

A Binuclear Trimethylenemethane Cobalt Carbonyl Providing the First Example of a Low-Energy Perpendicular Structure with Acyclic Hydrocarbon Ligands

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Supporting Information

Tables S1 to S4: Co-Co distances (Å), total energies (E, in hartree), relative energies (ΔE , in kcal/mol) and spin expectation values $\langle S^2 \rangle$ for all structures by the four DFT methods.

Tables S5 to S16: Atomic coordinates of the optimized structures for the all structures;

Tables S17 to S28: Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses in km/mol) for all structures.

Table S1. Co-Co distances (Å), total energies (E, in hartree), relative energies (ΔE , in kcal/mol) and spin expectation values $\langle S^2 \rangle$ for the $(C_4H_6)_2Co_2(CO)_2$ structures by the M06-L, B3LYP*, B3LYP and BP86 methods. None of these structures has an imaginary vibrational frequency.

		2S-1, C_{2v}	2T-2, C_i	2S-3, C_{2v}	2T-4, C_{2v}
M06-L	M-M	2.29	2.779	2.231	2.331
	E	-3304.24963	-3304.22953	-3304.21887	-3304.21207
	ΔE	0.0	12.6	19.3	23.6
	$\langle S^2 \rangle$	0.00	2.08	0.00	2.08
B3LYP*	M-M	2.300	3.019	2.231	2.349
	E	-3303.75108	-3303.74460	-3303.71603	-3303.71145
	ΔE	0.0	4.1	22.0	24.9
	$\langle S^2 \rangle$	0.00	2.05	0.00	2.11
B3LYP	M-M	2.292	3.064	2.232	2.349
	E	-3304.40861	-3304.41592	-3304.36920	-3304.36932
	ΔE	0.0	-4.6	24.7	24.7
	$\langle S^2 \rangle$	0.00	2.07	0.00	2.27
BP86	M-M	2.322	2.668	2.235	2.340
	E	-3304.89791	-3304.85823	-3304.87590	-3304.86448
	ΔE	0.0	24.9	13.8	21.0
	$\langle S^2 \rangle$	0.00	2.02	0.00	2.02

Table S2. Co-Co distances (Å), total energies (E, in hartree), relative energies (ΔE , in kcal/mol) and spin expectation values $\langle S^2 \rangle$ for the $(C_4H_6)_2Co_2(CO)_3$ structures by the M06-L, B3LYP*, B3LYP and BP86 methods. None of these structures has an imaginary vibrational frequency.

		3S-1, C_s	3S-2, C_s	3T-3, D_{3h}
M06-L	M-M	2.419	2.408	2.231
	E	-3417.59568	-3417.59338	-3417.59038
	ΔE	0.0	1.4	3.3
	$\langle S^2 \rangle$	0.00	0.00	2.01
B3LYP*	M-M	2.472	2.424	2.245
	E	-3417.04209	-3417.03919	-3417.03053
	ΔE	0.0	1.8	7.3
	$\langle S^2 \rangle$	0.00	0.00	2.02
B3LYP	M-M	2.487	2.437	2.252
	E	-3417.75986	-3417.75430	-3417.74577
	ΔE	0.0	3.5	8.8
	$\langle S^2 \rangle$	0.00	0.00	2.02
BP86	M-M	2.423	2.393	2.229
	E	-3418.25745	-3418.26200	-3418.25569
	ΔE	0.0	2.393	2.229

$\langle S^2 \rangle$	0.00	0.00	2.00
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Table S3. Co-Co distances (Å), total energies (E, in hartree), relative energies (ΔE , in kcal/mol) for the $(C_4H_6)_2Co_2(CO)_4$ structures by the M06-L, B3LYP*, B3LYP and BP86 methods. None of these structures has an imaginary vibrational frequency.

		4S-1, C_{2h}	4S-2, C_{2v}	4S-3, C_2
M06-L	M-M	2.504	2.507	2.678
	E	-3530.97710	-3530.97651	-3530.97440
	ΔE	0.0	0.4	1.7
B3LYP*	M-M	2.536	2.539	2.721
	E	-3530.36556	-3530.36412	-3530.36430
	ΔE	0.0	0.9	0.8
B3LYP	M-M	2.544	2.548	2.723
	E	-3531.14066	-3531.13917	-3531.14189
	ΔE	0.0	0.9	-0.8
BP86	M-M	2.514	2.516	2.712
	E	-3531.65758	-3531.65602	-3531.64828
	ΔE	0.0	1.0	5.8

Table S4. Co-Co distances (Å), total energies (E, in hartree) for the $(C_4H_6)_2Co_2(CO)_6$ and $(C_4H_6)_2Co_2(CO)_5$ structures by the M06-L, B3LYP*, B3LYP and BP86 methods. None of these structures has an imaginary vibrational frequency.

		5S, C_1	6S, C_2
M06-L	M-M	2.698	2.770
	E	-3644.28907	-3757.59869
B3LYP*	M-M	2.764	2.826
	E	-3643.63102	-3756.89359
B3LYP	M-M	2.782	2.824
	E	-3644.46912	-3757.79356
BP86	M-M	2.612	2.831
	E	-3644.98436	-3758.30885

