	0.00000000	2.23592000
O	0.00000000	0.00000000	3.41642500	0.00000000	0.00000000	3.41823500
C	0.00000000	0.00000000	-0.81103600	0.00000000	0.00000000	-0.82654600

Table S15. Theoretical Cartesian coordinates (in Å) for the structure **13T-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	-0.25781300	-0.23954000	-1.33198200	-0.26288100	-0.29149500	-1.30270500
Fe	0.97217000	1.49722100	0.27153000	0.93486300	1.48820900	0.21637200
Fe	1.29105100	-1.22323600	0.51900000	1.30958600	-1.17767100	0.53914200
Fe	-2.00619300	-0.11099100	0.61645500	-2.01344800	-0.08657800	0.60838400
C	-3.01012100	1.43331700	0.94825400	-3.02140400	1.42763800	0.81598700
O	-3.60114400	2.39019300	1.19617000	-3.68159800	2.37475200	0.98668700
C	-1.95094500	-0.56077100	2.37346800	-1.99376100	-0.39115700	2.37910000
O	-1.96021800	-0.81683100	3.49843200	-2.03251500	-0.55833700	3.53474200
C	-3.32225200	-1.36274500	0.24584400	-3.26167400	-1.39104300	0.30542200
O	-4.10419800	-2.17565100	0.00555300	-4.03967200	-2.24525100	0.13625300
C	1.46145500	1.99829700	1.92739500	1.40583000	2.01740400	1.85215400
O	1.76024200	2.31500700	2.99718900	1.70373300	2.37524300	2.92609100
C	2.49656200	1.94776700	-0.68230500	2.49083800	1.87028000	-0.66924500
O	3.45730100	2.20894900	-1.26343500	3.49612900	2.12476100	-1.20698600
C	0.05681700	3.00031600	-0.10279600	0.08730800	3.00718500	-0.20414500
O	-0.55863000	3.95194800	-0.32395600	-0.45554700	4.01431700	-0.45053600
C	1.26528900	-3.03388700	0.31001100	1.23223600	-2.96600900	0.37509900
O	1.21915800	-4.17802600	0.17996100	1.17594200	-4.12950100	0.28539600
C	1.20787600	-1.32139900	2.32845700	1.19071400	-1.26925500	2.33134000
O	1.20650000	-1.38805000	3.47862700	1.16703100	-1.36327200	3.49430500
C	3.12204000	-0.95029600	0.50396000	3.10703300	-0.93716900	0.57125900
O	4.26528900	-0.80799600	0.53712800	4.26500700	-0.80697500	0.63610700
C	0.18979000	1.01535900	-2.52058100	0.21533700	0.99282700	-2.44727200
O	0.43425600	1.76142700	-3.37118700	0.45527800	1.73439200	-3.32268600
C	-2.10163100	0.40242000	-1.37227000	-2.10165000	0.28325500	-1.42335400
O	-2.90962600	0.81968700	-2.11250400	-2.93899900	0.63329600	-2.18731100
C	-0.89789800	-1.55158300	-2.41100000	-0.82038400	-1.60530200	-2.40299100
O	-1.29305300	-2.38649000	-3.10096800	-1.16568400	-2.45396400	-3.12756500
C	1.42556200	-1.09397700	-1.57437600	1.46825400	-1.11366300	-1.51056000
O	2.21290900	-1.45611900	-2.36522700	2.25830800	-1.46787900	-2.32230200
C	-0.11085400	0.09148300	0.55988500	-0.13708300	0.05889000	0.58577300

Table S16. Theoretical Cartesian coordinates (in Å) for the structure **13T-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.00000000	1.35584100	0.77123500	0.00000000	1.31177500	0.78034700
Fe	-1.79565700	0.00000000	-0.81115300	-1.81046900	0.00000000	-0.79976100
Fe	0.00000000	-1.35584100	0.77123500	0.00000000	-1.31177500	0.78034700
Fe	1.79565700	0.00000000	-0.81115300	1.81046900	0.00000000	-0.79976100
C	2.24305700	1.27736700	-1.98090100	2.26031800	1.25725000	-1.96917900
O	2.51778900	2.08280600	-2.76308500	2.56443000	2.04977700	-2.77680700
C	2.24305700	-1.27736700	-1.98090100	2.26031800	-1.25725000	-1.96917900
O	2.51778900	-2.08280600	-2.76308500	2.56443000	-2.04977700	-2.77680700
C	3.33139600	0.00000000	0.21345400	3.35167700	0.00000000	0.19325300
O	4.28166100	0.00000000	0.86903400	4.33348500	0.00000000	0.82843600
C	-2.24305700	-1.27736700	-1.98090100	-2.26031800	-1.25725000	-1.96917900
O	-2.51778900	-2.08280600	-2.76308500	-2.56443000	-2.04977700	-2.77680700
C	-3.33139600	0.00000000	0.21345400	-3.35167700	0.00000000	0.19325300
O	-4.28166100	0.00000000	0.86903400	-4.33348500	0.00000000	0.82843600
C	-2.24305700	1.27736700	-1.98090100	-2.26031800	1.25725000	-1.96917900
O	-2.51778900	2.08280600	-2.76308500	-2.56443000	2.04977700	-2.77680700
C	1.38534200	-2.11707800	1.66220400	1.36828300	-2.09539100	1.64531400
O	2.24177000	-2.62163700	2.24622800	2.22535800	-2.63695500	2.22403300
C	0.00000000	-2.71176500	-0.49392200	0.00000000	-2.63814600	-0.48654100
O	0.00000000	-3.58399200	-1.24426900	0.00000000	-3.54468200	-1.21838300
C	-1.38534200	-2.11707800	1.66220400	-1.36828300	-2.09539100	1.64531400
O	-2.24177000	-2.62163700	2.24622800	-2.22535800	-2.63695500	2.22403300
C	-1.38534200	2.11707800	1.66220400	-1.36828300	2.09539100	1.64531400
O	-2.24177000	2.62163700	2.24622800	-2.22535800	2.63695500	2.22403300
C	0.00000000	2.71176500	-0.49392200	0.00000000	2.63814600	-0.48654100
O	0.00000000	3.58399200	-1.24426900	0.00000000	3.54468200	-1.21838300
C	1.38534200	2.11707800	1.66220400	1.36828300	2.09539100	1.64531400
O	2.24177000	2.62163700	2.24622800	2.22535800	2.63695500	2.22403300
C	0.00000000	0.00000000	2.22520800	0.00000000	0.00000000	2.26045900
O	0.00000000	0.00000000	3.40431100	0.00000000	0.00000000	3.45084400
C	0.00000000	0.00000000	-0.82541300	0.00000000	0.00000000	-0.82331200

Table S17. Theoretical Cartesian coordinates (in Å) for the structure **12S-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	1.84594600	0.01986100	0.60418500	1.85977400	0.02728100	0.59812400
Fe	-1.82926000	0.00366600	0.61504200	-1.84198800	0.04434300	0.62261300
Fe	-0.04554900	1.44330200	-0.52556800	-0.03120400	1.39332500	-0.51138000
Fe	0.06871600	-1.41210900	-0.56292300	0.05747100	-1.36886500	-0.53712400
C	-1.60337900	1.55709500	-1.40032600	-1.58662800	1.40464500	-1.40127600
C	0.04083700	3.21168500	-0.22046400	0.00746100	3.17438800	-0.37105000
C	1.22295500	1.55145000	-1.76543200	1.23470800	1.39096700	-1.74961600
C	1.66982900	-1.84732400	-1.25667200	1.68654700	-1.91533500	-1.06142700
C	-0.99044900	-1.56096200	-1.99874600	-0.79481200	-1.52586400	-2.09295400
C	-0.38880000	-3.05331300	-0.02779100	-0.56654000	-2.93502100	-0.00397900
C	-2.51275800	1.43306000	1.44314100	-2.65944200	1.49516200	1.25360300
C	-3.35958700	-0.53757200	-0.23933000	-3.26864100	-0.72213100	-0.19898600
C	-1.97452000	-1.09575500	2.01066400	-1.99982900	-0.86899600	2.13522800
C	2.07669500	1.40849800	1.69797700	2.13448800	1.52076300	1.51652600
C	3.48764400	0.13834800	-0.21764300	3.52057900	0.01050400	-0.15934700
C	2.30373000	-1.24709500	1.77141100	2.26944800	-1.09100400	1.91183400
O	-2.04463000	-1.78575900	2.93340200	-2.09567900	-1.44290900	3.14897900
O	-4.31254000	-0.91580600	-0.76626300	-4.17927300	-1.25430100	-0.70015600
O	-2.92815500	2.35355500	2.00462100	-3.18427100	2.44296900	1.69677900
O	2.21202800	2.28606300	2.43690800	2.32727200	2.47813700	2.16114300
O	4.52076400	0.23422700	-0.71829000	4.60098200	0.02021400	-0.59965500
O	2.56677500	-2.05798100	2.55026500	2.51616100	-1.81070400	2.79934200
O	2.56378500	-2.30074400	-1.84353600	2.58142000	-2.50078300	-1.55310600
O	-1.62065000	-1.64931000	-2.96365600	-1.31555300	-1.62705700	-3.13568500
O	-0.67699900	-4.10151900	0.36123800	-0.96449300	-3.97243200	0.36498600
O	-2.44761500	1.80060000	-2.16316200	-2.41408700	1.61063600	-2.21462300
O	0.10171300	4.33612100	0.02906600	0.03619200	4.33667300	-0.25167900
O	1.95450800	1.65853000	-2.65870500	1.96563000	1.45312900	-2.66660600
C	0.00313000	-0.00587400	0.70084100	-0.00063800	0.00079600	0.74214000

Table S18. Theoretical Cartesian coordinates (in Å) for the structure **12S-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	-1.01913500	-1.01913500	1.01913500	-1.02324300	-1.02324300	1.02324300
Fe	1.01913500	1.01913500	1.01913500	1.02324300	1.02324300	1.02324300
Fe	1.01913500	-1.01913500	-1.01913500	1.02324300	-1.02324300	-1.02324300
Fe	-1.01913500	1.01913500	-1.01913500	-1.02324300	1.02324300	-1.02324300
C	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
C	2.16937200	-0.22110600	-2.16937200	2.16791700	-0.24310700	-2.16791700
C	2.16937200	-2.16937200	-0.22110600	2.16791700	-2.16791700	-0.24310700
C	0.22110600	-2.16937200	-2.16937200	0.24310700	-2.16791700	-2.16791700
C	-2.16937200	0.22110600	-2.16937200	-2.16791700	0.24310700	-2.16791700
C	-0.22110600	2.16937200	-2.16937200	-0.24310700	2.16791700	-2.16791700
C	-2.16937200	2.16937200	-0.22110600	-2.16791700	2.16791700	-0.24310700
C	2.16937200	0.22110600	2.16937200	2.16791700	0.24310700	2.16791700
C	2.16937200	2.16937200	0.22110600	2.16791700	2.16791700	0.24310700
C	0.22110600	2.16937200	2.16937200	0.24310700	2.16791700	2.16791700
C	-0.22110600	-2.16937200	2.16937200	-0.24310700	-2.16791700	2.16791700
C	-2.16937200	-2.16937200	0.22110600	-2.16791700	-2.16791700	0.24310700
C	-2.16937200	-0.22110600	2.16937200	-2.16791700	-0.24310700	2.16791700
O	-0.29107800	2.90086300	2.90086300	-0.24884500	2.91812500	2.91812500
O	2.90086300	2.90086300	-0.29107800	2.91812500	2.91812500	-0.24884500
O	2.90086300	-0.29107800	2.90086300	2.91812500	-0.24884500	2.91812500
O	0.29107800	-2.90086300	2.90086300	0.24884500	-2.91812500	2.91812500
O	-2.90086300	-2.90086300	-0.29107800	-2.91812500	-2.91812500	-0.24884500
O	-2.90086300	0.29107800	2.90086300	-2.91812500	0.24884500	2.91812500
O	-2.90086300	-0.29107800	-2.90086300	-2.91812500	-0.24884500	-2.91812500
O	0.29107800	2.90086300	-2.90086300	0.24884500	2.91812500	-2.91812500
O	-2.90086300	2.90086300	0.29107800	-2.91812500	2.91812500	0.24884500
O	2.90086300	0.29107800	-2.90086300	2.91812500	0.24884500	-2.91812500
O	2.90086300	-2.90086300	0.29107800	2.91812500	-2.91812500	0.24884500
O	-0.29107800	-2.90086300	-2.90086300	-0.24884500	-2.91812500	-2.91812500

Table S19. Theoretical Cartesian coordinates (in Å) for the structure **12T-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.02180400	0.66917400	1.83226100	0.01969400	0.67655100	1.83304300
Fe	0.02180400	0.66917400	-1.83226100	0.01969400	0.67655100	-1.83304300
Fe	1.39973700	-0.70585300	0.00000000	1.34004300	-0.67476800	0.00000000
Fe	-1.40474900	-0.63376000	0.00000000	-1.36460800	-0.63186700	0.00000000
C	1.53332200	-1.91879200	-1.33306600	1.52622100	-1.86637000	-1.32357900
C	3.13189400	-0.08091900	0.00000000	3.02740900	-0.05408900	0.00000000
C	1.53332200	-1.91879200	1.33306600	1.52622100	-1.86637000	1.32357900
C	-1.82789600	-1.77602900	1.33771100	-1.66179300	-1.81233300	1.31521500
C	-1.82789600	-1.77602900	-1.33771100	-1.66179300	-1.81233300	-1.31521500
C	-2.93665000	0.29437900	0.00000000	-2.98406000	0.13476700	0.00000000
C	1.56298600	0.85249800	-2.74777400	1.44335900	0.60233700	-2.93554300
C	-0.99918900	0.21074800	-3.29658700	-1.26253600	0.46398800	-3.09458400
C	-0.37452800	2.43940200	-1.79988000	-0.07110200	2.45398400	-1.80723500
C	1.56298600	0.85249800	2.74777400	1.44335900	0.60233700	2.93554300
C	-0.99918900	0.21074800	3.29658700	-1.26253600	0.46398800	3.09458400
C	-0.37452800	2.43940200	1.79988000	-0.07110200	2.45398400	1.80723500
O	-0.63755300	3.56182300	-1.75000800	-0.12780200	3.62232700	-1.79453000
O	-1.62505000	-0.02439600	-4.23665800	-2.08473800	0.38669200	-3.92204800
O	2.53664100	0.98902700	-3.35619600	2.35831800	0.60394700	-3.66431800
O	2.53664100	0.98902700	3.35619600	2.35831800	0.60394700	3.66431800
O	-1.62505000	-0.02439600	4.23665800	-2.08473800	0.38669200	3.92204800
O	-0.63755300	3.56182300	1.75000800	-0.12780200	3.62232700	1.79453000
O	-2.12706900	-2.55863200	2.13349200	-1.89089100	-2.62976500	2.12174300
O	-2.12706900	-2.55863200	-2.13349200	-1.89089100	-2.62976500	-2.12174300
O	-3.90375100	0.92495000	0.00000000	-4.04064600	0.63564300	0.00000000
O	1.63328900	-2.71410800	-2.16677500	1.67900300	-2.68812100	-2.14406700
O	4.21449300	0.31355400	0.00000000	4.12792300	0.33997000	0.00000000
O	1.63328900	-2.71410800	2.16677500	1.67900300	-2.68812100	2.14406700
C	0.01977700	0.51512800	0.00000000	0.00405100	0.61372000	0.00000000

Table S20. Theoretical Cartesian coordinates (in Å) for the structure **11S-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	1.89153900	0.27030900	0.41561500	-1.87380800	-0.34901200	0.47145100
Fe	-1.71639800	0.12442100	0.72114500	1.80406400	-0.35214000	0.60575200
Fe	-0.09918600	1.02029800	-1.03090700	-0.02620700	-0.85538700	-1.13733600
Fe	0.10505600	-1.49170400	-0.23564900	0.04064000	1.43265800	-0.14504300
C	-1.64768500	1.28911600	-1.90862300	1.24098500	-1.88000400	-1.84866600
C	0.31819200	2.75612600	-0.92508400	-1.65354200	-1.74670700	-1.17584200
C	1.53751500	-2.60253900	-0.31634900	-1.18444400	2.71827600	-0.45036000
C	-1.32261200	-2.60781700	-0.32804900	1.47334000	2.49640200	-0.17275300
C	-2.08756200	1.67712700	1.51937400	2.19648100	-1.93145500	1.32986800
C	-3.37629300	-0.18912700	-0.02779800	3.35153600	-0.05171900	-0.33819700
C	-1.93484100	-0.84822900	2.20494400	2.23263400	0.51743300	2.08221900
C	2.27063200	1.78686100	1.26949000	-2.43111100	-1.77761300	1.39388000
C	3.09686700	0.38614400	-0.94978900	-3.39762100	0.19889500	-0.37963200
C	2.81277300	-0.73791300	1.58463200	-2.10309900	0.74204800	1.86931300
O	-2.04725600	-1.46092500	3.17789100	2.49869400	1.08357300	3.07204600
O	-4.41981300	-0.41355900	-0.46323600	4.33732700	0.14257900	-0.93128100
O	-2.28226900	2.69360900	2.03067400	2.42510600	-2.96455200	1.82739800
O	2.49189600	2.76196000	1.85014300	-2.78710700	-2.68855100	2.03347200
O	3.81639600	0.48483700	-1.85054400	-4.36471100	0.56675100	-0.91883200
O	3.39164200	-1.36602600	2.36477200	-2.26270800	1.42489100	2.80505000
O	2.39912600	-3.36572400	-0.41454000	-1.95425200	3.57066400	-0.67065600
O	-2.17836500	-3.37947200	-0.42426600	2.36658800	3.25361400	-0.22782300
O	-2.59890600	1.55719900	-2.51294300	2.05184900	-2.59475700	-2.30868400
O	0.57060200	3.87892000	-0.82942200	-2.39031900	-2.48621600	-1.73670800
C	0.11474000	0.23825100	0.67177400	-0.01353100	-0.34228100	0.62972400
C	0.18200200	-1.17972300	-1.96810900	0.23078700	0.90586100	-1.90201100
O	0.29586800	-1.11783300	-3.12650300	0.30248100	1.20776700	-3.05531600

Table S21. Theoretical Cartesian coordinates (in Å) for the structure **11S-2** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	0.15227000	0.58446100	1.82613600	0.23402600	0.54999000	1.84271400
Fe	0.15227000	0.58446100	-1.82613600	0.23402600	0.54999000	-1.84271400
Fe	1.11477600	-0.98083800	0.00000000	1.02088700	-1.03418700	0.00000000
Fe	-1.41583200	-0.42735700	0.00000000	-1.39836300	-0.29473100	0.00000000
C	2.17820900	-1.18912700	-1.42651600	2.04968900	-1.31307000	-1.44463300
C	2.17820900	-1.18912700	1.42651600	2.04968900	-1.31307000	1.44463300
C	-2.53673100	-0.69922500	1.39046600	-2.55517100	-0.53223000	1.35254100
C	-2.53673100	-0.69922500	-1.39046600	-2.55517100	-0.53223000	-1.35254100
C	1.54876100	1.60911100	-2.28619700	1.65585500	1.50520500	-2.34487700
C	-0.01953700	-0.42288400	-3.36121700	-0.06816300	-0.41737700	-3.37052500
C	-1.03714000	1.85767200	-2.20119700	-0.87320900	1.88557000	-2.19653200
C	1.54876100	1.60911100	2.28619700	1.65585500	1.50520500	2.34487700
C	-0.01953700	-0.42288400	3.36121700	-0.06816300	-0.41737700	3.37052500
C	-1.03714000	1.85767200	2.20119700	-0.87320900	1.88557000	2.19653200
O	-1.79546100	2.70159100	-2.42149100	-1.58922900	2.78323200	-2.42504000
O	-0.13549400	-1.06970400	-4.30861900	-0.26969100	-1.02841100	-4.34449400
O	2.43675900	2.29749700	-2.54928500	2.56569600	2.17016800	-2.65652700
O	2.43675900	2.29749700	2.54928500	2.56569600	2.17016800	2.65652700
O	-0.13549400	-1.06970400	4.30861900	-0.26969100	-1.02841100	4.34449400
O	-1.79546100	2.70159100	2.42149100	-1.58922900	2.78323200	2.42504000
O	-3.29852500	-0.91898800	2.23180400	-3.35054200	-0.72730300	2.18935100
O	-3.29852500	-0.91898800	-2.23180400	-3.35054200	-0.72730300	-2.18935100
O	2.98612000	-1.41414200	-2.22957900	2.84305300	-1.60950600	-2.26038300
O	2.98612000	-1.41414200	2.22957900	2.84305300	-1.60950600	2.26038300
C	0.22865100	0.67305100	0.00000000	0.29780600	0.65954000	0.00000000
C	-0.67211500	-2.02713000	0.00000000	-0.72362400	-1.95765600	0.00000000
O	-0.26586600	-3.13263000	0.00000000	-0.68708000	-3.15087100	0.00000000

Table S22. Theoretical Cartesian coordinates (in Å) for the structure **11T-1** using the B3LYP/DZP and BP86/DZP methods.

	B3LYP/DZP			BP86/DZP		
Fe	-1.81483400	-0.07668300	0.60193300	0.16895400	0.62153000	1.81736200
Fe	1.79999200	-0.08088100	0.61653900	0.16895400	0.62153000	-1.81736200
Fe	0.01366100	-1.35247800	-0.77491200	1.05936700	-0.96750100	0.00000000
Fe	-0.05539700	1.30445000	-0.68949900	-1.39070400	-0.45742000	0.00000000
C	1.53853700	-2.41068600	-1.08974400	2.20251700	-1.32092100	-1.38767900
C	-1.32208600	-2.62416800	-1.20180000	2.20251700	-1.32092100	1.38767900
C	-1.61684900	1.65720400	-1.49693500	-2.54086900	-0.68435100	1.35796700
C	0.34468400	3.00650400	-0.30111000	-2.54086900	-0.68435100	-1.35796700
C	2.25396300	-1.38669700	1.74765500	1.58398800	1.60108000	-2.26498100
C	3.35621900	0.03420400	-0.35820500	-0.00593600	-0.34502300	-3.35911200
C	2.14049700	1.24123300	1.76177600	-0.98734300	1.90624700	-2.20267400
C	-2.03456000	-1.35889900	1.82213000	1.58398800	1.60108000	2.26498100
C	-3.39777700	-0.30024600	-0.30045600	-0.00593600	-0.34502300	3.35911200
C	-2.33408300	1.27295900	1.64441600	-0.98734300	1.90624700	2.20267400
O	2.32502800	2.09082800	2.52280400	-1.72642800	2.78213300	-2.44139800
O	4.32817600	0.12012500	-0.97525100	-0.12812300	-0.96863000	-4.34006900
O	2.51405900	-2.21942900	2.50656600	2.50030500	2.27684300	-2.53625100
O	-2.14981200	-2.17072900	2.63678500	2.50030500	2.27684300	2.53625100
O	-4.38821900	-0.47621000	-0.86665500	-0.12812300	-0.96863000	4.34006900
O	-2.63030600	2.14960600	2.33649400	-1.72642800	2.78213300	2.44139800
O	-2.50957800	2.00005500	-2.15636100	-3.32266400	-0.88793100	2.20515700
O	0.60070800	4.09307600	-0.00685300	-3.32266400	-0.88793100	-2.20515700
O	2.41397100	-3.10852900	-1.37148900	2.98225800	-1.61918400	-2.20695300
O	-2.10805700	-3.41892400	-1.47948400	2.98225800	-1.61918400	2.20695300
C	-0.00010900	0.00478500	0.68811400	0.14640800	0.71503100	0.00000000
C	1.09100700	1.29841200	-2.05538900	-0.75345000	-2.10019500	0.00000000
O	1.77332700	1.28235300	-2.99259100	-0.55530800	-3.27209200	0.00000000

Table S23. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **16S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
15.8 (0.0), 25.2 (0.0), 46.3 (0.1), 46.3 (0.1), 54.5 (0.0), 54.7 (0.1), 54.7 (0.1), 58.8 (0.0), 76.4 (0.0), 81.7 (0.1), 81.7 (0.1), 82.2 (0.0), 83.1 (0.0), 87.4 (0.3), 87.4 (0.3), 90.3 (0.0), 91.9 (0.0), 98.5 (0.5), 98.5 (0.5), 102.9 (0.0), 106.5 (0.0), 107.4 (0.0), 107.9 (0.0), 112.2 (0.7), 112.2 (0.7), 114.3 (0.1), 114.3 (0.1), 114.5 (0.0), 120.9 (0.0), 140.5 (1.4), 140.5 (1.4), 140.9 (0.1), 142.5 (0.0), 144.6 (0.7), 144.6 (0.7), 151.5 (0.0), 196.9 (0.6), 203.7 (0.0), 337.2 (42.1), 337.2 (42.1), 389.6 (0.0), 394.6 (0.0), 395.7 (2.2), 396.8 (2.1), 396.8 (2.1), 399.7 (0.0), 404.8 (20.1), 404.8 (20.1), 413.8 (0.2), 413.8 (0.2), 418.0 (7.5), 418.2 (0.0), 419.9 (0.0), 420.1 (0.0), 438.5 (2.8), 438.5 (2.8), 446.0 (7.9), 446.0 (7.9), 452.3 (25.3), 455.6 (0.0), 476.7 (21.4), 476.7 (21.4), 478.5 (9.2), 481.8 (0.0), 495.7 (16.2), 495.7 (16.2), 506.0 (0.0), 510.2 (0.0), 510.9 (0.6), 513.5 (0.0), 534.5 (37.0), 534.5 (37.0), 554.5 (0.0), 561.9 (0.0), 565.3 (37.8), 565.3 (37.8), 569.4 (11.5), 593.1 (0.0), 600.8 (34.4), 600.8 (34.4), 602.8 (0.0), 639.0 (479.5), 641.4 (210.9), 641.4 (210.9), 646.1 (0.0), 646.3 (105.3), 646.3 (105.3), 654.6 (0.0), 679.0 (141.9) , 2054.8 (0.3), 2054.8 (0.3), 2055.5 (0.0), 2062.8 (0.0), 2066.0 (0.0), 2071.5 (36.7), 2071.5 (36.7), 2071.9 (853.2), 2083.8 (157.8), 2083.8 (157.8), 2093.7 (0.0), 2097.8 (934.7), 2111.1 (3287.2), 2111.1 (3287.2), 2132.9 (1479.4), 2173.5 (0.0)	10.6 (0.0), 14.0 (0.0), 41.2 (0.0), 41.2 (0.0), 50.4 (0.0), 52.1 (0.1), 52.1 (0.1), 55.7 (0.0), 68.9 (0.0), 76.1 (0.0), 78.0 (0.0), 79.0 (0.0), 79.0 (0.0), 83.4 (0.0), 83.4 (0.0), 86.2 (0.0), 89.0 (0.0), 93.9 (0.2), 93.9 (0.2), 99.2 (0.1), 101.4 (0.0), 102.2 (0.0), 103.5 (0.0), 107.6 (0.4), 107.6 (0.4), 109.1 (0.0), 109.2 (0.3), 109.2 (0.3), 115.5 (0.0), 134.2 (0.2), 136.3 (0.0), 137.6 (0.0), 137.6 (0.0), 140.8 (0.9), 140.8 (0.9), 150.5 (0.0), 198.9 (0.1), 205.8 (0.0), 346.5 (24.9), 346.5 (24.9), 386.8 (0.2), 387.8 (0.0), 389.7 (1.3), 389.7 (1.3), 391.2 (0.0), 392.6 (0.0), 406.8 (9.5), 406.8 (9.5), 417.7 (0.0), 420.1 (0.0), 434.4 (2.7), 434.4 (2.7), 439.9 (4.7), 440.9 (0.0), 443.3 (7.3), 443.3 (7.3), 455.2 (6.7), 455.2 (6.7), 462.3 (6.9), 464.2 (0.0), 480.1 (0.0), 484.6 (2.4), 484.9 (11.0), 484.9 (11.0), 495.0 (0.1), 495.0 (0.1), 507.8 (1.8), 509.1 (0.0), 522.8 (0.0), 523.8 (0.0), 536.2 (4.7), 536.2 (4.7), 540.9 (0.0), 546.8 (0.0), 553.9 (32.7), 553.9 (32.7), 566.9 (35.1), 581.7 (0.0), 587.7 (67.1), 587.7 (67.1), 594.0 (0.0), 630.9 (399.3), 633.3 (151.0), 633.3 (151.0), 641.6 (0.0), 645.9 (137.7), 645.9 (137.7), 646.2 (0.0), 675.4 (204.5), 1968.3 (0.0), 1975.1 (6.2), 1975.1 (6.2), 1978.1 (0.0), 1983.8 (0.0), 1991.1 (2.9), 1991.1 (2.9), 1993.8 (928.1), 2002.7 (770.7), 2002.7 (770.7), 2012.2 (0.0), 2015.7 (700.0), 2035.2 (1975.5), 2035.2 (1975.5), 2055.0 (1074.2), 2088.0 (0.0)

Table S24. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **16S-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
16.2 (0.0), 35.8 (0.0), 37.8 (0.1), 43.9 (0.1), 44.9 (0.0), 55.0 (0.2), 59.5 (0.1), 60.5 (0.0), 66.4 (0.0), 70.3 (0.0), 71.4 (0.2), 72.5 (0.1), 76.5 (0.0), 85.3 (0.0), 86.9 (0.5), 87.1 (0.1), 90.5 (0.1), 94.5 (0.0), 95.1 (0.0), 97.1 (0.5), 98.4 (0.1), 108.0 (0.7), 108.1 (0.0), 108.2 (0.1), 114.5 (0.0), 122.5 (0.0), 135.6 (0.0), 137.6 (0.2), 139.5 (2.5), 139.9 (0.0), 142.3 (0.1), 143.6 (0.0), 154.6 (0.1), 157.0 (0.0), 193.8 (0.0), 210.8 (0.0), 229.5 (0.5), 253.2 (0.1), 313.4 (0.2), 329.3 (0.0), 354.8 (36.2), 388.0 (0.0), 389.5 (0.7), 394.3 (0.0), 399.2 (0.6), 404.4 (0.2), 405.7 (2.0), 408.7 (4.7), 413.2 (0.2), 415.4 (0.0), 424.4 (11.6), 426.3 (0.4), 428.2 (0.0), 430.2 (1.1), 436.9 (8.5), 437.3 (0.3), 441.5 (87.4), 446.4 (2.0), 447.0 (1.4), 448.7 (46.5), 464.1 (0.0), 472.8 (12.6), 473.5 (11.3), 482.1 (2.2), 490.1 (0.9), 498.5 (23.5), 499.3 (8.3), 506.7 (0.0), 509.8 (0.1), 520.9 (8.6), 522.0 (0.0), 546.8 (38.6), 557.4 (0.8), 567.6 (58.4), 568.9 (0.0), 569.1 (3.8), 585.8 (0.0), 592.3 (111.4), 595.4 (0.0), 598.4 (30.3), 613.1 (90.7), 629.3 (0.0), 633.1 (133.8), 636.0 (193.2), 642.1 (391.7), 646.0 (8.0), 651.1 (86.1), 667.9 (66.5), 669.8 (488.8), 1906.1 (612.4), 1939.5 (207.9), 2057.5 (0.0), 2062.9 (42.4), 2074.4 (63.7), 2076.7 (1463.9), 2077.4 (281.3), 2081.6 (22.9), 2087.0 (0.0), 2089.0 (214.9), 2094.1 (35.6), 2095.8 (76.9), 2115.0 (2524.9), 2117.4 (3231.0), 2129.3 (1793.5), 2173.2 (18.8)	15.7 (0.0), 31.0 (0.0), 33.7 (0.1), 41.8 (0.0), 44.1 (0.0), 52.8 (0.1), 56.3 (0.1), 58.6 (0.0), 61.8 (0.0), 68.3 (0.0), 69.6 (0.1), 71.3 (0.0), 73.0 (0.0), 83.1 (0.0), 83.7 (0.3), 84.0 (0.0), 87.0 (0.1), 91.7 (0.0), 93.1 (0.3), 93.6 (0.0), 97.2 (0.0), 103.5 (0.0), 104.0 (0.0), 104.6 (0.2), 109.3 (0.0), 126.9 (0.0), 131.2 (0.0), 132.8 (0.2), 134.4 (0.0), 134.6 (0.7), 140.4 (0.6), 140.9 (0.0), 148.5 (0.1), 152.2 (0.1), 189.8 (0.0), 212.0 (0.1), 225.9 (1.3), 250.4 (0.0), 309.8 (0.5), 328.9 (0.0), 356.8 (23.9), 390.5 (0.1), 391.3 (0.7), 393.6 (0.0), 396.3 (1.0), 398.5 (0.7), 400.6 (0.2), 417.4 (0.0), 419.8 (2.9), 420.8 (0.0), 421.6 (5.6), 425.9 (0.5), 432.1 (3.5), 433.5 (0.5), 441.6 (0.3), 447.3 (1.5), 456.5 (27.9), 456.8 (10.1), 462.6 (0.0), 465.4 (4.6), 467.0 (13.4), 468.9 (11.0), 479.6 (4.8), 489.6 (0.5), 491.2 (6.3), 497.3 (7.6), 502.6 (1.4), 508.0 (7.8), 515.3 (0.0), 515.7 (0.2), 520.4 (0.0), 533.5 (17.8), 544.4 (0.0), 549.6 (0.0), 550.3 (1.7), 564.0 (86.5), 567.5 (1.3), 579.3 (52.0), 587.1 (0.0), 594.6 (45.5), 608.1 (61.5), 615.4 (0.0), 624.8 (271.2), 629.2 (12.1), 637.3 (234.4), 641.8 (91.5), 643.9 (136.4), 653.0 (558.2), 663.5 (132.7), 1859.3 (453.9), 1878.7 (134.2), 1969.1 (0.0), 1983.4 (87.8), 1987.9 (136.4), 1994.9 (1567.7), 1997.4 (517.1), 1999.0 (0.7), 1999.5 (0.0), 2003.4 (5.0), 2007.7 (286.4), 2011.7 (24.7), 2033.4 (2320.5), 2039.7 (1674.1), 2048.0 (1257.3), 2085.5 (47.0)