Table S5. Optimized coordinates of the 2S-1 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-1.767842	0.000000	-0.878038	-1.836502	0.000000	-0.893523	-1.842777	0.000000	-0.895351	-1.800106	0.000000	-0.894737
1	-2.004774	0.913710	-1.420710	-2.079881	0.915859	-1.434191	-2.091056	0.913544	-1.433577	-2.026579	0.923456	-1.445145
1	-2.004774	-0.913710	-1.420710	-2.079881	-0.915859	-1.434191	-2.091056	-0.913544	-1.433577	-2.026579	-0.923456	-1.445145
6	-1.730592	0.000000	0.555335	-1.757518	0.000000	0.536977	-1.764125	0.000000	0.533817	-1.740027	0.000000	0.545384
6	-1.501268	1.284279	1.183079	-1.522807	1.288868	1.171488	-1.526326	1.288433	1.165441	-1.515224	1.294008	1.187834
1	-1.248653	1.275198	2.244673	-1.274171	1.278347	2.235862	-1.282504	1.278705	2.228838	-1.260243	1.282113	2.257952
8	0.000000	-3.918714	-1.032115	0.000000	-3.932412	-1.009745	0.000000	-3.936258	-0.996639	0.000000	-3.932714	-1.040101
6	0.000000	-2.801582	-0.698701	0.000000	-2.814565	-0.683219	0.000000	-2.820323	-0.679728	0.000000	-2.805986	-0.690905
1	-2.163147	2.101299	0.900496	-2.186282	2.109615	0.890856	-2.189910	2.106421	0.883923	-2.181283	2.120561	0.905600
6	-1.501268	-1.284279	1.183079	-1.522807	-1.288868	1.171488	-1.526326	-1.288433	1.165441	-1.515224	-1.294008	1.187834
1	-2.163147	-2.101299	0.900496	-2.186282	-2.109615	0.890856	-2.189910	-2.106421	0.883923	-2.181283	-2.120561	0.905600
1	-1.248653	-1.275198	2.244673	-1.274171	-1.278347	2.235862	-1.282504	-1.278705	2.228838	-1.260243	-1.282113	2.257952
6	1.767842	0.000000	-0.878038	1.836502	0.000000	-0.893523	1.842777	0.000000	-0.895351	1.800106	0.000000	-0.894737
1	2.004774	-0.913710	-1.420710	2.079881	-0.915859	-1.434191	2.091056	-0.913544	-1.433577	2.026579	-0.923456	-1.445145
1	2.004774	0.913710	-1.420710	2.079881	0.915859	-1.434191	2.091056	0.913544	-1.433577	2.026579	0.923456	-1.445145
6	1.730592	0.000000	0.555335	1.757518	0.000000	0.536977	1.764125	0.000000	0.533817	1.740027	0.000000	0.545384
6	1.501268	-1.284279	1.183079	1.522807	-1.288868	1.171488	1.526326	-1.288433	1.165441	1.515224	-1.294008	1.187834
1	1.248653	-1.275198	2.244673	1.274171	-1.278347	2.235862	1.282504	-1.278705	2.228838	1.260243	-1.282113	2.257952
6	0.000000	2.801582	-0.698701	0.000000	2.814565	-0.683219	0.000000	2.820323	-0.679728	0.000000	2.805986	-0.690905
8	0.000000	3.918714	-1.032115	0.000000	3.932412	-1.009745	0.000000	3.936258	-0.996639	0.000000	3.932714	-1.040101
1	2.163147	-2.101299	0.900496	2.186282	-2.109615	0.890856	2.189910	-2.106421	0.883923	2.181283	-2.120561	0.905600
6	1.501268	1.284279	1.183079	1.522807	1.288868	1.171488	1.526326	1.288433	1.165441	1.515224	1.294008	1.187834
1	2.163147	2.101299	0.900496	2.186282	2.109615	0.890856	2.189910	2.106421	0.883923	2.181283	2.120561	0.905600
1	1.248653	1.275198	2.244673	1.274171	1.278347	2.235862	1.282504	1.278705	2.228838	1.260243	1.282113	2.257952
27	0.000000	-1.145033	-0.120760	0.000000	-1.150124	-0.115791	0.000000	-1.146019	-0.115666	0.000000	-1.160959	-0.115869
27	0.000000	1.145033	-0.120760	0.000000	1.150124	-0.115791	0.000000	1.146019	-0.115666	0.000000	1.160959	-0.115869