Table S25. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **16S-3** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-28.1 (0.0), -16.7 (0.0), -16.7 (0.0), 26.1 (0.0), 47.5 (0.4), 54.1 (0.0), 54.5 (0.0), 54.5 (0.0), 62.5 (0.0), 62.5 (0.0), 68.7 (0.0), 78.6 (0.2), 78.6 (0.2), 80.2 (0.0), 84.8 (0.0), 86.7 (0.0), 86.7 (0.0), 89.9 (0.5), 89.9 (0.5), 92.2 (0.0), 92.2 (0.0), 99.6 (0.0), 99.8 (0.0), 99.8 (0.0), 107.7 (0.9), 128.0 (0.0), 128.0 (0.0), 146.2 (0.0), 160.5 (0.0), 169.6 (0.2), 169.6 (0.2), 169.7 (0.0), 181.2 (0.0), 196.7 (0.0), 225.1 (0.9), 225.1 (0.9), 240.8 (0.0), 245.9 (0.0), 304.7 (0.0), 304.7 (0.0), 318.6 (0.0), 323.9 (0.0), 387.7 (4.3), 390.9 (0.9), 390.9 (0.9), 392.6 (0.0), 407.1 (1.2), 407.1 (1.2), 413.8 (0.0), 418.7 (0.0), 422.0 (4.4), 427.3 (0.0), 427.3 (0.0), 429.9 (0.0), 431.0 (1.9), 431.0 (1.9), 432.9 (89.5), 436.8 (0.0), 439.7 (0.0), 446.8 (0.0), 447.5 (51.3), 447.5 (51.3), 490.1 (7.3), 494.1 (0.1), 494.1 (0.1), 502.0 (0.0), 513.2 (9.5), 513.2 (9.5), 517.5 (0.0), 528.7 (0.0), 546.3 (71.5), 548.2 (0.0), 549.3 (6.1), 549.3 (6.1), 567.8 (2.4), 567.8 (2.4), 581.1 (30.4), 595.8 (57.4), 595.8 (57.4), 615.2 (11.4), 615.2 (11.4), 620.3 (0.0), 629.1 (0.0), 633.9 (0.0), 635.1 (366.0), 645.0 (0.0), 657.9 (106.7), 660.4 (576.3), 660.4 (576.3), 1903.4 (739.8), 1903.4 (739.8), 1940.7 (0.0), 1941.6 (308.7), 2072.2 (0.0), 2075.8 (5.9), 2075.8 (5.9), 2085.1 (1156.6), 2094.6 (17.2), 2094.6 (17.2), 2098.1 (0.0), 2105.9 (0.0), 2122.7 (2948.7), 2122.7 (2948.7), 2126.3 (2302.3), 2171.9 (0.0)	-25.2 (0.0), -18.4 (0.0), -18.4 (0.0), 30.5 (0.0), 46.4 (0.1), 52.6 (0.0), 52.6 (0.0), 59.2 (0.0), 60.7 (0.0), 65.3 (0.0), 66.7 (0.0), 76.2 (0.2), 76.2 (0.2), 82.7 (0.0), 83.3 (0.0), 83.3 (0.0), 84.9 (0.0), 86.5 (0.3), 86.5 (0.3), 88.7 (0.0), 90.1 (0.0), 96.0 (0.0), 96.0 (0.0), 104.2 (0.2), 105.0 (0.0), 130.3 (0.0), 130.3 (0.0), 145.9 (0.0), 151.1 (0.0), 159.7 (0.3), 159.7 (0.3), 160.6 (0.0), 179.8 (0.0), 193.6 (0.0), 220.1 (1.6), 220.1 (1.6), 239.3 (0.3), 243.9 (0.0), 298.4 (0.2), 298.4 (0.2), 321.9 (0.0), 325.6 (0.0), 389.5 (4.8), 394.4 (0.8), 394.4 (0.8), 394.6 (0.0), 403.4 (1.4), 403.4 (1.4), 408.5 (0.0), 410.7 (0.0), 414.2 (5.7), 421.6 (0.0), 426.8 (0.0), 426.8 (0.0), 437.7 (1.8), 437.7 (1.8), 441.3 (0.0), 447.1 (0.0), 450.0 (41.3), 452.2 (0.0), 463.0 (17.0), 463.0 (17.0), 492.7 (0.0), 492.7 (0.0), 503.8 (6.7), 505.9 (3.8), 505.9 (3.8), 507.8 (0.0), 510.0 (0.0), 516.6 (0.0), 535.1 (47.2), 537.7 (0.0), 538.1 (6.7), 538.1 (6.7), 554.0 (0.5), 554.0 (0.5), 569.6 (40.1), 579.4 (24.2), 579.4 (24.2), 606.9 (0.5), 606.9 (0.5), 613.2 (0.0), 614.7 (0.0), 620.7 (0.0), 624.8 (338.1), 633.1 (0.0), 647.3 (621.1), 647.3 (621.1), 650.6 (183.3), 1859.9 (545.8), 1859.9 (545.8), 1880.3 (0.0), 1882.2 (204.0), 1985.7 (0.0), 1989.0 (13.5), 1989.0 (13.5), 1997.3 (1191.4), 2007.7 (108.9), 2007.7 (108.9), 2009.0 (0.0), 2016.6 (0.0), 2038.1 (2259.9), 2038.1 (2259.9), 2043.6 (1625.6), 2079.7 (0.0)

Table S26. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
20.2 (0.1), 25.1 (0.5), 33.5 (0.0), 45.8 (0.1), 48.7 (0.4), 52.7 (0.6), 62.5 (0.2), 64.6 (0.0), 70.2 (0.0), 75.1 (0.1), 77.6 (0.2), 83.1 (0.2), 84.0 (0.1), 84.8 (0.2), 89.4 (0.5), 94.4 (0.1), 96.3 (0.2), 97.4 (0.1), 98.5 (0.6), 101.6 (0.3), 106.7 (0.1), 111.0 (1.0), 112.2 (0.3), 114.7 (0.1), 118.8 (0.1), 122.0 (0.6), 123.6 (0.1), 126.5 (0.8), 130.6 (0.5), 135.3 (0.4), 142.9 (1.3), 148.7 (0.2), 157.5 (0.7), 167.1 (2.6), 197.2 (0.8), 216.5 (4.2), 340.2 (8.9), 371.0 (1.8), 377.5 (4.5), 378.7 (24.1), 385.4 (11.2), 392.7 (17.6), 397.4 (4.9), 403.2 (4.5), 405.2 (3.5), 409.6 (4.3), 413.2 (0.3), 414.0 (0.4), 417.3 (3.5), 419.9 (4.2), 423.4 (7.2), 435.1 (6.5), 439.3 (7.7), 448.4 (17.3), 454.7 (18.3), 464.1 (20.8), 467.4 (1.5), 467.9 (5.1), 470.6 (7.2), 481.7 (5.2), 496.1 (0.5), 497.6 (8.4), 505.3 (8.3), 511.4 (1.8), 514.5 (1.6), 519.9 (10.3), 525.6 (6.8), 537.8 (5.0), 553.6 (9.6), 560.7 (3.4), 566.6 (5.6), 577.0 (43.0), 584.3 (131.8), 585.6 (14.0), 594.4 (24.9), 599.8 (8.2), 610.0 (253.5), 619.4 (239.9), 626.6 (134.8), 635.9 (348.0), 636.9 (16.0), 647.2 (5.9), 658.6 (45.4), 756.6 (226.6), 2026.8 (92.5), 2035.6 (177.1), 2045.7 (266.4), 2056.2 (245.8), 2059.6 (200.2), 2068.5 (473.6), 2070.0 (205.5), 2080.8 (211.3), 2086.0 (102.4), 2090.1 (380.0), 2102.4 (1690.1), 2106.7 (2003.3), 2120.4 (2244.6), 2121.6 (1842.8), 2172.4 (87.6)	28.1 (1.2), 41.5 (0.0), 44.7 (0.4), 52.9 (0.0), 53.3 (0.5), 57.4 (0.0), 58.8 (1.7), 61.1 (0.0), 72.3 (0.5), 74.5 (0.0), 75.3 (0.0), 79.0 (0.0), 81.0 (0.2), 81.0 (0.0), 87.0 (0.5), 87.8 (0.1), 90.1 (0.0), 90.3 (0.5), 92.0 (0.0), 96.6 (0.0), 99.3 (0.1), 101.5 (0.1), 103.5 (1.6), 114.5 (0.1), 121.2 (0.0), 122.6 (0.6), 136.7 (1.6), 155.5 (0.1), 162.4 (2.5), 166.7 (0.0), 192.7 (0.1), 194.8 (19.6), 210.0 (8.3), 234.9 (6.5), 259.9 (22.1), 260.0 (0.2), 298.6 (7.1), 318.0 (2.1), 322.3 (0.4), 355.5 (35.8), 372.9 (1.1), 375.1 (2.7), 377.1 (1.4), 396.4 (1.8), 402.7 (6.0), 404.6 (4.9), 408.2 (3.2), 409.4 (6.9), 425.0 (0.0), 428.9 (1.5), 429.1 (0.6), 442.2 (0.2), 442.9 (12.8), 448.8 (2.2), 456.2 (0.1), 456.9 (17.4), 456.9 (0.2), 459.4 (24.3), 461.6 (30.9), 472.7 (5.1), 473.2 (14.0), 486.2 (2.4), 488.4 (2.7), 495.0 (2.3), 498.6 (0.2), 504.8 (10.5), 511.6 (6.7), 516.7 (3.6), 525.3 (4.3), 545.3 (11.0), 556.3 (5.2), 557.5 (59.0), 573.6 (30.9), 591.9 (3.4), 598.5 (0.0), 600.7 (24.8), 605.9 (257.3), 607.0 (19.3), 613.3 (3.3), 619.4 (9.5), 621.0 (39.1), 646.5 (367.1), 690.6 (588.5), 734.9 (359.1), 1865.1 (109.7), 1868.7 (638.2), 1875.7 (309.0), 1891.3 (484.7), 1898.9 (151.0), 1996.4 (30.4), 1999.7 (8.4), 2003.1 (849.7), 2007.7 (18.7), 2015.2 (514.9), 2015.2 (27.9), 2031.1 (1656.8), 2035.4 (2090.8), 2043.3 (1685.6), 2077.4 (49.2)

Table S27. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15S-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
11.2 (0.0), 18.0 (0.0), 23.4 (0.2), 28.9 (0.0), 38.5 (0.0), 42.3 (0.1), 49.5 (0.0), 53.6 (0.1), 57.9 (0.3), 64.9 (0.1), 68.5 (0.0), 69.2 (0.0), 73.4 (0.3), 75.6 (0.0), 78.9 (0.0), 83.1 (0.3), 86.4 (0.1), 87.4 (0.1), 92.4 (0.1), 93.6 (0.1), 95.5 (0.1), 99.3 (0.0), 101.6 (0.1), 104.0 (0.7), 106.6 (0.1), 111.1 (1.0), 111.6 (0.6), 117.7 (0.8), 125.2 (0.0), 128.0 (0.9), 135.0 (0.1), 145.9 (3.1), 154.8 (3.2), 186.7 (0.1), 237.5 (12.3), 283.2 (4.8), 316.5 (7.6), 359.5 (80.6), 371.5 (8.1), 380.2 (7.2), 384.7 (0.7), 387.2 (1.9), 392.0 (23.8), 393.0 (14.1), 398.4 (19.9), 401.1 (0.9), 403.3 (2.2), 406.5 (17.5), 412.4 (2.7), 418.8 (55.0), 423.0 (4.0), 427.5 (6.0), 433.0 (33.8), 441.5 (39.3), 447.4 (38.7), 457.6 (17.5), 465.6 (51.0), 469.0 (5.3), 472.4 (8.7), 475.4 (26.6), 481.9 (26.6), 484.7 (12.1), 489.3 (0.9), 493.7 (2.7), 503.1 (11.9), 509.3 (17.8), 524.1 (51.0), 533.6 (139.6), 551.2 (2.1), 556.4 (21.3), 563.7 (70.5), 565.1 (7.6), 571.6 (27.1), 589.2 (31.7), 594.0 (20.9), 602.8 (74.8), 618.4 (170.9), 623.2 (114.2), 631.1 (199.9), 633.3 (294.0), 643.0 (67.6), 652.9 (65.2), 657.1 (141.7), 976.3 (248.1), 1879.6 (317.5), 2027.4 (74.1), 2045.6 (125.5), 2060.2 (670.4), 2068.7 (1020.5), 2077.6 (35.8), 2081.2 (511.7), 2089.5 (101.1), 2095.3 (186.7), 2101.5 (1004.8), 2112.0 (819.8), 2120.1 (2306.1), 2124.1 (1372.3), 2133.3 (1648.5), 2177.5 (181.4)	14.6 (0.0), 20.8 (0.2), 24.0 (0.1), 27.1 (0.0), 31.3 (0.0), 39.0 (0.1), 48.6 (0.0), 50.7 (0.1), 59.4 (0.2), 62.4 (0.2), 65.5 (0.1), 66.2 (0.1), 70.8 (0.1), 73.8 (0.0), 75.5 (0.0), 79.2 (0.2), 83.9 (0.1), 84.6 (0.1), 89.4 (0.0), 90.9 (0.3), 91.9 (0.1), 97.2 (0.5), 98.7 (0.1), 100.1 (0.3), 104.3 (0.1), 106.2 (0.4), 107.5 (0.4), 112.3 (0.3), 117.5 (0.1), 118.7 (0.5), 126.3 (0.2), 143.7 (5.4), 151.3 (1.0), 188.7 (0.2), 237.0 (3.3), 283.4 (8.0), 306.3 (1.4), 362.3 (22.2), 372.5 (2.3), 373.8 (4.5), 379.5 (6.7), 382.2 (16.4), 386.3 (16.7), 388.1 (0.6), 389.9 (1.0), 397.8 (8.1), 406.1 (6.7), 414.3 (9.0), 419.9 (5.8), 428.9 (5.5), 434.0 (5.3), 443.8 (32.0), 446.4 (8.6), 448.7 (11.8), 457.3 (31.0), 459.6 (31.5), 468.3 (6.2), 470.9 (0.5), 472.3 (7.5), 480.7 (8.8), 487.9 (6.1), 491.3 (27.3), 495.4 (3.1), 501.8 (17.1), 504.9 (1.3), 514.1 (3.5), 520.7 (50.8), 531.6 (61.5), 536.7 (4.0), 542.1 (14.1), 546.2 (7.8), 554.2 (68.4), 568.3 (20.5), 578.5 (43.4), 582.2 (29.9), 601.9 (53.8), 613.3 (168.9), 618.6 (219.8), 622.7 (201.0), 626.3 (198.4), 634.2 (45.9), 648.0 (83.1), 655.2 (180.4), 964.3 (287.8), 1820.1 (254.6), 1953.2 (49.4), 1970.1 (481.5), 1975.0 (226.8), 1990.9 (531.8), 1996.4 (260.6), 1999.2 (10.7), 2000.2 (515.5), 2010.6 (202.8), 2014.9 (676.9), 2022.4 (1491.0), 2029.2 (1048.8), 2043.9 (1344.0), 2052.4 (1516.7), 2090.3 (167.8)

Table S28. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15S-3** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
13.8 (0.0), 23.7 (0.0), 33.7 (0.0), 50.9 (0.3), 52.7 (0.6), 53.6 (0.1), 53.7 (0.1), 58.4 (0.0), 59.3 (0.3), 64.1 (0.2), 70.5 (0.0), 75.3 (0.1), 80.4 (0.0), 82.9 (0.0), 83.6 (0.8), 85.1 (1.7), 89.2 (0.0), 92.0 (0.2), 93.2 (0.5), 94.5 (0.7), 98.2 (0.5), 103.3 (0.1), 105.1 (0.1), 109.7 (0.4), 111.0 (0.1), 115.8 (0.4), 116.1 (0.0), 136.0 (0.9), 137.0 (0.2), 141.1 (0.1), 156.4 (5.4), 165.3 (2.1), 170.1 (0.0), 220.2 (1.6), 235.1 (5.2), 271.3 (5.4), 285.6 (11.2), 310.3 (1.6), 316.5 (0.0), 355.7 (0.6), 357.3 (6.3), 382.5 (0.0), 387.0 (0.4), 400.6 (0.9), 401.3 (1.8), 404.3 (2.2), 414.7 (20.2), 414.7 (4.7), 420.5 (0.9), 429.5 (9.6), 430.6 (14.0), 431.2 (92.3), 433.0 (6.4), 435.7 (17.3), 445.0 (10.0), 446.5 (65.9), 450.2 (3.4), 456.5 (0.0), 466.3 (0.2), 472.8 (21.8), 481.8 (2.8), 484.5 (1.3), 487.9 (0.8), 494.7 (12.1), 501.6 (1.8), 504.9 (0.6), 511.1 (4.6), 541.4 (7.7), 543.8 (35.6), 552.0 (13.0), 573.9 (7.9), 575.1 (60.6), 583.2 (104.4), 593.6 (10.0), 601.1 (156.2), 612.3 (15.4), 616.3 (27.9), 616.7 (0.3), 618.7 (2.3), 619.5 (237.8), 632.6 (4.2), 648.0 (181.7), 675.0 (514.4), 776.5 (485.3), 1919.7 (717.6), 1948.9 (593.7), 1953.6 (410.0), 2044.2 (44.4), 2058.9 (376.1), 2070.0 (636.1), 2072.0 (840.8), 2082.4 (323.3), 2098.6 (5.7), 2101.1 (48.8), 2101.4 (560.1), 2108.0 (2351.6), 2124.8 (2491.6), 2125.2 (1589.7), 2167.4 (56.3)	-7.3 (0.1), 24.3 (0.1), 28.6 (0.0), 35.3 (4.4), 47.6 (0.0), 47.6 (0.2), 50.5 (0.1), 54.3 (0.1), 59.0 (0.5), 64.1 (0.0), 70.3 (0.2), 72.7 (0.0), 75.1 (0.1), 76.0 (0.0), 77.7 (2.0), 80.6 (0.1), 83.7 (0.0), 85.2 (0.0), 86.4 (0.3), 87.2 (0.1), 92.6 (0.1), 97.3 (0.0), 99.5 (0.0), 102.8 (0.2), 104.0 (0.2), 107.4 (1.2), 108.1 (0.1), 120.3 (0.1), 132.4 (0.1), 138.8 (0.0), 139.2 (0.1), 159.9 (4.7), 167.3 (0.0), 211.4 (2.0), 227.2 (11.6), 268.6 (3.2), 286.6 (7.3), 294.9 (0.1), 314.7 (0.0), 347.0 (2.8), 356.2 (0.0), 379.4 (0.1), 381.7 (0.2), 388.1 (0.1), 393.4 (29.4), 393.9 (0.0), 406.3 (5.7), 417.0 (0.0), 424.5 (31.4), 425.6 (7.1), 429.4 (0.3), 433.8 (15.9), 437.6 (0.4), 440.1 (0.8), 443.1 (11.7), 452.2 (50.6), 454.7 (0.1), 456.9 (15.4), 460.5 (6.0), 473.4 (1.9), 481.0 (0.6), 481.4 (1.0), 493.0 (0.1), 495.6 (5.5), 505.6 (12.4), 508.2 (2.2), 517.0 (21.2), 526.2 (5.1), 527.4 (15.2), 535.5 (9.5), 545.2 (0.2), 568.7 (69.9), 574.4 (140.3), 581.0 (53.8), 592.4 (32.3), 597.1 (189.1), 601.7 (1.6), 604.3 (2.3), 608.6 (10.8), 614.8 (80.7), 620.3 (45.5), 628.1 (170.4), 656.3 (520.0), 809.1 (541.2), 1873.0 (543.5), 1893.3 (278.7), 1928.9 (475.4), 1949.4 (5.5), 1965.3 (48.4), 1976.6 (1031.7), 1991.3 (305.4), 2002.0 (675.5), 2012.8 (2.0), 2016.0 (0.0), 2017.3 (459.2), 2024.3 (2116.4), 2037.0 (1298.0), 2043.7 (1780.3), 2077.8 (92.3)

Table S29. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15T-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
10.8 (0.0), 34.2 (0.2), 37.9 (0.1), 49.1 (0.1), 52.4 (0.0), 61.5 (0.2), 62.2 (0.1), 63.5 (0.1), 65.7 (0.1), 69.8 (0.0), 70.9 (0.0), 74.0 (0.1), 77.4 (0.1), 80.5 (0.2), 83.3 (0.0), 85.1 (0.2), 87.9 (0.0), 92.0 (0.9), 92.3 (0.7), 94.5 (0.1), 100.6 (0.4), 103.0 (0.1), 104.9 (0.2), 105.8 (0.5), 109.4 (0.2), 113.6 (0.0), 116.2 (0.7), 124.9 (0.1), 128.3 (0.1), 130.2 (0.4), 133.0 (0.5), 151.1 (1.4), 175.5 (0.1), 199.5 (1.0), 221.0 (0.8), 252.4 (0.4), 296.8 (0.0), 301.2 (0.0), 318.4 (0.4), 348.2 (38.3), 356.0 (17.8), 373.9 (0.7), 374.8 (5.3), 378.1 (0.2), 387.1 (0.9), 392.7 (1.2), 402.9 (13.0), 403.5 (3.2), 413.0 (8.9), 415.1 (0.1), 423.4 (1.9), 424.4 (0.7), 430.2 (1.0), 434.3 (0.2), 435.9 (29.9), 437.5 (37.1), 438.9 (7.6), 444.9 (25.5), 450.3 (1.7), 452.0 (13.1), 472.0 (1.3), 475.0 (5.0), 481.3 (5.8), 483.3 (0.3), 494.2 (14.6), 496.5 (18.7), 500.6 (0.5), 506.7 (1.6), 515.4 (2.7), 521.2 (31.3), 542.9 (20.1), 548.6 (4.5), 558.0 (5.4), 571.7 (1.9), 586.2 (99.7), 593.5 (26.0), 606.7 (79.2), 608.8 (36.8), 619.0 (8.3), 624.9 (246.2), 635.4 (99.9), 648.9 (224.0), 660.0 (467.6), 671.3 (133.7), 1913.4 (603.3), 1947.8 (253.5), 2041.9 (400.9), 2043.1 (143.9), 2071.4 (289.7), 2074.8 (219.6), 2077.8 (474.3), 2087.0 (112.5), 2088.8 (557.3), 2096.0 (153.5), 2096.1 (136.6), 2100.9 (2530.9), 2118.3 (2609.7), 2124.8 (2049.0), 2166.5 (52.6)	9.9 (0.0), 31.7 (0.1), 34.5 (0.1), 45.6 (0.0), 48.7 (0.0), 59.0 (0.1), 61.0 (0.0), 62.7 (0.1), 65.5 (0.3), 66.8 (0.0), 70.3 (0.0), 74.3 (0.1), 79.4 (0.0), 79.8 (0.1), 82.5 (0.0), 86.6 (0.1), 88.2 (0.0), 88.8 (0.1), 90.0 (0.6), 94.1 (0.0), 98.5 (0.1), 101.6 (0.3), 102.1 (0.7), 103.1 (0.1), 105.5 (0.1), 108.5 (0.0), 112.8 (0.4), 122.0 (0.3), 123.5 (0.0), 125.0 (0.2), 131.1 (0.3), 152.0 (0.4), 173.2 (0.1), 205.5 (1.9), 213.4 (1.0), 247.0 (0.5), 289.8 (0.4), 318.3 (0.7), 323.5 (0.0), 363.9 (3.2), 375.6 (0.1), 376.6 (0.0), 382.5 (2.1), 386.8 (2.3), 389.6 (0.0), 396.5 (3.6), 410.0 (0.1), 411.0 (2.0), 416.3 (1.0), 426.3 (2.8), 429.9 (8.2), 437.1 (4.7), 437.7 (4.3), 444.9 (2.0), 447.6 (2.0), 453.2 (31.7), 455.8 (6.6), 456.8 (1.2), 465.3 (6.2), 472.1 (5.1), 480.9 (5.5), 483.6 (0.0), 486.0 (6.0), 493.2 (0.0), 496.3 (1.3), 497.7 (6.4), 503.5 (2.1), 506.5 (20.5), 524.0 (1.3), 524.5 (10.6), 527.6 (15.8), 542.5 (9.3), 545.2 (3.8), 560.1 (3.3), 571.5 (69.5), 591.1 (27.3), 599.7 (37.5), 601.4 (55.4), 602.5 (1.3), 611.2 (224.9), 629.6 (107.5), 642.3 (499.9), 648.4 (206.2), 668.0 (202.3), 1866.7 (437.9), 1886.5 (169.3), 1954.5 (360.3), 1955.3 (124.5), 1981.5 (297.1), 1989.9 (237.6), 1995.5 (415.1), 2000.6 (121.4), 2004.3 (867.8), 2008.3 (117.6), 2011.4 (12.7), 2013.9 (1856.4), 2035.1 (2054.4), 2044.7 (1417.6), 2077.9 (97.4)

Table S30. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **15T-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
15.7 (0.0), 18.5 (0.0), 20.2 (0.0), 27.4 (0.2), 36.3 (0.0), 42.1 (0.2), 44.2 (0.1), 50.7 (0.0), 52.1 (0.2), 57.4 (0.0), 58.6 (0.4), 63.5 (0.0), 67.7 (0.0), 69.6 (0.1), 73.2 (0.0), 77.7 (0.4), 79.9 (0.0), 80.5 (0.3), 90.1 (0.1), 90.9 (0.0), 93.0 (0.1), 93.3 (0.4), 98.4 (0.0), 100.5 (0.3), 102.9 (0.1), 106.1 (0.8), 110.3 (0.2), 113.1 (0.1), 114.0 (1.0), 121.8 (1.6), 130.0 (0.1), 132.4 (0.0), 158.5 (0.7), 180.4 (0.5), 235.8 (14.1), 252.6 (4.1), 303.6 (10.0), 334.3 (6.8), 350.5 (7.2), 355.7 (8.2), 370.2 (1.2), 375.5 (1.2), 377.7 (9.0), 384.5 (0.6), 386.4 (9.5), 391.4 (5.7), 393.0 (74.5), 397.6 (11.1), 402.5 (24.4), 407.5 (71.6), 409.0 (6.4), 413.4 (5.3), 416.3 (27.1), 423.0 (6.7), 427.2 (13.2), 430.8 (12.1), 437.8 (12.3), 444.6 (26.2), 451.9 (16.2), 455.8 (77.2), 462.5 (1.8), 468.2 (10.3), 472.0 (15.6), 478.9 (15.8), 480.1 (2.7), 483.2 (12.4), 486.8 (20.0), 500.5 (7.5), 526.2 (117.2), 542.4 (0.5), 545.5 (4.0), 546.7 (6.1), 557.4 (29.2), 562.1 (1.0), 585.0 (23.8), 591.7 (51.1), 604.3 (106.6), 609.4 (18.7), 623.8 (431.1), 626.2 (286.5), 631.2 (2.6), 637.4 (70.3), 649.0 (169.9), 778.1 (175.3), 1871.7 (279.3), 2038.4 (31.8), 2046.8 (89.3), 2062.7 (643.4), 2069.4 (705.4), 2073.8 (140.2), 2078.6 (305.1), 2080.1 (288.6), 2087.0 (781.2), 2093.0 (597.6), 2103.4 (1554.4), 2112.1 (1703.2), 2119.2 (2021.6), 2128.9 (1418.1), 2172.5 (111.7)	14.3 (0.0), 20.2 (0.0), 23.2 (0.0), 38.0 (0.2), 40.0 (0.1), 43.6 (0.0), 50.2 (0.2), 52.5 (0.1), 55.4 (0.0), 61.4 (0.0), 63.7 (0.0), 65.8 (0.1), 68.6 (0.1), 71.1 (0.1), 77.2 (0.2), 79.3 (0.1), 80.1 (0.2), 81.3 (0.6), 83.8 (0.1), 84.7 (0.2), 85.0 (0.1), 86.1 (0.0), 89.5 (0.1), 95.2 (0.2), 96.6 (0.2), 98.5 (0.4), 101.7 (0.3), 103.5 (0.3), 107.5 (0.3), 136.2 (0.5), 157.0 (0.4), 162.1 (0.1), 199.1 (2.7), 219.7 (0.9), 241.8 (0.7), 264.5 (8.5), 279.7 (0.3), 310.4 (0.2), 319.0 (4.3), 345.3 (21.1), 359.7 (3.0), 368.8 (5.7), 380.7 (0.6), 382.5 (0.4), 385.5 (5.3), 388.7 (28.6), 391.3 (0.9), 399.0 (18.2), 413.3 (1.2), 420.3 (5.0), 430.8 (51.6), 434.7 (0.6), 437.2 (14.8), 444.3 (22.4), 444.9 (11.2), 450.1 (2.9), 451.9 (54.6), 455.8 (6.5), 460.5 (3.5), 467.2 (5.8), 470.3 (8.3), 475.5 (9.8), 482.9 (3.4), 484.0 (25.5), 490.5 (1.4), 494.4 (0.5), 508.6 (22.5), 511.9 (14.3), 520.6 (4.0), 523.3 (54.4), 526.5 (3.1), 539.3 (57.7), 540.8 (21.9), 549.7 (19.9), 569.3 (103.3), 597.4 (8.3), 599.9 (52.6), 602.3 (85.9), 606.0 (290.0), 611.3 (76.7), 622.3 (170.4), 632.0 (294.9), 639.6 (326.2), 787.1 (165.1), 1816.1 (303.2), 1871.2 (550.1), 1892.3 (317.9), 1946.7 (178.2), 1972.3 (248.4), 1992.9 (635.3), 2000.9 (630.5), 2009.2 (313.0), 2010.0 (333.7), 2014.2 (69.2), 2015.3 (594.5), 2021.9 (1591.4), 2041.9 (1658.4), 2050.2 (1723.1), 2077.2 (14.4)

Table S31. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
15.9 (0.2), 21.3 (0.0), 33.9 (0.2), 40.9 (0.1), 45.0 (0.1), 54.9 (0.3), 59.4 (0.1), 65.7 (0.1), 74.2 (0.7), 75.2 (0.2), 79.0 (0.1), 83.4 (0.0), 86.1 (0.3), 89.7 (0.1), 92.0 (0.4), 93.6 (0.2), 94.6 (0.6), 99.2 (1.4), 104.1 (0.9), 106.1 (0.8), 108.3 (0.9), 109.3 (1.0), 113.6 (0.4), 122.0 (0.4), 123.0 (0.2), 126.9 (0.0), 130.8 (0.2), 144.5 (0.3), 159.8 (1.4), 172.7 (2.9), 185.4 (1.0), 189.9 (3.8), 204.0 (3.7), 232.7 (5.3), 327.1 (2.2), 372.8 (7.8), 386.3 (6.4), 391.5 (8.7), 393.3 (10.5), 396.4 (10.9), 399.1 (5.1), 403.9 (1.2), 405.9 (5.5), 413.8 (4.5), 420.0 (2.3), 426.2 (9.0), 429.9 (4.6), 435.9 (16.4), 440.9 (2.4), 454.1 (4.2), 459.1 (7.2), 464.3 (3.2), 470.8 (7.1), 473.9 (17.1), 477.7 (6.0), 484.0 (12.2), 488.7 (1.5), 498.4 (3.2), 508.3 (10.6), 512.1 (6.8), 515.0 (10.1), 522.6 (11.4), 541.1 (7.4), 550.7 (23.6), 562.4 (28.4), 564.3 (26.3), 573.0 (35.8), 585.0 (62.0), 587.8 (14.0), 593.9 (63.9), 604.9 (110.9), 606.6 (108.3), 609.8 (33.3), 618.5 (11.7), 628.5 (193.8), 638.2 (165.6), 642.9 (51.4), 689.1 (230.0), 759.9 (325.5), 1927.6 (369.6), 2038.8 (118.5), 2057.4 (154.5), 2060.9 (200.6), 2064.9 (52.3), 2068.4 (301.1), 2075.3 (175.9), 2088.1 (159.4), 2094.3 (367.8), 2100.7 (1635.7), 2106.7 (1898.5), 2112.3 (2608.2), 2125.3 (1931.5), 2169.8 (117.9)	18.6 (0.1), 27.6 (0.0), 31.2 (0.2), 40.0 (0.1), 45.6 (0.0), 55.4 (0.1), 58.6 (0.2), 67.7 (0.1), 73.3 (0.1), 76.4 (0.1), 77.7 (0.1), 81.0 (0.1), 83.0 (0.1), 86.4 (0.0), 89.1 (0.0), 90.8 (0.1), 92.1 (0.2), 97.2 (0.3), 101.2 (0.8), 104.1 (0.7), 105.7 (0.1), 108.8 (0.5), 111.0 (1.7), 119.2 (0.1), 120.5 (0.4), 123.5 (0.1), 130.1 (0.1), 133.5 (0.2), 165.3 (0.6), 183.7 (1.5), 190.2 (1.2), 201.2 (3.5), 210.5 (5.5), 242.2 (2.7), 331.9 (2.7), 363.0 (3.2), 381.2 (2.6), 381.4 (4.0), 386.8 (9.9), 389.6 (1.3), 396.4 (7.0), 397.9 (1.9), 410.7 (5.0), 411.7 (3.9), 417.7 (8.1), 427.0 (0.2), 430.8 (0.0), 446.0 (1.1), 457.0 (1.0), 457.8 (9.4), 464.5 (5.6), 470.8 (2.5), 477.3 (3.4), 481.8 (0.6), 486.3 (5.1), 493.0 (3.9), 497.0 (0.5), 504.7 (4.9), 509.8 (0.3), 513.0 (2.7), 516.2 (5.7), 527.0 (11.4), 528.6 (10.3), 541.4 (4.7), 556.8 (19.5), 558.9 (21.4), 565.9 (75.3), 578.9 (83.9), 580.4 (12.4), 582.5 (23.8), 593.1 (18.6), 598.1 (2.8), 612.6 (71.7), 616.2 (18.7), 620.0 (55.4), 630.9 (169.8), 633.8 (246.5), 683.6 (237.3), 751.1 (335.4), 1848.6 (287.2), 1958.8 (20.2), 1970.8 (270.1), 1979.3 (76.4), 1981.4 (15.0), 1986.2 (516.8), 1996.7 (181.5), 2009.9 (66.2), 2010.9 (79.6), 2018.8 (1157.5), 2025.2 (1807.9), 2026.9 (2062.8), 2046.7 (1363.9), 2084.4 (174.4)