Table S6. Optimized coordinates of the 2T-2 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	0.006349	-1.555186	1.206564	-0.044297	-1.549508	1.233282	-0.052107	-1.546290	1.233767	0.016948	-1.676959	1.255009
1	1.050879	-1.449180	1.489497	0.988816	-1.362366	1.525294	0.975402	-1.344381	1.528750	1.073050	-1.607820	1.532131
1	-0.640397	-1.876108	2.028914	-0.675599	-1.918999	2.050790	-0.678344	-1.927323	2.047018	-0.648721	-1.992299	2.076897
6	-0.360899	-1.891876	-0.135620	-0.378815	-1.870618	-0.118169	-0.377977	-1.866962	-0.116728	-0.379055	-1.941479	-0.106943
6	0.608224	-1.590871	-1.225107	0.618498	-1.561468	-1.204806	0.623235	-1.558347	-1.200749	0.582841	-1.600402	-1.210581
1	0.117787	-1.530730	-2.201925	0.132522	-1.491622	-2.186027	0.139086	-1.492972	-2.181161	0.080533	-1.530121	-2.190792
8	-3.963539	0.916158	-0.268060	-4.050736	0.961435	-0.210172	-4.068963	0.979885	-0.194371	-3.862263	0.857019	-0.363851
6	-2.899249	0.521889	-0.022768	-2.996764	0.537617	0.028382	-3.022710	0.546100	0.039925	-2.795116	0.471135	-0.059247
1	1.405285	-2.339467	-1.268899	1.380399	-2.351281	-1.249295	1.375342	-2.355637	-1.241770	1.417912	-2.319040	-1.274165
6	-1.751043	-2.035410	-0.363342	-1.763777	-2.068604	-0.372684	-1.760894	-2.069656	-0.375197	-1.784198	-2.068973	-0.325026
1	-2.381582	-2.459963	0.417773	-2.390861	-2.537568	0.389931	-2.383699	-2.548141	0.382519	-2.426287	-2.495915	0.457567
1	-2.120219	-2.147646	-1.379756	-2.115661	-2.171797	-1.398862	-2.107755	-2.176318	-1.400720	-2.170036	-2.135792	-1.349198
6	1.751043	2.035410	0.363342	1.763777	2.068604	0.372684	1.760894	2.069656	0.375197	1.784198	2.068973	0.325026
1	2.120219	2.147646	1.379756	2.115661	2.171797	1.398862	2.107755	2.176318	1.400720	2.170036	2.135792	1.349198
1	2.381582	2.459963	-0.417773	2.390861	2.537568	-0.389931	2.383699	2.548141	-0.382519	2.426287	2.495915	-0.457567
6	0.360899	1.891876	0.135620	0.378815	1.870618	0.118169	0.377977	1.866962	0.116728	0.379055	1.941479	0.106943
6	-0.608224	1.590871	1.225107	-0.618498	1.561468	1.204806	-0.623235	1.558347	1.200749	-0.582841	1.600402	1.210581
1	-1.405285	2.339467	1.268899	-1.380399	2.351281	1.249295	-1.375342	2.355637	1.241770	-1.417912	2.319040	1.274165
6	2.899249	-0.521889	0.022768	2.996764	-0.537617	-0.028382	3.022710	-0.546100	-0.039925	2.795116	-0.471135	0.059247
8	3.963539	-0.916158	0.268060	4.050736	-0.961435	0.210172	4.068963	-0.979885	0.194371	3.862263	-0.857019	0.363851
1	-0.117787	1.530730	2.201925	-0.132522	1.491622	2.186027	-0.139086	1.492972	2.181161	-0.080533	1.530121	2.190792
6	-0.006349	1.555186	-1.206564	0.044297	1.549508	-1.233282	0.052107	1.546290	-1.233767	-0.016948	1.676959	-1.255009
1	0.640397	1.876108	-2.028914	0.675599	1.918999	-2.050790	0.678344	1.927323	-2.047018	0.648721	1.992299	-2.076897
1	-1.050879	1.449180	-1.489497	-0.988816	1.362366	-1.525294	-0.975402	1.344381	-1.528750	-1.073050	1.607820	-1.532131
27	-1.313780	-0.150963	0.426266	-1.422816	-0.163773	0.477088	-1.443396	-0.167153	0.485796	-1.239538	-0.178895	0.458768
27	1.313780	0.150963	-0.426266	1.422816	0.163773	-0.477088	1.443396	0.167153	-0.485796	1.239538	0.178895	-0.458768

Table S7. Optimized coordinates of the 2S-3 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-1.177499	2.768504	-0.354465	-1.185962	2.809153	-0.336466	-1.184560	2.806590	-0.335131	-1.191589	2.812719	-0.347742
1	-1.187864	3.108754	-1.387366	-1.196270	3.160246	-1.368513	-1.196395	3.161171	-1.363987	-1.197284	3.155173	-1.389620
1	-2.148401	2.670045	0.126578	-2.157844	2.712367	0.147983	-2.154243	2.714025	0.150228	-2.170784	2.709850	0.135666
6	0.000000	2.957009	0.437720	0.000000	2.965632	0.453844	0.000000	2.964854	0.453913	0.000000	2.972799	0.449193
6	1.177499	2.768504	-0.354465	1.185962	2.809153	-0.336466	1.184560	2.806590	-0.335131	1.191589	2.812719	-0.347742
1	2.148401	2.670045	0.126578	2.157844	2.712367	0.147983	2.154243	2.714025	0.150228	2.170784	2.709850	0.135666
8	-2.578602	0.000000	-0.883252	-2.582294	0.000000	-0.892710	-2.593889	0.000000	-0.878193	-2.566739	0.000000	-0.915401
6	-1.461435	0.000000	-0.503896	-1.465006	0.000000	-0.517676	-1.477972	0.000000	-0.514313	-1.439626	0.000000	-0.520820
1	1.187864	3.108754	-1.387366	1.196270	3.160246	-1.368513	1.196395	3.161171	-1.363987	1.197284	3.155173	-1.389620
6	0.000000	2.256427	1.692529	0.000000	2.266765	1.712377	0.000000	2.263909	1.708907	0.000000	2.273127	1.718402
1	-0.922715	2.190588	2.264009	-0.925541	2.187984	2.282556	-0.923660	2.185774	2.278544	-0.931649	2.194617	2.291534
1	0.922715	2.190588	2.264009	0.925541	2.187984	2.282556	0.923660	2.185774	2.278544	0.931649	2.194617	2.291534
6	-1.177499	-2.768504	-0.354465	-1.185962	-2.809153	-0.336466	-1.184560	-2.806590	-0.335131	-1.191589	-2.812719	-0.347742
1	-2.148401	-2.670045	0.126578	-2.157844	-2.712367	0.147983	-2.154243	-2.714025	0.150228	-2.170784	-2.709850	0.135666
1	-1.187864	-3.108754	-1.387366	-1.196270	-3.160246	-1.368513	-1.196395	-3.161171	-1.363987	-1.197284	-3.155173	-1.389620
6	0.000000	-2.957009	0.437720	0.000000	-2.965632	0.453844	0.000000	-2.964854	0.453913	0.000000	-2.972799	0.449193
6	0.000000	-2.256427	1.692529	0.000000	-2.266765	1.712377	0.000000	-2.263909	1.708907	0.000000	-2.273127	1.718402
1	0.922715	-2.190588	2.264009	0.925541	-2.187984	2.282556	0.923660	-2.185774	2.278544	0.931649	-2.194617	2.291534
6	1.461435	0.000000	-0.503896	1.465006	0.000000	-0.517676	1.477972	0.000000	-0.514313	1.439626	0.000000	-0.520820
8	2.578602	0.000000	-0.883252	2.582294	0.000000	-0.892710	2.593889	0.000000	-0.878193	2.566739	0.000000	-0.915401
1	-0.922715	-2.190588	2.264009	-0.925541	-2.187984	2.282556	-0.923660	-2.185774	2.278544	-0.931649	-2.194617	2.291534
6	1.177499	-2.768504	-0.354465	1.185962	-2.809153	-0.336466	1.184560	-2.806590	-0.335131	1.191589	-2.812719	-0.347742
1	1.187864	-3.108754	-1.387366	1.196270	-3.160246	-1.368513	1.196395	-3.161171	-1.363987	1.197284	-3.155173	-1.389620
1	2.148401	-2.670045	0.126578	2.157844	-2.712367	0.147983	2.154243	-2.714025	0.150228	2.170784	-2.709850	0.135666
27	0.000000	-1.115379	-0.016480	0.000000	-1.115632	-0.030965	0.000000	-1.115944	-0.036055	0.000000	-1.117282	-0.017026
27	0.000000	1.115379	-0.016480	0.000000	1.115632	-0.030965	0.000000	1.115944	-0.036055	0.000000	1.117282	-0.017026