Table S32. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
15.9 (0.1), 22.5 (0.6), 27.5 (0.2), 34.3 (3.0), 45.0 (0.1), 58.0 (3.2), 58.6 (0.1), 61.4 (0.6), 71.8 (0.0), 72.2 (0.7), 80.3 (1.7), 80.9 (0.7), 86.8 (0.1), 87.4 (0.8), 93.6 (0.0), 95.6 (2.3), 97.3 (0.0), 98.9 (0.9), 102.9 (0.0), 105.0 (1.9), 107.5 (0.0), 108.9 (0.2), 110.8 (0.0), 113.0 (0.5), 116.9 (0.8), 119.3 (0.1), 124.1 (0.0), 127.5 (0.0), 129.1 (0.8), 155.7 (0.1), 157.6 (3.7), 170.8 (2.9), 175.2 (1.8), 221.6 (1.3), 239.8 (57.8), 359.7 (5.4), 369.0 (7.1), 374.8 (6.0), 380.2 (1.8), 383.4 (30.8), 389.2 (2.9), 390.6 (11.7), 394.5 (2.2), 398.4 (1.3), 400.8 (0.4), 406.5 (0.3), 420.1 (1.7), 436.0 (0.7), 443.3 (0.6), 447.5 (5.2), 451.2 (21.1), 453.3 (31.5), 459.6 (0.1), 460.9 (10.1), 469.7 (0.0), 473.2 (3.8), 478.1 (0.6), 478.3 (24.4), 488.0 (4.1), 491.7 (0.3), 496.3 (34.0), 520.6 (0.1), 520.7 (32.9), 536.5 (20.1), 538.9 (34.1), 557.4 (4.2), 559.3 (1.8), 577.1 (25.1), 584.8 (64.2), 585.2 (27.7), 590.2 (5.1), 591.7 (38.5), 608.5 (26.2), 611.0 (73.0), 618.8 (46.7), 626.8 (206.0), 639.8 (128.1), 729.2 (523.3), 767.4 (239.6), 2017.5 (25.3), 2024.7 (180.0), 2043.0 (86.8), 2049.1 (837.6), 2052.7 (744.8), 2077.2 (411.0), 2079.0 (287.6), 2094.1 (21.7), 2096.3 (1088.4), 2101.9 (2227.4), 2113.7 (2164.7), 2116.5 (368.9), 2137.4 (1423.1), 2177.8 (169.1)	-52.7 (11.3), 22.7 (2.0), 27.9 (0.1), 29.4 (1.9), 41.7 (0.2), 49.7 (0.8), 55.2 (0.0), 56.6 (0.9), 66.2 (0.3), 66.6 (0.1), 71.2 (0.7), 73.5 (0.0), 79.0 (0.0), 80.2 (0.0), 84.4 (2.1), 86.8 (0.0), 87.9 (0.0), 89.2 (1.5), 89.7 (0.9), 93.9 (0.0), 96.1 (1.0), 98.0 (0.1), 103.6 (0.0), 105.2 (1.2), 106.2 (0.9), 109.2 (0.8), 120.0 (5.5), 122.5 (0.0), 122.6 (3.7), 153.0 (2.1), 155.7 (2.4), 175.1 (4.4), 185.5 (8.4), 233.9 (1.7), 252.2 (29.5), 323.8 (5.6), 335.6 (30.8), 349.4 (11.9), 356.4 (8.4), 365.1 (1.0), 374.1 (0.3), 386.8 (0.9), 388.9 (0.5), 401.2 (7.3), 403.2 (0.9), 413.5 (1.1), 420.8 (0.0), 424.5 (2.4), 425.0 (0.5), 443.5 (17.1), 447.9 (7.5), 448.2 (1.8), 455.0 (0.8), 461.6 (7.2), 471.2 (11.4), 473.0 (4.5), 474.6 (2.4), 476.1 (5.0), 481.8 (0.7), 488.2 (2.6), 493.7 (18.4), 503.2 (1.3), 509.5 (3.7), 524.4 (50.4), 529.4 (11.7), 529.4 (29.5), 548.0 (23.2), 560.7 (19.1), 565.4 (21.2), 577.6 (49.9), 581.6 (0.7), 582.3 (17.9), 583.8 (0.0), 595.4 (162.2), 615.8 (20.9), 618.4 (121.4), 630.4 (112.5), 767.5 (342.9), 800.0 (467.4), 1944.1 (169.6), 1952.0 (59.6), 1960.8 (5.9), 1963.4 (11.5), 1974.0 (54.4), 1974.8 (467.5), 1985.3 (35.4), 1987.2 (1105.9), 2004.4 (2120.7), 2014.3 (453.0), 2020.0 (1134.9), 2020.4 (1421.2), 2045.2 (1306.0), 2083.4 (146.7)

Table S33. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14S-3** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
11.7 (0.0), 16.7 (0.0), 21.4 (0.0), 30.4 (0.0), 34.4 (0.1), 47.3 (0.3), 49.5 (0.2), 53.1 (0.2), 57.6 (0.5), 63.9 (0.3), 68.4 (0.4), 71.3 (0.0), 73.9 (0.1), 80.8 (0.1), 83.5 (0.0), 88.5 (0.2), 89.4 (0.1), 93.4 (0.1), 95.7 (0.6), 97.3 (0.1), 102.3 (0.1), 103.6 (0.2), 107.2 (0.4), 114.0 (0.1), 114.9 (0.2), 118.9 (0.2), 126.3 (0.5), 130.0 (0.1), 136.0 (3.4), 165.0 (0.1), 183.2 (0.1), 206.5 (1.3), 248.8 (0.5), 279.6 (15.4), 342.1 (1.4), 352.2 (14.5), 373.2 (1.7), 380.9 (3.1), 383.1 (9.9), 389.5 (5.8), 395.5 (0.2), 397.0 (9.9), 403.5 (7.2), 404.5 (2.0), 410.6 (8.8), 413.9 (2.7), 422.0 (31.2), 429.9 (30.0), 432.2 (2.1), 443.4 (16.1), 449.6 (16.8), 461.0 (1.7), 461.7 (16.9), 466.4 (16.8), 470.0 (12.2), 476.1 (11.1), 478.2 (12.4), 482.7 (3.4), 496.0 (7.7), 497.1 (3.1), 500.2 (2.3), 512.7 (9.5), 519.0 (3.5), 545.1 (4.6), 549.9 (2.2), 554.7 (22.3), 564.8 (3.2), 579.3 (27.9), 589.9 (14.5), 593.7 (104.3), 608.1 (280.3), 614.7 (80.5), 624.5 (112.1), 629.8 (243.0), 634.6 (51.2), 640.1 (131.7), 645.1 (74.4), 654.7 (128.7), 901.6 (282.0), 1887.7 (618.0), 1894.4 (11.1), 2055.4 (464.8), 2059.5 (597.5), 2073.7 (691.1), 2078.0 (29.6), 2084.4 (36.6), 2097.4 (402.0), 2100.4 (236.9), 2107.6 (1785.7), 2113.2 (2178.5), 2120.5 (1431.7), 2126.6 (1583.8), 2175.2 (209.1)	7.6 (0.0), 17.4 (0.1), 22.3 (0.0), 27.0 (0.0), 31.6 (0.1), 41.0 (0.2), 47.6 (0.2), 48.9 (0.3), 54.6 (0.3), 60.1 (0.2), 66.6 (0.1), 68.9 (0.1), 70.9 (0.1), 77.5 (0.0), 81.2 (0.1), 82.9 (0.2), 85.8 (0.1), 87.6 (0.1), 92.0 (0.4), 92.9 (0.1), 99.6 (0.1), 100.2 (0.3), 103.3 (0.1), 106.0 (0.0), 110.2 (0.1), 114.9 (0.2), 115.3 (0.3), 120.0 (0.1), 135.7 (2.6), 166.6 (0.1), 193.9 (0.3), 213.7 (0.3), 264.4 (0.3), 288.0 (17.5), 331.2 (1.3), 342.5 (4.2), 366.8 (2.1), 373.5 (4.1), 378.4 (3.1), 383.1 (5.5), 385.8 (0.5), 392.2 (2.3), 395.5 (1.4), 406.1 (19.0), 415.3 (3.0), 429.6 (12.0), 432.7 (1.5), 435.2 (5.6), 441.5 (2.2), 446.9 (7.2), 453.4 (8.5), 456.0 (17.4), 461.1 (3.7), 462.2 (1.1), 473.6 (7.0), 474.5 (1.0), 483.7 (8.6), 485.5 (2.4), 490.2 (3.1), 496.8 (0.5), 508.4 (3.5), 512.1 (2.1), 519.3 (1.5), 532.4 (3.7), 535.0 (1.4), 542.1 (12.4), 547.2 (2.9), 562.0 (2.7), 578.6 (16.3), 587.7 (42.5), 600.6 (329.1), 608.8 (19.6), 617.6 (104.6), 620.6 (225.4), 625.1 (169.5), 630.2 (52.8), 637.0 (76.1), 645.0 (127.8), 899.8 (286.7), 1815.9 (454.7), 1828.8 (47.1), 1978.9 (282.6), 1982.4 (486.7), 1992.1 (76.6), 1994.6 (479.3), 1997.5 (85.5), 2011.6 (458.5), 2014.3 (497.1), 2020.3 (1414.4), 2030.3 (800.2), 2033.3 (2058.6), 2048.5 (1278.2), 2087.5 (206.3)

Table S34. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14T-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
25.6 (0.3), 31.9 (0.0), 35.0 (0.1), 38.3 (0.2), 50.4 (0.1), 52.7 (0.1), 64.6 (0.1), 69.4 (0.2), 73.1 (0.1), 74.8 (0.1), 78.6 (0.3), 79.7 (0.5), 81.5 (0.5), 84.6 (0.2), 86.9 (0.1), 89.7 (0.6), 91.0 (0.1), 95.5 (0.5), 96.8 (0.1), 97.8 (0.4), 100.9 (3.4), 105.6 (0.0), 106.0 (0.1), 106.7 (0.6), 110.6 (0.8), 117.0 (0.8), 117.4 (0.3), 139.3 (2.5), 144.1 (0.4), 157.9 (0.8), 183.4 (6.0), 196.5 (14.3), 204.7 (1.5), 236.8 (3.0), 307.1 (11.1), 341.0 (0.9), 352.2 (14.2), 358.4 (0.6), 376.1 (16.9), 382.5 (8.9), 384.5 (0.5), 389.2 (4.3), 392.5 (3.0), 395.1 (0.0), 404.1 (10.9), 411.1 (4.2), 414.2 (2.2), 416.3 (26.2), 421.7 (1.9), 424.9 (2.6), 433.7 (4.2), 441.8 (13.4), 444.5 (13.1), 448.9 (15.1), 460.8 (11.3), 466.5 (2.4), 470.5 (0.4), 478.4 (2.6), 487.3 (1.5), 494.9 (0.6), 505.2 (6.4), 509.0 (4.8), 516.2 (29.6), 526.4 (28.6), 535.4 (3.6), 539.4 (9.7), 552.0 (10.9), 558.3 (26.7), 562.5 (68.9), 567.0 (58.9), 571.6 (95.7), 580.0 (31.2), 596.6 (34.2), 606.5 (70.0), 608.8 (70.1), 619.0 (150.9), 629.3 (126.4), 648.3 (231.2), 734.8 (256.1), 1951.7 (390.7), 2037.7 (230.7), 2047.6 (40.8), 2059.6 (374.5), 2067.8 (39.3), 2073.5 (66.6), 2074.8 (336.4), 2080.2 (648.7), 2088.2 (39.3), 2090.1 (133.6), 2098.5 (2797.4), 2111.9 (2581.3), 2117.4 (2339.2), 2161.3 (51.7)	26.4 (0.0), 27.8 (0.2), 33.7 (0.1), 38.5 (0.1), 48.2 (0.5), 51.5 (0.0), 60.6 (0.1), 63.7 (0.4), 68.3 (0.4), 71.4 (0.1), 72.2 (0.2), 77.0 (0.2), 80.0 (0.3), 80.5 (0.2), 84.7 (0.1), 86.3 (0.1), 87.9 (0.2), 89.7 (0.2), 91.5 (0.4), 94.8 (1.0), 95.1 (0.4), 99.3 (0.1), 102.5 (0.9), 107.1 (0.2), 107.9 (0.0), 108.4 (0.5), 115.1 (1.2), 133.5 (0.0), 149.9 (0.9), 157.2 (0.3), 187.0 (1.9), 207.5 (9.7), 212.9 (4.0), 241.3 (1.2), 308.3 (6.9), 355.6 (7.5), 361.4 (5.0), 362.2 (7.0), 367.3 (1.2), 372.8 (8.7), 381.0 (1.8), 390.9 (2.9), 394.0 (3.3), 394.9 (5.2), 402.8 (3.2), 413.3 (2.1), 416.3 (4.5), 425.9 (1.9), 437.2 (2.7), 449.2 (0.7), 457.3 (5.7), 457.6 (20.5), 462.6 (1.0), 465.1 (2.5), 473.7 (0.8), 477.3 (1.6), 481.7 (0.2), 486.2 (1.4), 492.0 (4.0), 501.5 (2.1), 507.2 (12.3), 508.8 (2.7), 510.9 (4.9), 527.2 (10.1), 532.2 (5.4), 541.6 (12.1), 551.7 (20.3), 554.0 (17.9), 561.1 (4.9), 564.6 (63.0), 574.9 (84.9), 579.3 (42.4), 594.0 (47.7), 597.0 (45.1), 601.6 (169.3), 609.4 (46.0), 621.7 (132.1), 642.3 (240.9), 718.8 (226.5), 1873.1 (302.8), 1956.1 (90.4), 1960.7 (151.6), 1973.6 (255.7), 1984.8 (41.7), 1988.0 (194.8), 1991.2 (411.7), 1998.8 (374.0), 2002.7 (129.3), 2005.4 (36.4), 2015.1 (2246.7), 2025.2 (2067.2), 2036.0 (2015.3), 2071.6 (67.2)

Table S35. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **14T-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
8.0 (0.0), 10.5 (0.0), 17.8 (0.0), 26.4 (0.0), 39.6 (0.0), 43.8 (0.2), 52.8 (0.1), 56.4 (0.2), 58.9 (0.3), 64.0 (0.2), 66.6 (0.1), 68.2 (0.2), 70.9 (0.2), 75.9 (0.0), 77.2 (0.1), 80.9 (0.2), 84.4 (0.5), 86.9 (0.1), 87.5 (0.2), 91.2 (0.1), 94.6 (0.1), 97.0 (0.2), 98.4 (0.2), 107.6 (0.1), 114.1 (0.7), 114.5 (0.3), 128.4 (1.8), 130.3 (0.2), 135.3 (0.1), 138.8 (2.1), 148.4 (23.7), 168.1 (3.5), 180.5 (1.1), 272.7 (16.3), 285.9 (4.4), 310.2 (0.1), 338.8 (146.0), 351.2 (0.9), 362.6 (1.5), 370.7 (1.9), 373.8 (10.6), 388.4 (2.4), 391.5 (0.1), 396.7 (13.8), 400.0 (1.6), 404.2 (10.4), 409.2 (5.7), 412.1 (0.2), 417.8 (9.9), 419.6 (5.1), 432.7 (17.6), 434.6 (19.5), 438.2 (7.8), 451.9 (31.1), 458.1 (23.6), 467.8 (15.1), 471.6 (1.9), 475.7 (46.7), 484.2 (52.4), 486.6 (20.1), 487.7 (4.0), 489.7 (15.2), 500.1 (30.0), 509.9 (11.5), 521.6 (12.1), 534.2 (8.1), 547.6 (25.7), 551.2 (6.0), 555.9 (23.1), 562.8 (9.1), 583.4 (28.9), 591.2 (9.1), 595.7 (25.4), 621.6 (115.5), 626.2 (77.4), 633.3 (222.3), 641.4 (151.0), 664.4 (131.6), 997.5 (264.1), 1961.1 (411.3), 1973.3 (7.4), 2033.3 (626.3), 2042.0 (969.9), 2069.7 (537.1), 2077.3 (104.3), 2089.8 (136.8), 2095.8 (4.1), 2102.7 (801.9), 2106.3 (2416.9), 2116.8 (263.4), 2123.1 (1748.4), 2128.8 (1472.6), 2177.6 (365.3)	9.8 (0.1), 17.0 (0.1), 19.2 (0.1), 21.2 (0.4), 30.0 (0.1), 37.5 (0.1), 51.5 (0.1), 54.5 (0.4), 58.4 (0.2), 63.3 (0.0), 65.8 (0.1), 66.9 (0.1), 72.8 (0.1), 74.8 (0.2), 79.7 (0.2), 83.0 (0.1), 85.3 (0.2), 85.9 (0.1), 89.7 (0.5), 89.9 (0.1), 95.9 (0.0), 97.4 (0.4), 102.0 (0.3), 106.0 (0.0), 106.6 (0.3), 111.8 (0.3), 115.0 (0.2), 119.2 (0.3), 148.3 (1.5), 155.8 (0.7), 188.2 (1.3), 201.5 (0.2), 207.9 (1.8), 258.6 (4.8), 287.8 (5.5), 298.1 (14.4), 338.8 (3.5), 351.5 (1.3), 360.9 (1.7), 376.5 (8.5), 379.1 (3.9), 384.1 (0.4), 389.2 (3.1), 396.9 (3.1), 405.8 (3.6), 410.5 (1.1), 420.8 (1.5), 427.1 (6.4), 431.4 (7.0), 434.6 (3.3), 443.6 (6.0), 448.0 (7.0), 457.2 (3.5), 458.6 (6.0), 464.5 (2.1), 471.2 (2.1), 478.1 (22.0), 480.3 (1.2), 486.4 (0.1), 490.4 (2.8), 493.8 (16.4), 496.1 (7.5), 502.7 (3.4), 516.3 (5.7), 522.4 (10.4), 535.9 (4.1), 540.8 (13.3), 551.6 (3.4), 556.9 (23.7), 565.2 (32.3), 574.7 (7.0), 580.8 (135.5), 583.0 (46.3), 591.1 (94.0), 611.4 (97.6), 618.6 (212.2), 626.3 (147.7), 649.2 (133.3), 944.5 (330.5), 1827.5 (327.9), 1840.0 (170.8), 1972.8 (404.1), 1978.2 (350.8), 1983.6 (555.0), 1992.3 (223.4), 1995.2 (181.9), 2006.9 (105.1), 2012.4 (306.3), 2018.2 (1705.6), 2022.9 (2374.8), 2031.7 (582.9), 2044.8 (1153.6), 2086.1 (399.2)