Table S8. Optimized coordinates of the 2T-4 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-1.200671	2.844717	-0.396773	-1.208309	2.880883	-0.442889	-1.206706	2.874483	-0.472043	-1.216900	2.892708	-0.369050
1	-1.228137	3.249444	-1.407118	-1.235845	3.239337	-1.473410	-1.233616	3.230458	-1.501499	-1.244844	3.272023	-1.398850
1	-2.158874	2.753148	0.108485	-2.168027	2.808590	0.067387	-2.164905	2.815742	0.038925	-2.181457	2.797363	0.142077
6	0.000000	2.964394	0.372622	0.000000	3.008939	0.317616	0.000000	3.014866	0.288399	0.000000	2.991883	0.395435
6	1.200671	2.844717	-0.396773	1.208309	2.880883	-0.442889	1.206706	2.874483	-0.472043	1.216900	2.892708	-0.369050
1	2.158874	2.753148	0.108485	2.168027	2.808590	0.067387	2.164905	2.815742	0.038925	2.181457	2.797363	0.142077
8	-2.705479	0.000000	-0.127618	-2.693046	0.000000	-0.046928	-2.698582	0.000000	0.068050	-2.687358	0.000000	-0.336099
6	-1.526953	0.000000	-0.201343	-1.516293	0.000000	-0.148342	-1.535211	0.000000	-0.096979	-1.491160	0.000000	-0.278079
1	1.228137	3.249444	-1.407118	1.235845	3.239337	-1.473410	1.233616	3.230458	-1.501499	1.244844	3.272023	-1.398850
6	0.000000	2.149361	1.560577	0.000000	2.257163	1.550405	0.000000	2.304797	1.541779	0.000000	2.186304	1.606220
1	-0.923846	2.027798	2.122454	-0.925849	2.157963	2.117612	-0.924894	2.217063	2.108254	-0.932030	2.060208	2.171033
1	0.923846	2.027798	2.122454	0.925849	2.157963	2.117612	0.924894	2.217063	2.108254	0.932030	2.060208	2.171033
6	-1.200671	-2.844717	-0.396773	-1.208309	-2.880883	-0.442889	-1.206706	-2.874483	-0.472043	-1.216900	-2.892708	-0.369050
1	-2.158874	-2.753148	0.108485	-2.168027	-2.808590	0.067387	-2.164905	-2.815742	0.038925	-2.181457	-2.797363	0.142077
1	-1.228137	-3.249444	-1.407118	-1.235845	-3.239337	-1.473410	-1.233616	-3.230458	-1.501499	-1.244844	-3.272023	-1.398850
6	0.000000	-2.964394	0.372622	0.000000	-3.008939	0.317616	0.000000	-3.014866	0.288399	0.000000	-2.991883	0.395435
6	0.000000	-2.149361	1.560577	0.000000	-2.257163	1.550405	0.000000	-2.304797	1.541779	0.000000	-2.186304	1.606220
1	0.923846	-2.027798	2.122454	0.925849	-2.157963	2.117612	0.924894	-2.217063	2.108254	0.932030	-2.060208	2.171033
6	1.526953	0.000000	-0.201343	1.516293	0.000000	-0.148342	1.535211	0.000000	-0.096979	1.491160	0.000000	-0.278079
8	2.705479	0.000000	-0.127618	2.693046	0.000000	-0.046928	2.698582	0.000000	0.068050	2.687358	0.000000	-0.336099
1	-0.923846	-2.027798	2.122454	-0.925849	-2.157963	2.117612	-0.924894	-2.217063	2.108254	-0.932030	-2.060208	2.171033
6	1.200671	-2.844717	-0.396773	1.208309	-2.880883	-0.442889	1.206706	-2.874483	-0.472043	1.216900	-2.892708	-0.369050
1	1.228137	-3.249444	-1.407118	1.235845	-3.239337	-1.473410	1.233616	-3.230458	-1.501499	1.244844	-3.272023	-1.398850
1	2.158874	-2.753148	0.108485	2.168027	-2.808590	0.067387	2.164905	-2.815742	0.038925	2.181457	-2.797363	0.142077
27	0.000000	-1.165317	-0.231724	0.000000	-1.174703	-0.224117	0.000000	-1.174442	-0.243350	0.000000	-1.169830	-0.187132
27	0.000000	1.165317	-0.231724	0.000000	1.174703	-0.224117	0.000000	1.174442	-0.243350	0.000000	1.169830	-0.187132