Table S36. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **13S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
23.8 (0.0), 31.3 (0.2), 31.5 (0.2), 43.2 (0.1), 55.2 (0.0), 61.9 (0.4), 68.0 (0.1), 75.6 (1.8), 78.4 (0.4), 80.1 (0.0), 83.5 (0.0), 84.6 (0.0), 85.1 (0.0), 85.5 (0.0), 90.7 (0.1), 95.7 (0.1), 98.5 (0.0), 102.5 (0.4), 103.6 (0.1), 104.0 (0.0), 110.1 (0.1), 110.1 (0.2), 110.2 (0.0), 111.1 (0.0), 112.9 (0.0), 162.4 (0.0), 164.2 (7.1), 171.2 (0.0), 195.6 (9.6), 199.4 (3.8), 222.6 (3.8), 261.3 (0.2), 324.8 (7.5), 381.5 (0.3), 381.7 (0.0), 382.1 (0.0), 388.7 (0.2), 408.8 (0.0), 416.1 (10.8), 419.6 (13.5), 423.0 (0.1), 433.1 (0.0), 435.3 (5.9), 445.8 (1.6), 448.2 (2.8), 448.9 (0.0), 455.8 (8.8), 457.3 (3.0), 478.6 (26.9), 480.4 (5.5), 488.6 (0.5), 491.9 (6.8), 493.2 (0.0), 494.3 (0.3), 498.6 (8.1), 506.1 (13.7), 507.4 (1.4), 517.1 (0.0), 527.8 (0.8), 542.4 (0.0), 559.0 (0.1), 564.5 (0.0), 570.8 (65.4), 585.5 (88.7), 591.5 (0.0), 597.0 (159.2), 609.2 (141.4), 617.2 (53.2), 620.5 (14.4), 625.7 (109.0), 629.8 (260.0), 635.8 (3.6), 682.2 (208.6), 915.9 (129.5), 1984.4 (398.1), 2055.8 (18.3), 2062.0 (0.0), 2063.0 (253.4), 2063.7 (0.4), 2071.6 (0.0), 2077.9 (6.3), 2080.9 (217.9), 2084.9 (850.0), 2101.1 (2140.1), 2110.8 (3403.8), 2120.4 (2496.6), 2164.0 (13.1)	18.7 (0.0), 23.5 (0.1), 33.1 (0.0), 41.2 (0.0), 51.5 (0.0), 57.6 (0.3), 65.5 (0.0), 75.1 (0.2), 75.9 (0.0), 77.3 (0.1), 80.7 (0.0), 81.7 (0.0), 82.4 (0.0), 86.9 (0.1), 87.8 (0.0), 94.8 (0.0), 98.3 (0.2), 98.9 (0.0), 100.7 (0.0), 102.1 (0.0), 102.5 (0.0), 104.3 (0.3), 105.5 (0.2), 107.1 (0.0), 109.6 (0.1), 158.2 (0.1), 173.8 (0.0), 176.7 (2.1), 198.6 (5.6), 219.1 (10.7), 227.2 (1.1), 259.4 (0.1), 340.2 (11.0), 369.9 (0.0), 370.5 (1.5), 386.7 (2.8), 399.6 (0.1), 404.8 (0.0), 412.7 (5.9), 417.3 (10.4), 419.1 (0.6), 430.0 (0.0), 436.5 (0.4), 442.4 (0.0), 446.6 (0.0), 447.7 (5.4), 468.6 (3.1), 468.9 (3.2), 485.0 (0.0), 486.9 (0.7), 488.6 (0.0), 491.4 (0.0), 495.2 (3.6), 503.3 (13.3), 504.8 (0.0), 513.1 (5.3), 522.4 (6.8), 522.6 (0.0), 523.9 (0.7), 543.8 (2.8), 550.4 (0.7), 565.5 (65.8), 571.4 (0.0), 585.3 (78.7), 586.6 (106.4), 587.9 (0.0), 601.7 (143.9), 611.3 (26.7), 617.0 (1.7), 618.3 (9.2), 627.9 (309.3), 628.3 (0.1), 680.1 (193.9), 904.4 (191.2), 1896.5 (294.2), 1974.4 (1.5), 1975.5 (0.0), 1976.0 (360.4), 1979.3 (65.2), 1994.4 (0.0), 1999.0 (80.0), 2004.4 (95.2), 2014.7 (405.2), 2018.3 (1877.5), 2029.8 (2543.1), 2043.2 (1989.0), 2075.7 (2.9)

Table S37. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **13T-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
15.6 (0.1), 27.6 (0.0), 32.1 (0.0), 39.6 (0.0), 44.7 (0.1), 51.8 (0.1), 56.9 (0.0), 64.6 (0.0), 68.9 (0.1), 73.6 (0.3), 75.1 (0.4), 76.3 (0.2), 80.4 (0.0), 81.7 (0.1), 84.1 (0.0), 87.5 (0.3), 88.6 (0.0), 90.9 (0.4), 94.3 (0.5), 99.0 (1.1), 100.1 (0.8), 104.8 (0.1), 106.4 (0.0), 109.1 (0.1), 117.4 (0.9), 150.2 (0.5), 179.0 (2.7), 187.8 (2.8), 193.3 (1.7), 208.0 (1.3), 220.7 (16.3), 241.3 (5.3), 325.2 (4.4), 337.9 (2.0), 351.5 (4.2), 356.8 (13.6), 370.6 (12.3), 379.4 (31.2), 383.9 (6.4), 384.8 (13.8), 391.5 (8.9), 395.2 (8.0), 401.9 (1.3), 411.3 (3.3), 416.5 (1.0), 421.4 (6.6), 424.3 (12.8), 426.2 (3.0), 434.3 (17.0), 440.7 (18.2), 447.3 (11.0), 469.7 (1.2), 472.3 (6.8), 480.1 (1.1), 482.9 (14.3), 483.9 (3.2), 489.6 (1.7), 507.6 (10.7), 520.3 (31.7), 526.3 (15.2), 535.1 (15.8), 537.7 (9.0), 548.0 (31.0), 556.4 (13.8), 559.9 (99.1), 569.8 (14.5), 574.3 (22.8), 583.9 (64.0), 594.0 (62.4), 598.8 (79.7), 606.7 (52.3), 615.3 (46.7), 659.8 (247.3), 753.6 (118.0), 1926.3 (768.6), 1952.2 (295.6), 2053.5 (54.8), 2065.7 (61.3), 2070.5 (236.8), 2073.8 (146.6), 2076.3 (55.0), 2084.4 (235.6), 2088.5 (61.9), 2102.1 (2964.3), 2106.6 (2933.0), 2107.5 (2531.5), 2157.6 (50.3)	15.8 (0.0), 28.2 (0.1), 31.8 (0.0), 40.2 (0.0), 42.4 (0.0), 51.0 (0.1), 55.6 (0.0), 63.5 (0.1), 67.2 (0.0), 73.0 (0.1), 75.2 (0.1), 79.0 (0.1), 79.8 (0.1), 81.6 (0.0), 83.9 (0.0), 84.6 (0.2), 87.8 (0.0), 89.2 (0.2), 93.9 (0.6), 97.4 (0.1), 98.4 (0.1), 100.3 (0.3), 103.6 (0.0), 107.5 (0.2), 124.5 (0.4), 153.5 (0.2), 185.2 (1.8), 187.8 (1.1), 194.5 (0.8), 213.6 (1.8), 231.8 (10.1), 249.7 (3.2), 328.6 (2.3), 342.6 (4.4), 352.4 (1.2), 362.6 (5.3), 377.3 (5.1), 377.7 (11.1), 381.8 (0.7), 397.6 (0.1), 403.5 (0.7), 409.8 (4.2), 418.0 (16.7), 422.2 (1.8), 424.9 (2.8), 435.6 (1.4), 438.7 (5.2), 444.0 (12.2), 449.6 (2.7), 454.7 (4.0), 464.8 (5.2), 475.1 (3.7), 478.6 (1.2), 483.0 (8.1), 489.5 (5.4), 493.5 (4.3), 497.2 (4.5), 508.9 (4.4), 515.9 (1.0), 527.4 (3.9), 531.4 (33.0), 542.2 (81.4), 553.6 (14.5), 555.9 (40.0), 558.3 (17.4), 565.5 (8.4), 572.3 (27.1), 580.7 (35.2), 588.2 (19.5), 594.3 (49.5), 605.7 (39.1), 615.0 (168.1), 652.1 (185.3), 763.6 (173.8), 1861.7 (434.4), 1879.3 (221.6), 1968.1 (12.8), 1978.5 (48.2), 1987.5 (254.8), 1990.0 (190.1), 1991.1 (196.8), 1998.1 (166.8), 2002.6 (34.0), 2015.3 (2531.4), 2020.7 (2488.0), 2022.0 (2001.5), 2066.8 (91.6)

Table S38. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **13T-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-53.1 (2.3), -9.0 (0.0), 20.7 (0.1), 43.3 (0.0), 45.0 (0.0), 45.3 (0.7), 51.7 (6.4), 65.4 (0.1), 66.3 (0.1), 66.5 (0.0), 76.7 (0.0), 76.9 (0.0), 80.1 (0.3), 83.4 (0.1), 85.6 (0.0), 90.4 (0.0), 93.9 (0.7), 95.6 (0.0), 97.7 (0.0), 98.8 (0.6), 100.6 (0.0), 104.7 (0.3), 107.4 (0.2), 110.5 (0.1), 111.1 (0.0), 135.1 (1.4), 137.8 (0.3), 141.1 (5.2), 144.2 (0.0), 185.2 (0.0), 251.8 (0.0), 257.0 (0.0), 314.8 (0.6), 341.1 (16.5), 344.3 (24.0), 371.1 (0.0), 379.3 (0.9), 384.6 (0.0), 389.4 (3.1), 395.6 (3.8), 399.3 (0.1), 399.4 (18.8), 404.5 (14.6), 406.3 (0.0), 415.8 (8.2), 424.5 (8.1), 431.3 (0.0), 444.7 (0.8), 445.4 (15.4), 457.6 (1.6), 462.3 (3.1), 465.1 (9.0), 466.8 (11.5), 469.7 (1.2), 476.0 (14.7), 479.1 (15.5), 492.8 (0.0), 493.1 (0.4), 502.4 (0.0), 511.1 (4.3), 528.2 (1.4), 551.6 (31.4), 552.2 (0.0), 559.2 (0.0), 565.6 (45.7), 566.4 (57.7), 584.1 (184.6), 584.8 (161.5), 590.3 (94.8), 601.8 (20.4), 608.5 (0.1), 631.4 (139.7), 652.2 (167.1), 861.0 (34.5), 1902.4 (450.3), 2056.5 (104.7), 2057.8 (338.2), 2060.1 (0.0), 2062.2 (135.8), 2078.2 (142.2), 2081.5 (0.0), 2085.2 (205.8), 2085.5 (583.3), 2104.6 (2557.5), 2105.2 (3561.6), 2108.0 (2575.8), 2160.2 (0.0)	-22.0 (0.0), -9.9 (0.0), -7.4 (0.1), 35.1 (0.0), 40.4 (0.0), 44.7 (0.4), 53.5 (0.3), 55.9 (0.9), 60.0 (0.0), 65.2 (1.1), 73.0 (0.0), 73.2 (0.0), 76.4 (0.2), 77.8 (0.0), 81.5 (0.0), 83.4 (0.0), 88.9 (1.0), 91.5 (0.0), 92.8 (0.0), 93.3 (0.0), 97.0 (0.0), 102.1 (0.2), 102.5 (0.2), 105.0 (0.0), 106.8 (0.0), 136.9 (0.3), 136.9 (0.0), 139.7 (0.0), 140.7 (1.0), 192.3 (0.5), 249.2 (0.3), 251.7 (0.4), 303.5 (1.0), 360.8 (0.6), 361.9 (0.0), 373.7 (0.1), 375.3 (0.0), 392.5 (2.0), 397.9 (12.5), 398.9 (0.0), 399.9 (0.0), 403.2 (0.0), 408.1 (0.5), 413.6 (8.1), 419.2 (0.2), 425.8 (0.0), 437.9 (0.8), 447.7 (30.5), 456.0 (0.8), 456.3 (6.2), 468.2 (0.0), 473.9 (1.2), 479.8 (2.2), 481.0 (1.3), 487.0 (6.1), 494.4 (0.0), 495.6 (8.3), 505.2 (1.6), 510.3 (0.0), 514.7 (1.0), 515.3 (0.7), 544.2 (36.3), 553.0 (0.0), 558.5 (0.0), 560.5 (38.7), 566.6 (80.8), 580.1 (136.7), 586.3 (104.3), 588.3 (65.2), 597.8 (2.3), 606.6 (10.6), 628.6 (175.0), 649.5 (171.1), 860.9 (54.7), 1849.8 (359.7), 1968.7 (398.6), 1969.9 (0.0), 1970.8 (87.4), 1975.5 (187.6), 1997.4 (15.8), 1997.7 (0.0), 2004.8 (4.0), 2007.6 (0.3), 2018.4 (2136.0), 2019.6 (2981.6), 2030.2 (2242.2), 2068.3 (5.2)

Table S39. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
8.5 (0.0), 17.3 (0.0), 26.9 (0.0), 38.2 (0.0), 43.3 (0.1), 53.2 (0.0), 62.1 (0.0), 66.4 (0.7), 69.2 (0.0), 72.1 (0.1), 77.9 (0.2), 80.6 (0.1), 83.5 (0.2), 83.9 (0.1), 86.9 (0.3), 89.5 (0.1), 93.0 (0.4), 95.1 (0.3), 95.5 (0.1), 98.7 (0.4), 99.6 (1.2), 106.1 (0.9), 120.9 (1.0), 125.0 (2.3), 148.2 (1.6), 169.4 (0.1), 176.9 (3.2), 180.2 (2.7), 186.4 (3.8), 252.1 (0.0), 347.9 (6.3), 366.8 (16.8), 385.4 (4.5), 388.7 (1.4), 393.5 (2.9), 394.8 (1.1), 402.9 (3.9), 416.6 (4.5), 422.9 (7.8), 424.3 (5.3), 432.4 (3.3), 445.5 (0.9), 452.1 (2.6), 455.1 (6.0), 470.2 (5.2), 473.7 (6.4), 483.8 (9.8), 487.8 (1.3), 496.5 (9.1), 498.0 (9.2), 507.6 (1.1), 525.2 (15.0), 530.9 (6.3), 534.0 (3.6), 538.8 (32.7), 549.8 (6.0), 557.1 (53.0), 570.3 (82.9), 576.5 (101.0), 585.8 (1.8), 589.1 (1.4), 596.3 (11.9), 601.2 (19.5), 607.1 (99.3), 614.1 (60.4), 634.3 (18.6), 659.7 (135.2), 687.7 (148.3), 813.1 (38.7), 2016.0 (252.4), 2028.6 (235.0), 2047.7 (254.4), 2066.1 (154.2), 2069.3 (27.5), 2072.6 (22.5), 2082.6 (94.1), 2085.1 (493.0), 2095.8 (2123.3), 2103.0 (3003.2), 2114.7 (3182.4), 2157.6 (19.0)	19.2 (0.0), 25.9 (0.0), 28.9 (0.0), 37.7 (0.0), 43.1 (0.0), 55.8 (0.0), 59.3 (0.1), 63.6 (0.4), 66.9 (0.1), 71.4 (0.0), 76.1 (0.0), 78.0 (0.1), 80.1 (0.4), 82.7 (0.0), 85.9 (0.2), 89.3 (0.1), 90.7 (0.2), 92.7 (0.1), 93.3 (0.1), 96.4 (0.2), 98.1 (0.5), 104.5 (1.3), 121.7 (0.8), 127.5 (2.4), 151.8 (1.3), 174.2 (0.9), 178.0 (0.6), 186.4 (1.0), 203.5 (2.4), 250.9 (0.7), 330.9 (4.9), 359.6 (11.9), 383.2 (2.8), 387.3 (4.1), 389.0 (1.3), 393.4 (2.3), 395.2 (1.1), 415.3 (4.3), 420.1 (3.2), 423.8 (7.5), 429.3 (0.5), 441.2 (1.4), 462.6 (1.0), 467.5 (1.3), 473.7 (0.8), 488.5 (0.1), 491.6 (1.5), 497.6 (1.0), 500.4 (1.6), 503.2 (0.2), 508.7 (3.5), 516.1 (18.7), 526.6 (7.0), 530.9 (15.6), 537.8 (17.2), 545.8 (16.4), 563.9 (35.8), 567.9 (17.2), 570.3 (105.3), 584.6 (10.1), 586.3 (7.8), 593.4 (7.1), 596.2 (69.7), 601.3 (14.0), 606.8 (30.9), 626.3 (32.4), 664.7 (135.1), 702.2 (129.9), 788.0 (76.5), 1935.0 (174.7), 1943.3 (223.8), 1967.1 (114.2), 1983.6 (128.3), 1985.6 (86.9), 1989.3 (37.0), 1998.7 (231.8), 2003.3 (147.4), 2014.5 (1966.7), 2016.9 (2482.8), 2033.5 (2308.4), 2067.8 (29.4)