Table S9. Optimized coordinates of the 3S-1 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-0.788545	2.379188	1.193538	-0.812132	2.348184	1.204180	-0.813271	2.336500	1.203246	-0.808987	2.404125	1.208681
1	-1.850082	2.143599	1.211318	-1.861807	2.060898	1.231513	-1.859681	2.044873	1.233003	-1.874782	2.151182	1.228282
1	-0.333234	2.614551	2.153122	-0.366886	2.616227	2.162739	-0.373088	2.613167	2.159598	-0.346070	2.640316	2.174536
6	-0.220275	2.938124	0.000000	-0.268542	2.918404	0.000000	-0.278925	2.914604	0.000000	-0.230103	2.946198	0.000000
6	-0.788545	2.379188	-1.193538	-0.812132	2.348184	-1.204180	-0.813271	2.336500	-1.203246	-0.808987	2.404125	-1.208681
1	-0.333234	2.614551	-2.153122	-0.366886	2.616227	-2.162739	-0.373088	2.613167	-2.159598	-0.346070	2.640316	-2.174536
6	-1.870037	-0.235282	0.000000	-1.987169	-0.346948	0.000000	-2.010472	-0.363101	0.000000	-1.892579	-0.287778	0.000000
8	-2.928131	0.260904	0.000000	-3.058181	0.112946	0.000000	-3.079118	0.090149	0.000000	-2.980611	0.174159	0.000000
8	1.711378	-0.084548	2.327981	1.861220	0.043074	2.321913	1.881785	0.059998	2.320723	1.785307	-0.004413	2.328093
6	1.177289	0.330435	1.378055	1.285480	0.422318	1.382263	1.304142	0.435354	1.385184	1.208002	0.374857	1.373712
1	-1.850082	2.143599	-1.211318	-1.861807	2.060898	-1.231513	-1.859681	2.044873	-1.233003	-1.874782	2.151182	-1.228282
6	1.202599	3.061877	0.000000	1.142216	3.151810	0.000000	1.127286	3.163762	0.000000	1.200782	3.098673	0.000000
1	1.714647	3.321240	0.922850	1.641338	3.436453	0.925585	1.621648	3.455795	0.923634	1.717814	3.355091	0.931699
1	1.714647	3.321240	-0.922850	1.641338	3.436453	-0.925585	1.621648	3.455795	-0.923634	1.717814	3.355091	-0.931699
6	-0.788545	-2.766805	1.167997	-0.812132	-2.822298	1.175304	-0.813271	-2.827502	1.174890	-0.808987	-2.802163	1.178810
1	-0.303089	-2.637345	2.135963	-0.330406	-2.685206	2.146145	-0.330297	-2.696561	2.143722	-0.326128	-2.661792	2.156252
1	-1.824721	-3.094814	1.191058	-1.842879	-3.175671	1.197218	-1.840594	-3.184860	1.198506	-1.855571	-3.128791	1.196529
6	0.010872	-3.031228	0.000000	-0.007842	-3.052094	0.000000	-0.011194	-3.055467	0.000000	-0.001016	-3.056257	0.000000
6	1.309238	-2.439217	0.000000	1.289700	-2.455642	0.000000	1.280734	-2.449528	0.000000	1.323089	-2.502959	0.000000
1	1.884939	-2.430994	-0.922693	1.864472	-2.425576	-0.925255	1.855317	-2.419045	-0.923166	1.900034	-2.489013	-0.931841
6	1.177289	0.330435	-1.378055	1.285480	0.422318	-1.382263	1.304142	0.435354	-1.385184	1.208002	0.374857	-1.373712
8	1.711378	-0.084548	-2.327981	1.861220	0.043074	-2.321913	1.881785	0.059998	-2.320723	1.785307	-0.004413	-2.328093
1	1.884939	-2.430994	0.922693	1.864472	-2.425576	0.925255	1.855317	-2.419045	0.923166	1.900034	-2.489013	0.931841
6	-0.788545	-2.766805	-1.167997	-0.812132	-2.822298	-1.175304	-0.813271	-2.827502	-1.174890	-0.808987	-2.802163	-1.178810
1	-1.824721	-3.094814	-1.191058	-1.842879	-3.175671	-1.197218	-1.840594	-3.184860	-1.198506	-1.855571	-3.128791	-1.196529
1	-0.303089	-2.637345	-2.135963	-0.330406	-2.685206	-2.146145	-0.330297	-2.696561	-2.143722	-0.326128	-2.661792	-2.156252
27	-0.388700	-1.177786	0.000000	-0.452768	-1.189213	0.000000	-0.460174	-1.193478	0.000000	-0.403999	-1.182809	0.000000
27	0.376452	1.116808	0.000000	0.435490	1.118153	0.000000	0.445433	1.123043	0.000000	0.380593	1.110004	0.000000

Table S10. Optimized coordinates of the 3S-2 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	0.556669	-2.952244	1.220694	0.725934	-2.945490	1.228452	0.703584	-2.955878	1.226565	0.788674	-2.911458	1.234786
1	1.607796	-3.234155	1.273192	1.805055	-3.105333	1.282275	1.778213	-3.132659	1.280192	1.880144	-3.025339	1.287303
1	0.015965	-2.933630	2.162856	0.184053	-2.980584	2.172185	0.162979	-2.987492	2.168948	0.244437	-2.961328	2.184034
6	-0.160701	-3.144316	0.000000	0.033063	-3.190372	0.000000	0.007838	-3.194278	0.000000	0.100947	-3.181822	0.000000
6	0.556669	-2.952244	-1.220694	0.725934	-2.945490	-1.228452	0.703584	-2.955878	-1.226565	0.788674	-2.911458	-1.234786
1	0.015965	-2.933630	-2.162856	0.184053	-2.980584	-2.172185	0.162979	-2.987492	-2.168948	0.244437	-2.961328	-2.184034
6	1.781533	1.473610	0.000000	1.729594	1.470310	0.000000	1.741656	1.474746	0.000000	1.697681	1.451827	0.000000
8	2.899809	1.782036	0.000000	2.853467	1.758287	0.000000	2.862172	1.760646	0.000000	2.835080	1.738775	0.000000
8	-0.423737	-0.153821	2.617506	-0.461874	-0.157149	2.611671	-0.455735	-0.152857	2.609153	-0.472099	-0.170122	2.627795
6	-0.108378	-0.156712	1.475786	-0.159363	-0.158503	1.466270	-0.154656	-0.154734	1.467085	-0.173481	-0.168863	1.468265
1	1.607796	-3.234155	-1.273192	1.805055	-3.105333	-1.282275	1.778213	-3.132659	-1.280192	1.880144	-3.025339	-1.287303
6	-1.403477	-2.401442	0.000000	-1.291602	-2.597355	0.000000	-1.307328	-2.583585	0.000000	-1.250687	-2.634492	0.000000
1	-1.971695	-2.310871	0.924989	-1.867817	-2.573041	0.926084	-1.883287	-2.556564	0.923861	-1.828564	-2.619931	0.933144
1	-1.971695	-2.310871	-0.924989	-1.867817	-2.573041	-0.926084	-1.883287	-2.556564	-0.923861	-1.828564	-2.619931	-0.933144
6	-0.423737	2.773163	1.218639	-0.461874	2.826146	1.225355	-0.455735	2.826528	1.223198	-0.472099	2.824744	1.233014
1	-0.884777	2.492028	2.162059	-0.924584	2.548734	2.171366	-0.918317	2.553236	2.168249	-0.939612	2.542303	2.182797
1	0.352751	3.532541	1.268997	0.330528	3.572653	1.274853	0.332517	3.574785	1.271931	0.335389	3.564327	1.284349
6	-1.159813	2.607742	0.000000	-1.191789	2.653687	0.000000	-1.187148	2.655083	0.000000	-1.203809	2.657628	0.000000
6	-2.007135	1.454591	0.000000	-2.080140	1.528562	0.000000	-2.071414	1.528414	0.000000	-2.107177	1.535197	0.000000
1	-2.490288	1.146751	-0.925413	-2.572882	1.234335	-0.926765	-2.565964	1.237181	-0.924457	-2.598298	1.236483	-0.934030
6	-0.108378	-0.156712	-1.475786	-0.159363	-0.158503	-1.466270	-0.154656	-0.154734	-1.467085	-0.173481	-0.168863	-1.468265
8	-0.423737	-0.153821	-2.617506	-0.461874	-0.157149	-2.611671	-0.455735	-0.152857	-2.609153	-0.472099	-0.170122	-2.627795
1	-2.490288	1.146751	0.925413	-2.572882	1.234335	0.926765	-2.565964	1.237181	0.924457	-2.598298	1.236483	0.934030
6	-0.423737	2.773163	-1.218639	-0.461874	2.826146	-1.225355	-0.455735	2.826528	-1.223198	-0.472099	2.824744	-1.233014
1	0.352751	3.532541	-1.268997	0.330528	3.572653	-1.274853	0.332517	3.574785	-1.271931	0.335389	3.564327	-1.284349
1	-0.884777	2.492028	-2.162059	-0.924584	2.548734	-2.171366	-0.918317	2.553236	-2.168249	-0.939612	2.542303	-2.182797
27	0.037845	1.105256	0.000000	-0.016480	1.115953	0.000000	-0.010121	1.121029	0.000000	-0.040055	1.103505	0.000000
27	0.248255	-1.293851	0.000000	0.246199	-1.293740	0.000000	0.245757	-1.302130	0.000000	0.245503	-1.272556	0.000000