Table S40. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12S-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
32.2 (1.1), 32.2 (1.1), 32.2 (1.1), 32.4 (0.0), 41.8 (0.0), 41.8 (0.0), 41.8 (0.0), 46.0 (0.0), 46.0 (0.0), 72.7 (0.0), 72.7 (0.0), 72.7 (0.0), 76.6 (0.0), 76.6 (0.0), 78.0 (0.3), 78.0 (0.3), 78.0 (0.3), 83.1 (0.0), 83.1 (0.0), 83.1 (0.0), 85.3 (0.0), 93.2 (0.0), 93.2 (0.0), 93.2 (0.0), 134.9 (5.9), 134.9 (5.9), 134.9 (5.9), 143.5 (0.0), 143.5 (0.0), 272.0 (0.0), 387.9 (0.0), 387.9 (0.0), 387.9 (0.0), 391.6 (0.0), 392.7 (0.0), 392.7 (0.0), 392.7 (0.0), 416.2 (15.9), 416.2 (15.9), 416.2 (15.9), 436.2 (0.0), 436.2 (0.0), 443.1 (3.0), 443.1 (3.0), 443.1 (3.0), 460.1 (0.0), 460.9 (0.9), 460.9 (0.9), 460.9 (0.9), 477.4 (0.0), 477.4 (0.0), 477.4 (0.0), 487.3 (0.0), 487.3 (0.0), 542.8 (193.3), 542.8 (193.3), 542.8 (193.3), 543.5 (0.0), 543.5 (0.0), 543.5 (0.0), 574.9 (0.0), 574.9 (0.0), 583.6 (3.4), 583.6 (3.4), 583.6 (3.4), 600.0 (0.0), 786.5 (259.9), 786.5 (259.9), 786.5 (259.9), 2061.1 (0.0), 2061.1 (0.0), 2061.1 (0.0), 2068.6 (0.0), 2068.6 (0.0), 2072.1 (106.9), 2072.1 (106.9), 2072.1 (106.9), 2106.0 (3192.3), 2106.0 (3192.3), 2106.0 (3192.3), 2158.0 (0.0)	29.9 (0.0), 32.0 (0.9), 32.0 (0.9), 32.0 (0.9), 39.8 (0.0), 39.8 (0.0), 39.8 (0.0), 44.3 (0.0), 44.3 (0.0), 72.1 (0.0), 72.1 (0.0), 72.1 (0.0), 74.7 (0.0), 74.7 (0.0), 77.6 (0.2), 77.6 (0.2), 77.6 (0.2), 81.9 (0.0), 82.6 (0.0), 82.6 (0.0), 82.6 (0.0), 89.6 (0.0), 89.6 (0.0), 89.6 (0.0), 133.4 (5.4), 133.4 (5.4), 133.4 (5.4), 135.9 (0.0), 135.9 (0.0), 269.1 (0.0), 381.6 (0.0), 381.6 (0.0), 381.6 (0.0), 385.1 (0.0), 391.2 (0.0), 391.2 (0.0), 391.2 (0.0), 413.7 (11.0), 413.7 (11.0), 413.7 (11.0), 430.8 (0.0), 430.8 (0.0), 457.6 (2.4), 457.6 (2.4), 457.6 (2.4), 463.9 (0.0), 470.0 (3.6), 470.0 (3.6), 470.0 (3.6), 475.8 (0.0), 475.8 (0.0), 475.8 (0.0), 492.1 (0.0), 492.1 (0.0), 545.2 (111.0), 545.2 (111.0), 545.2 (111.0), 561.0 (0.0), 561.0 (0.0), 561.0 (0.0), 578.2 (0.0), 578.2 (0.0), 580.8 (9.9), 580.8 (9.9), 580.8 (9.9), 589.1 (0.0), 797.7 (261.4), 797.7 (261.4), 797.7 (261.4), 1971.4 (0.0), 1971.4 (0.0), 1971.4 (0.0), 1980.4 (0.0), 1980.4 (0.0), 1991.3 (36.6), 1991.3 (36.6), 1991.3 (36.6), 2021.3 (2453.5), 2021.3 (2453.5), 2021.3 (2453.5), 2064.5 (0.0)

Table S41. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **12T-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
13.5(0.0), 19.3(0.0), 31.3(0.0), 40.8(0.1), 43.0(0.0), 52.2(0.1), 54.3(0.1), 57.8(0.2), 62.7(0.1), 69.8(0.1), 72.2(0.1), 77.6(0.0), 78.0(0.1), 80.0(0.1), 82.9(0.1), 83.0(0.1), 86.6(0.4), 88.1(0.1), 90.6(0.1), 91.3(0.0), 93.9(0.2), 95.7(0.4), 101.7(0.7), 105.7(0.1), 132.8(0.1), 148.1(1.0), 165.4(0.0), 179.9(2.8), 189.6(13.7), 232.2(0.3), 352.6(0.4), 353.2(0.2), 366.8(1.1), 375.1(2.4), 377.0(2.7), 385.1(8.6), 394.9(14.0), 400.3(6.7), 402.2(2.9), 412.1(6.8), 419.7(2.9), 423.3(3.5), 425.0(8.7), 431.5(0.1), 437.5(5.6), 447.0(6.9), 460.3(5.5), 460.9(5.8), 478.8(7.7), 480.8(1.6), 483.9(6.7), 489.2(0.9), 494.0(4.9), 498.4(1.7), 514.6(13.8), 530.0(12.8), 533.2(49.9), 540.8(20.3), 548.0(82.8), 552.1(32.5), 554.8(18.2), 568.7(40.1), 574.4(34.7), 580.3(55.8), 586.9(74.9), 589.5(14.7), 631.9(102.9), 676.7(240.4), 815.3(335.5), 2044.5(49.7), 2045.7(87.8), 2058.6(53.1), 2064.0(81.7), 2066.3(65.9), 2074.2(4.3), 2076.8(45.1), 2079.0(51.3), 2092.7(3004.6), 2097.5(3375.3), 2104.5(3125.8), 2153.1(1.6)	19.5(0.0), 20.1(0.0), 34.7(0.0), 38.9(0.1), 42.6(0.0), 52.0(0.0), 52.8(0.2), 58.2(0.0), 68.1(0.1), 68.3(0.2), 75.7(0.4), 77.2(0.0), 77.3(0.0), 79.8(0.0), 81.3(0.0), 81.7(0.1), 85.4(0.2), 86.6(0.1), 88.1(0.4), 89.2(0.0), 90.9(0.0), 92.2(0.2), 102.9(1.0), 106.2(0.3), 139.5(0.0), 160.0(2.2), 168.7(0.0), 193.0(0.8), 202.4(8.5), 246.1(0.3), 356.4(1.0), 357.9(0.3), 366.2(0.2), 367.8(9.0), 384.7(13.4), 388.4(0.0), 389.8(2.3), 400.0(1.4), 400.4(8.3), 416.7(2.8), 422.1(0.7), 433.7(0.0), 445.4(4.5), 449.0(0.2), 453.0(1.5), 469.2(0.6), 471.7(0.7), 480.4(2.0), 480.9(0.8), 487.7(1.8), 493.8(0.1), 494.0(1.3), 500.6(3.9), 506.4(12.5), 513.9(20.9), 533.5(45.3), 538.1(42.7), 552.9(0.0), 556.6(24.4), 559.0(28.1), 563.2(38.4), 567.9(27.7), 571.4(1.0), 581.7(2.0), 588.9(14.9), 593.4(59.0), 640.0(227.6), 654.6(85.9), 837.9(249.6), 1952.6(61.4), 1954.9(89.3), 1975.5(109.0), 1980.8(25.4), 1983.2(34.5), 1988.7(79.1), 1991.7(0.5), 1995.0(385.6), 2011.3(2519.8), 2011.4(2359.2), 2019.4(2457.7), 2061.3(5.6)

Table S42. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **11T-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
9.9 (0.0), 27.9 (0.0), 33.1 (0.2), 38.4 (0.2), 41.0 (0.3), 52.4 (0.1), 57.8 (0.1), 60.7 (0.5), 65.6 (0.0), 71.5 (0.1), 78.1 (0.4), 79.1 (0.1), 80.3 (0.1), 82.5 (0.3), 86.4 (1.0), 88.1 (1.3), 89.3 (0.1), 94.0 (0.7), 96.8 (0.5), 97.9 (0.6), 103.2 (1.4), 121.5 (1.9), 129.8 (1.1), 151.2 (0.3), 168.0 (2.1), 184.8 (8.6), 191.7 (4.2), 255.9 (0.1), 329.8 (9.4), 334.8 (13.7), 353.9 (16.5), 376.4 (15.0), 388.3 (1.1), 392.3 (3.8), 394.5 (21.5), 399.0 (4.9), 399.7 (10.5), 405.9 (6.2), 428.6 (11.1), 431.4 (8.2), 436.4 (0.3), 446.3 (0.0), 453.1 (10.0), 459.1 (2.9), 470.8 (3.6), 483.8 (2.1), 491.9 (1.6), 494.0 (21.3), 497.4 (2.0), 502.0 (13.1), 515.5 (3.8), 534.3 (5.8), 539.0 (3.5), 547.1 (44.5), 562.5 (56.8), 566.9 (54.3), 583.2 (24.5), 587.3 (49.0), 603.7 (59.2), 607.6 (63.8), 616.1 (58.0), 638.1 (101.3), 693.1 (161.6), 882.3 (109.5), 2027.0 (142.0), 2044.9 (210.1), 2046.2 (154.0), 2063.9 (9.7), 2066.0 (18.3), 2072.0 (84.7), 2076.4 (245.3), 2083.4 (2257.4), 2097.1 (3239.1), 2107.0 (3221.8), 2150.6 (18.0)	12.1 (0.0), 26.2 (0.1), 28.3 (0.2), 33.7 (0.0), 41.4 (0.0), 47.7 (0.0), 57.2 (0.1), 60.3 (0.2), 64.9 (0.0), 65.3 (0.1), 74.7 (0.1), 75.1 (0.0), 78.2 (0.4), 80.7 (0.5), 84.9 (0.0), 89.3 (0.2), 90.5 (0.0), 91.3 (0.1), 93.1 (0.5), 97.1 (0.4), 98.7 (1.3), 148.9 (0.5), 150.9 (0.1), 159.9 (1.0), 175.0 (0.6), 191.3 (3.4), 207.5 (2.5), 257.0 (0.3), 300.6 (2.8), 327.5 (4.2), 362.6 (0.2), 366.2 (9.6), 375.5 (3.8), 386.7 (2.2), 388.2 (0.4), 397.5 (2.6), 398.8 (8.5), 422.1 (8.1), 427.1 (1.7), 432.8 (1.7), 451.5 (8.6), 455.4 (0.5), 462.1 (3.6), 480.4 (1.7), 481.9 (10.5), 482.9 (1.7), 487.3 (1.6), 493.7 (2.3), 494.1 (0.0), 502.9 (0.5), 509.0 (0.8), 509.4 (29.5), 516.6 (12.8), 545.1 (19.8), 556.8 (70.6), 561.1 (33.7), 572.5 (24.0), 581.4 (1.3), 592.0 (65.9), 594.7 (66.1), 597.7 (41.6), 617.4 (35.6), 684.1 (156.2), 850.4 (93.3), 1879.3 (279.2), 1965.1 (56.9), 1971.8 (17.9), 1975.0 (191.5), 1983.5 (73.4), 1988.2 (227.1), 1989.6 (86.9), 1999.3 (2162.3), 2003.5 (2412.9), 2025.3 (2362.5), 2058.5 (50.5)

Table S43. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **11S-1** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
9.6 (0.4), 22.2 (0.0), 33.4 (0.1), 37.0 (0.1), 43.1 (0.1), 60.3 (0.2), 63.8 (0.2), 66.2 (0.3), 69.6 (0.1), 74.3 (0.1), 78.1 (0.2), 79.9 (0.2), 83.6 (0.1), 87.7 (0.2), 91.4 (0.1), 92.2 (0.2), 96.1 (0.2), 99.5 (0.1), 100.8 (0.3), 104.7 (0.4), 110.4 (1.0), 119.9 (0.7), 137.3 (0.7), 157.5 (1.2), 174.6 (3.6), 179.6 (2.9), 206.9 (1.3), 256.3 (0.2), 353.6 (5.7), 372.6 (0.6), 379.4 (2.4), 384.1 (11.7), 395.2 (7.8), 405.7 (2.2), 409.9 (2.2), 415.9 (13.8), 421.9 (5.8), 430.1 (6.2), 442.5 (1.1), 446.5 (2.4), 453.2 (7.7), 455.7 (0.6), 470.4 (3.1), 474.2 (5.9), 481.8 (8.5), 483.9 (8.2), 489.9 (5.6), 494.4 (11.4), 496.6 (5.3), 511.6 (1.9), 523.4 (18.4), 539.0 (17.4), 541.5 (29.9), 558.7 (0.4), 564.2 (53.6), 570.0 (3.8), 573.9 (128.3), 589.4 (38.7), 591.2 (80.1), 605.4 (92.8), 614.5 (134.2), 621.7 (38.2), 688.8 (136.2), 835.6 (50.1), 2000.4 (231.7), 2044.3 (297.4), 2053.2 (20.0), 2057.3 (446.5), 2061.4 (137.2), 2069.1 (318.6), 2074.4 (207.6), 2083.5 (1598.4), 2095.2 (3144.7), 2103.2 (3154.2), 2149.4 (93.9)	27.7 (0.4), 31.8 (0.1), 36.2 (0.0), 40.6 (0.1), 51.0 (0.2), 56.7 (0.3), 58.9 (0.1), 62.8 (0.1), 67.3 (0.1), 72.1 (0.2), 75.5 (0.4), 76.4 (0.2), 80.6 (0.4), 85.4 (0.5), 86.2 (0.0), 91.4 (0.1), 92.3 (0.1), 93.4 (0.0), 99.2 (0.1), 102.3 (0.8), 143.4 (2.2), 154.8 (1.1), 158.1 (0.7), 176.8 (3.3), 204.1 (1.9), 221.3 (1.4), 244.0 (0.4), 261.5 (3.5), 299.6 (7.1), 367.9 (0.7), 378.0 (3.6), 384.0 (1.6), 386.1 (2.3), 391.8 (2.4), 404.0 (0.1), 408.4 (4.4), 413.6 (0.5), 429.5 (7.1), 436.6 (4.2), 438.3 (2.0), 439.9 (1.1), 449.4 (2.5), 459.7 (2.4), 462.2 (2.5), 478.2 (1.7), 485.1 (5.4), 486.7 (1.6), 493.0 (11.7), 502.8 (3.4), 506.9 (7.9), 522.2 (16.0), 526.7 (5.6), 538.5 (9.9), 548.1 (4.4), 554.6 (42.1), 565.8 (5.6), 571.3 (49.2), 580.9 (36.7), 586.6 (23.5), 595.5 (67.8), 614.4 (83.4), 629.2 (145.6), 717.8 (89.4), 825.1 (101.0), 1830.9 (286.6), 1879.0 (496.0), 1960.4 (555.6), 1970.1 (145.9), 1987.5 (99.5), 1989.1 (250.5), 1996.4 (167.6), 2000.6 (1107.1), 2007.2 (2252.9), 2030.4 (2358.6), 2059.5 (118.0)

Table S44. Theoretical harmonic vibrational frequencies (in cm^{-1}) for the structure **11S-2** using the B3LYP/DZP and BP86/DZP methods