Table S11. Optimized coordinates of the 3T-3 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	1.202604	0.694324	2.677150	1.210003	0.698595	2.715021	1.208320	0.697624	2.710878	1.216465	0.702326	2.721851
1	1.231875	1.779456	2.748922	1.239448	1.785832	2.786409	1.238581	1.782621	2.787450	1.243884	1.796684	2.783277
1	2.156992	0.177107	2.748922	2.166300	0.180477	2.786409	2.163085	0.181332	2.787450	2.177916	0.178894	2.783277
6	0.000000	0.000000	3.027954	0.000000	0.000000	3.045527	0.000000	0.000000	3.045858	0.000000	0.000000	3.047609
6	-1.202604	0.694324	2.677150	-1.210003	0.698595	2.715021	-1.208320	0.697624	2.710878	-1.216465	0.702326	2.721851
1	-2.156992	0.177107	2.748922	-2.166300	0.180477	2.786409	-2.163085	0.181332	2.787450	-2.177916	0.178894	2.783277
6	0.000000	1.610594	0.000000	0.000000	1.603275	0.000000	0.000000	1.611226	0.000000	0.000000	1.592328	0.000000
8	0.000000	2.783486	0.000000	0.000000	2.776598	0.000000	0.000000	2.780354	0.000000	0.000000	2.779615	0.000000
8	2.410570	-1.391743	0.000000	2.404605	-1.388299	0.000000	2.407857	-1.390177	0.000000	2.407217	-1.389807	0.000000
6	1.394815	-0.805297	0.000000	1.388477	-0.801637	0.000000	1.395363	-0.805613	0.000000	1.378996	-0.796164	0.000000
1	-1.231875	1.779456	2.748922	-1.239448	1.785832	2.786409	-1.238581	1.782621	2.787450	-1.243884	1.796684	2.783277
6	0.000000	-1.388648	2.677150	0.000000	-1.397191	2.715021	0.000000	-1.395247	2.710878	0.000000	-1.404652	2.721851
1	0.925117	-1.956563	2.748922	0.926852	-1.966309	2.786409	0.924505	-1.963953	2.787450	0.934032	-1.975577	2.783277
1	-0.925117	-1.956563	2.748922	-0.926852	-1.966309	2.786409	-0.924505	-1.963953	2.787450	-0.934032	-1.975577	2.783277
6	1.202604	0.694324	-2.677150	1.210003	0.698595	-2.715021	1.208320	0.697624	-2.710878	1.216465	0.702326	-2.721851
1	2.156992	0.177107	-2.748922	2.166300	0.180477	-2.786409	2.163085	0.181332	-2.787450	2.177916	0.178894	-2.783277
1	1.231875	1.779456	-2.748922	1.239448	1.785832	-2.786409	1.238581	1.782621	-2.787450	1.243884	1.796684	-2.783277
6	0.000000	0.000000	-3.027954	0.000000	0.000000	-3.045527	0.000000	0.000000	-3.045858	0.000000	0.000000	-3.047609
6	0.000000	-1.388648	-2.677150	0.000000	-1.397191	-2.715021	0.000000	-1.395247	-2.710878	0.000000	-1.404652	-2.721851
1	-0.925117	-1.956563	-2.748922	-0.926852	-1.966309	-2.786409	-0.924505	-1.963953	-2.787450	-0.934032	-1.975577	-2.783277
6	-1.394815	-0.805297	0.000000	-1.388477	-0.801637	0.000000	-1.395363	-0.805613	0.000000	-1.378996	-0.796164	0.000000
8	-2.410570	-1.391743	0.000000	-2.404605	-1.388299	0.000000	-2.407857	-1.390177	0.000000	-2.407217	-1.389807	0.000000
1	0.925117	-1.956563	-2.748922	0.926852	-1.966309	-2.786409	0.924505	-1.963953	-2.787450	0.934032	-1.975577	-2.783277
6	-1.202604	0.694324	-2.677150	-1.210003	0.698595	-2.715021	-1.208320	0.697624	-2.710878	-1.216465	0.702326	-2.721851
1	-1.231875	1.779456	-2.748922	-1.239448	1.785832	-2.786409	-1.238581	1.782621	-2.787450	-1.243884	1.796684	-2.783277
1	-2.156992	0.177107	-2.748922	-2.166300	0.180477	-2.786409	-2.163085	0.181332	-2.787450	-2.177916	0.178894	-2.783277
27	0.000000	0.000000	-1.115591	0.000000	0.000000	-1.122733	0.000000	0.000000	-1.126118	0.000000	0.000000	-1.114348
27	0.000000	0.000000	1.115591	0.000000	0.000000	1.122733	0.000000	0.000000	1.126118	0.000000	0.000000	1.114348

Table S12. Optimized coordinates of the 4S-1 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-1.758691	1.856207	0.000000	-1.783217	1.920246	0.000000	-1.781556	1.923402	0.000000	-1.792318	1.910269	0.000000
1	-2.284189	1.621383	0.924158	-2.312451	1.693996	0.925997	-2.312564	1.701697	0.923875	-2.318791	1.675036	0.932917
1	-2.284189	1.621383	-0.924158	-2.312451	1.693996	-0.925997	-2.312564	1.701697	-0.923875	-2.318791	1.675036	-0.932917
6	-0.759120	2.876729	0.000000	-0.754723	2.913378	0.000000	-0.755546	2.917324	0.000000	-0.756650	2.906297	0.000000
6	0.000000	2.933205	1.214254	0.000000	2.982564	1.220690	0.000000	2.983730	1.218865	0.000000	2.978020	1.227411
1	0.877466	3.573329	1.261869	0.883052	3.619440	1.268151	0.880373	3.621173	1.266166	0.891056	3.614753	1.274984
6	2.015999	1.313288	0.000000	2.013666	1.356156	0.000000	2.018710	1.357907	0.000000	1.999975	1.358776	0.000000
8	3.170685	1.409486	0.000000	3.166327	1.473821	0.000000	3.167671	1.472979	0.000000	3.164224	1.494341	0.000000
8	0.000000	0.000000	2.667109	0.000000	0.000000	2.650701	0.000000	0.000000	2.647911	0.000000	0.000000	2.665112
6	0.000000	0.000000	1.486345	0.000000	0.000000	1.468884	0.000000	0.000000	1.469415	0.000000	0.000000	1.471355
1	-0.491026	2.723005	2.160892	-0.490333	2.770751	2.169862	-0.490623	2.776705	2.166748	-0.491908	2.757062	2.181202
6	0.000000	2.933205	-1.214254	0.000000	2.982564	-1.220690	0.000000	2.983730	-1.218865	0.000000	2.978020	-1.227411
1	-0.491026	2.723005	-2.160892	-0.490333	2.770751	-2.169862	-0.490623	2.776705	-2.166748	-0.491908	2.757062	-2.181202
1	0.877466	3.573329	-1.261869	0.883052	3.619440	-1.268151	0.880373	3.621173	-1.266166	0.891056	3.614753	-1.274984
6	0.000000	-2.933205	1.214254	0.000000	-2.982564	1.220690	0.000000	-2.983730	1.218865	0.000000	-2.978020	1.227411
1	-0.877466	-3.573329	1.261869	-0.883052	-3.619440	1.268151	-0.880373	-3.621173	1.266166	-0.891056	-3.614753	1.274984
1	0.491026	-2.723005	2.160892	0.490333	-2.770751	2.169862	0.490623	-2.776705	2.166748	0.491908	-2.757062	2.181202
6	0.759120	-2.876729	0.000000	0.754723	-2.913378	0.000000	0.755546	-2.917324	0.000000	0.756650	-2.906297	0.000000
6	0.000000	-2.933205	-1.214254	0.000000	-2.982564	-1.220690	0.000000	-2.983730	-1.218865	0.000000	-2.978020	-1.227411
1	0.491026	-2.723005	-2.160892	0.490333	-2.770751	-2.169862	0.490623	-2.776705	-2.166748	0.491908	-2.757062	-2.181202
6	0.000000	0.000000	-1.486345	0.000000	0.000000	-1.468884	0.000000	0.000000	-1.469415	0.000000	0.000000	-1.471355
8	0.000000	0.000000	-2.667109	0.000000	0.000000	-2.650701	0.000000	0.000000	-2.647911	0.000000	0.000000	-2.665112
8	-3.170685	-1.409486	0.000000	-3.166327	-1.473821	0.000000	-3.167671	-1.472979	0.000000	-3.164224	-1.494341	0.000000
6	-2.015999	-1.313288	0.000000	-2.013666	-1.356156	0.000000	-2.018710	-1.357907	0.000000	-1.999975	-1.358776	0.000000
1	-0.877466	-3.573329	-1.261869	-0.883052	-3.619440	-1.268151	-0.880373	-3.621173	-1.266166	-0.891056	-3.614753	-1.274984
6	1.758691	-1.856207	0.000000	1.783217	-1.920246	0.000000	1.781556	-1.923402	0.000000	1.792318	-1.910269	0.000000
1	2.284189	-1.621383	0.924158	2.312451	-1.693996	0.925997	2.312564	-1.701697	0.923875	2.318791	-1.675036	0.932917
1	2.284189	-1.621383	-0.924158	2.312451	-1.693996	-0.925997	2.312564	-1.701697	-0.923875	2.318791	-1.675036	-0.932917
27	-0.230655	-1.230531	0.000000	-0.230001	-1.246896	0.000000	-0.227594	-1.251587	0.000000	-0.231418	-1.235629	0.000000
27	0.230655	1.230531	0.000000	0.230001	1.246896	0.000000	0.227594	1.251587	0.000000	0.231418	1.235629	0.000000