B3LYP/DZP	BP86/DZP
-27.6 (1.2), 36.8 (0.0), 42.9 (0.0), 44.5 (0.1), 49.0 (0.1), 58.2 (0.1), 66.0 (0.1), 71.2 (0.0), 72.3 (0.1), 77.7 (0.0), 77.9 (0.2), 78.2 (0.3), 81.4 (1.2), 83.2 (0.4), 87.6 (0.3), 90.5 (0.3), 94.2 (0.1), 97.5 (0.2), 98.6 (0.4), 102.6 (0.0), 111.0 (0.6), 133.6 (2.9), 152.4 (3.0), 162.0 (0.9), 186.2 (2.6), 191.9 (2.8), 208.1 (1.8), 259.7 (0.0), 323.4 (2.9), 340.9 (14.1), 349.1 (10.6), 375.6 (4.4), 388.2 (0.2), 397.9 (8.5), 410.0 (3.5), 413.0 (25.9), 417.1 (16.5), 431.3 (4.3), 439.9 (8.8), 447.1 (2.7), 447.7 (1.4), 454.9 (10.2), 466.8 (1.5), 470.2 (0.3), 478.0 (5.1), 481.3 (29.0), 496.2 (16.0), 498.6 (0.2), 501.6 (4.7), 526.6 (8.5), 528.7 (75.7), 532.8 (0.1), 539.4 (19.4), 549.5 (42.3), 557.0 (11.3), 564.4 (15.6), 569.4 (143.4), 574.1 (1.8), 598.4 (55.4), 602.2 (103.7), 602.3 (121.4), 625.2 (30.8), 705.6 (135.6), 820.6 (37.1), 1928.4 (382.7), 2024.0 (182.3), 2038.4 (969.8), 2056.6 (24.8), 2066.7 (174.3), 2071.4 (0.3), 2081.4 (41.4), 2081.8 (1797.9), 2093.1 (2687.2), 2108.3 (3427.7), 2149.6 (73.2)	-16.1 (0.0), 24.3 (0.5), 40.0 (0.0), 40.2 (0.0), 43.8 (0.1), 53.3 (0.0), 61.8 (0.0), 63.5 (0.1), 71.6 (0.1), 71.9 (0.5), 73.9 (0.1), 75.9 (0.2), 79.8 (0.1), 80.8 (0.0), 87.0 (0.0), 90.6 (0.2), 92.7 (0.1), 93.3 (0.1), 94.2 (0.1), 100.3 (0.5), 112.6 (0.5), 156.0 (1.8), 156.0 (1.8), 165.7 (1.4), 199.5 (3.1), 200.2 (0.2), 234.2 (0.4), 254.9 (0.4), 259.4 (1.0), 341.2 (3.4), 365.7 (13.8), 375.4 (5.2), 385.4 (0.2), 386.0 (8.9), 394.5 (7.9), 401.8 (1.0), 413.7 (6.3), 424.9 (0.3), 435.0 (8.1), 439.3 (2.3), 451.2 (1.4), 456.0 (2.5), 464.1 (7.3), 468.5 (0.4), 474.4 (2.4), 481.9 (1.5), 494.8 (2.4), 495.0 (2.7), 499.3 (2.7), 515.3 (20.9), 518.8 (14.3), 531.5 (11.7), 537.9 (1.1), 551.2 (6.2), 556.8 (4.9), 562.5 (2.3), 564.9 (115.3), 575.0 (20.7), 586.2 (19.6), 596.9 (36.2), 607.7 (144.4), 623.9 (80.4), 725.2 (98.8), 796.0 (67.3), 1841.2 (291.1), 1934.7 (215.2), 1956.0 (654.9), 1970.7 (62.7), 1983.7 (45.1), 1986.2 (26.1), 1994.2 (126.2), 1996.6 (1442.9), 2005.1 (2344.1), 2026.9 (2502.3), 2057.8 (100.6)

Table 45. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{16}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
16S-1(D_{2d})	6906.745796	0	0	6907.779281	0	0
16S-2(C_{2v})	6906.740425	3.4	0	6907.782876	-2.3	0
16S-3(D_{2d})	6906.718346	17.2	3(28*i*,17*i*,17*i*)	6907.772434	4.3	3(25*i*,18*i*,18*i*)

Table 46. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{15}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
15S-1(C_1/C_2)	6793.419162	0	0	6794.45733	0	0
15S-2(C_1)	6793.416231	1.8	0	6794.444079	8.3	0
15T-1(C_s)	6793.400068	12.0	0	6794.419826	23.5	0
15T-2(C_1)	6793.400732	11.6	0	6794.419188	23.9	0
15S-3(C_s)	6793.375076	27.7	0	6794.414989	26.6	1(7*i*)

Table 47. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{14}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
14S-1(C_1)	6680.086278	0	0	6681.117140	0	0
14T-1(C_1)	6680.078815	4.7	0	6681.091739	15.9	0
14T-2(C_1)	6680.063049	14.6	0	6681.070460	29.3	0
14S-2(C_2)	6680.059756	16.6	0	6681.088644	17.9	1(53*i*)
14S-3(C_1)	6680.053914	20.3	0	6681.083698	21.0	0

Table 48. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{13}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
13S-1(C_{2v})	6566.764692	0	0	6567.784903	0	0
13T-1(C_1)	6566.739968	15.5	0	6567.752300	20.5	0
13T-2(C_{2v})	6566.727134	23.6	2(53*i*,9*i*)	6567.737988	29.4	3(22*i*,10*i*,7*i*)

Table 49. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{12}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
12S-1(C_1)	6453.408285	0	0	6454.420837	0	0
12T-1(C_1)	6453.405371	1.8	0	6454.405884	9.4	0
12S-2(T_d)	6453.390477	11.2	0	6454.395447	15.9	0

Table 50. The zero point energies (E, in hartrees), relative energies (ΔE, in kcal/mol), and number of imaginary vibrational frequencies (Nimag) for the optimized $Fe_4C(CO)_{11}$ isomers

Species	B3LYP			BP86		
	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag	$-E_{ZPVE}$	ΔE_{ZPVE}	NImag
11T-1(C_s/C_1)	6340.045541	0	0	6341.028663	0	0
11S-1(C_1)	6340.013395	20.2	0	6341.026369	1.4	0
11S-2(C_s)	6340.011375	21.4	1(28*i*)	6341.026431	1.4	1(16*i*)

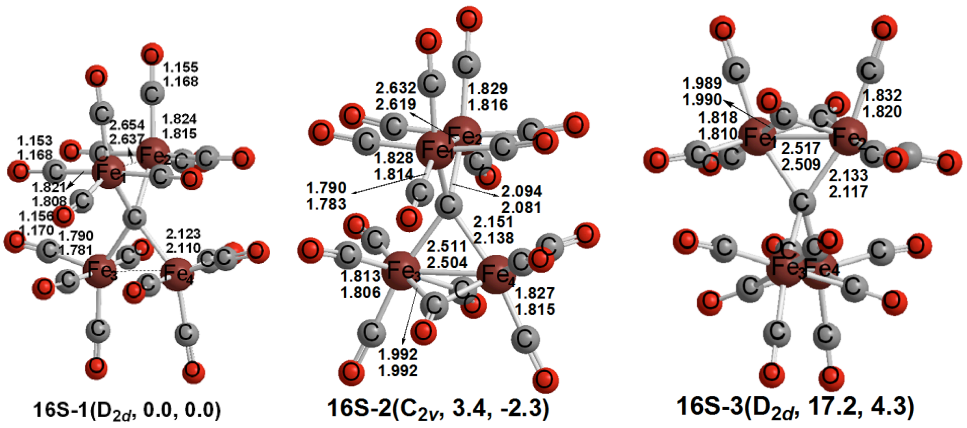

Figure 1. Three optimized singlet $Fe_4C(CO)_{16}$ structures. In Figures 1 to 6 the top numbers obtained by the B3LYP and the bottom numbers refer to distances obtained by the BP86 method. The relative energies (in kcal/mol) by B3LYP and BP86, respectively, are shown under each structure. All the bond distances in Figures 1 to 7 are given in Å.

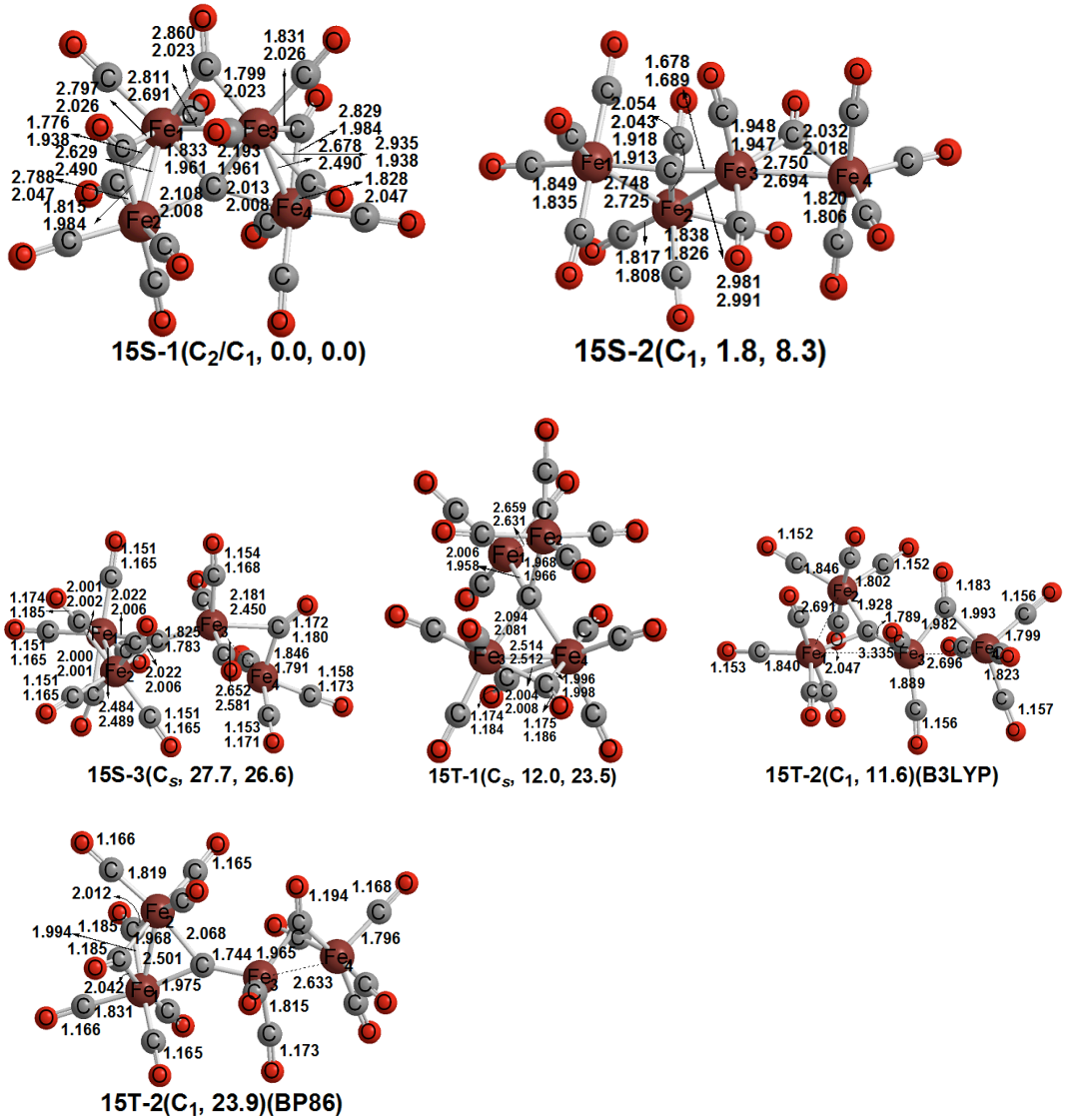

Figure 2. Three optimized singlet $Fe_4C(CO)_{15}$ structures and two optimized triplet $Fe_4C(CO)_{15}$ structures.

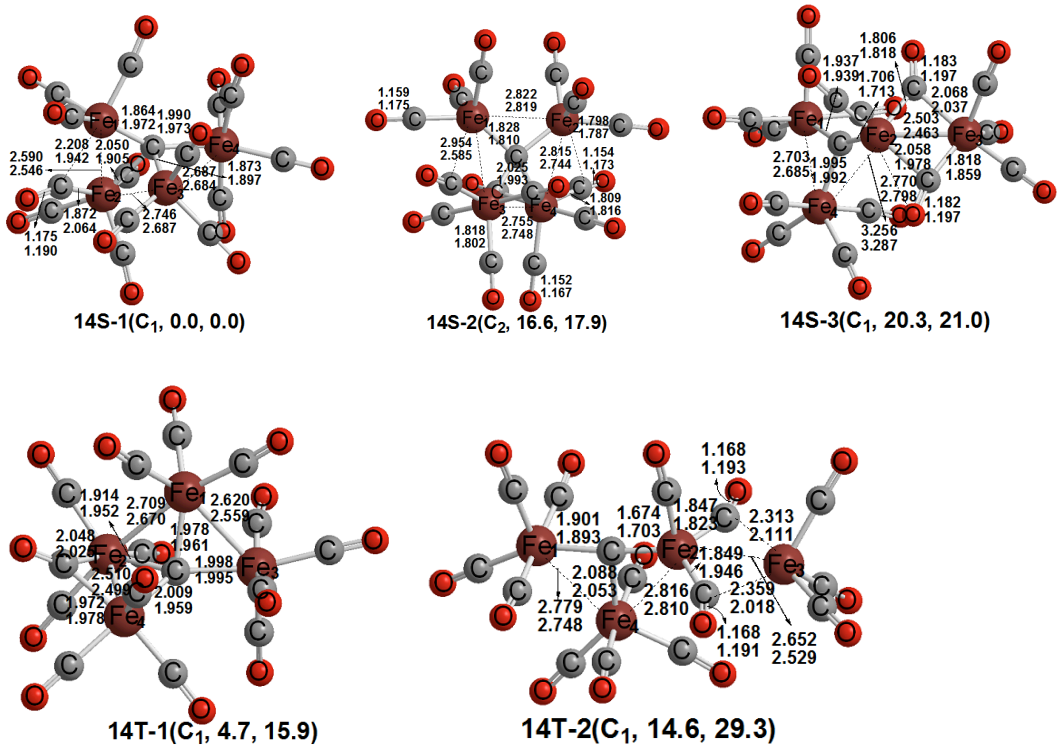

Figure 3. Three optimized singlet $Fe_4C(CO)_{14}$ structures and two optimized triplet $Fe_4C(CO)_{14}$ structures.

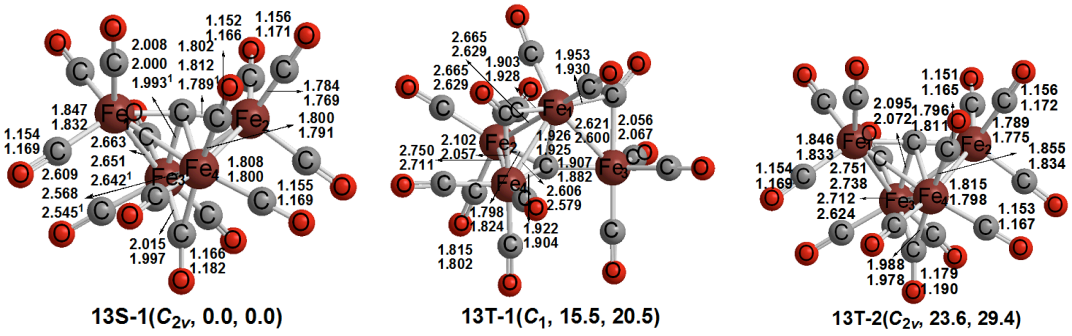

Figure 4. One optimized singlet $Fe_4C(CO)_{13}$ structures and two optimized triplet $Fe_4C(CO)_{13}$ structures.

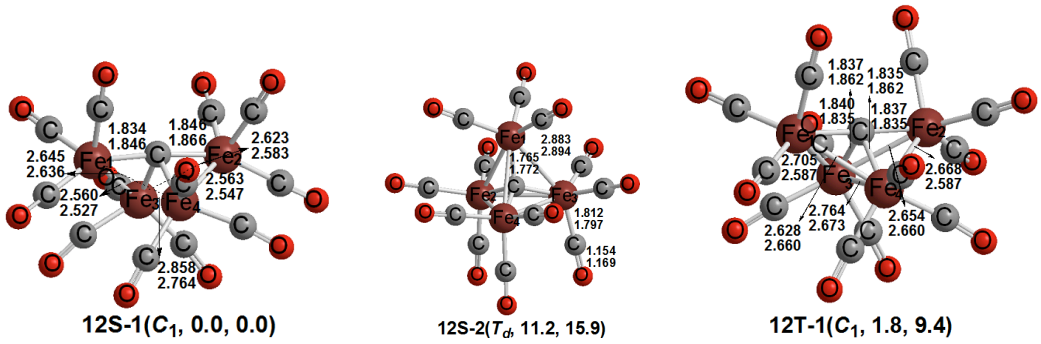

Figure 5. Two optimized singlet $Fe_4C(CO)_{12}$ structures and one optimized triplet $Fe_4C(CO)_{12}$ structures.

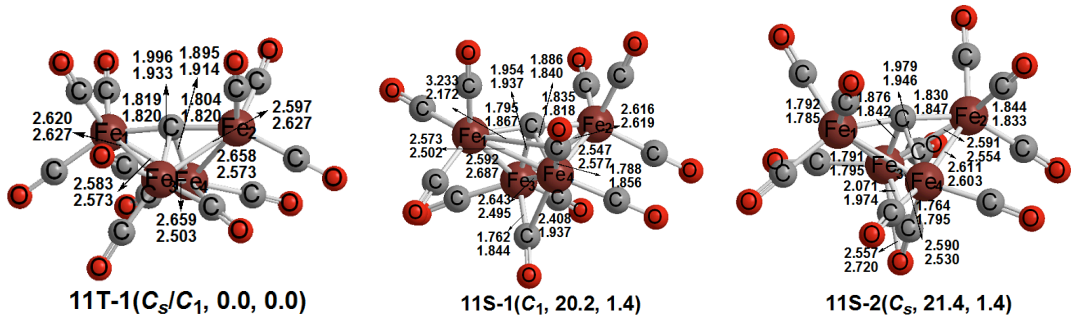

Figure 6. Two optimized singlet $Fe_4C(CO)_{11}$ structures and one optimized triplet $Fe_4C(CO)_{11}$ structures.

Complete Gaussian 03 reference (Reference 37)

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