Table S13. Optimized coordinates of the 4S-2 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	0.000000	1.652845	-2.032992	0.000000	1.699062	-2.070570	0.000000	1.703729	-2.068435	0.000000	1.689219	-2.081067
1	-0.924898	1.364094	-2.529124	-0.926211	1.414671	-2.569827	-0.924010	1.422455	-2.569327	-0.933344	1.400138	-2.578783
1	0.924898	1.364094	-2.529124	0.926211	1.414671	-2.569827	0.924010	1.422455	-2.569327	0.933344	1.400138	-2.578783
6	0.000000	2.778598	-1.153740	0.000000	2.808413	-1.168606	0.000000	2.813029	-1.168608	0.000000	2.801323	-1.170904
6	-1.213910	2.920003	-0.404304	-1.220432	2.966975	-0.426452	-1.218600	2.968706	-0.425127	-1.227146	2.961693	-0.427145
1	-1.261047	3.658192	0.392564	-1.267638	3.706927	0.372261	-1.265598	3.708704	0.371042	-1.274663	3.701509	0.380395
6	0.000000	1.570872	1.773541	0.000000	1.619375	1.759587	0.000000	1.622416	1.764527	0.000000	1.615642	1.744454
8	0.000000	1.833576	2.901332	0.000000	1.903688	2.882109	0.000000	1.904209	2.883822	0.000000	1.914203	2.876710
8	2.630342	0.000000	-0.402633	2.632926	0.000000	-0.283676	2.630067	0.000000	-0.283435	2.650069	0.000000	-0.264633
6	1.474104	0.000000	-0.160023	1.462082	0.000000	-0.120766	1.462399	0.000000	-0.122124	1.465594	0.000000	-0.112875
1	-2.160541	2.651595	-0.866431	-2.169720	2.694993	-0.885907	-2.166622	2.701656	-0.885538	-2.181058	2.681030	-0.887445
6	1.213910	2.920003	-0.404304	1.220432	2.966975	-0.426452	1.218600	2.968706	-0.425127	1.227146	2.961693	-0.427145
1	2.160541	2.651595	-0.866431	2.169720	2.694993	-0.885907	2.166622	2.701656	-0.885538	2.181058	2.681030	-0.887445
1	1.261047	3.658192	0.392564	1.267638	3.706927	0.372261	1.265598	3.708704	0.371042	1.274663	3.701509	0.380395
6	-1.213910	-2.920003	-0.404304	-1.220432	-2.966975	-0.426452	-1.218600	-2.968706	-0.425127	-1.227146	-2.961693	-0.427145
1	-2.160541	-2.651595	-0.866431	-2.169720	-2.694993	-0.885907	-2.166622	-2.701656	-0.885538	-2.181058	-2.681030	-0.887445
1	-1.261047	-3.658192	0.392564	-1.267638	-3.706927	0.372261	-1.265598	-3.708704	0.371042	-1.274663	-3.701509	0.380395
6	0.000000	-2.778598	-1.153740	0.000000	-2.808413	-1.168606	0.000000	-2.813029	-1.168608	0.000000	-2.801323	-1.170904
6	0.000000	-1.652845	-2.032992	0.000000	-1.699062	-2.070570	0.000000	-1.703729	-2.068435	0.000000	-1.689219	-2.081067
1	0.924898	-1.364094	-2.529124	0.926211	-1.414671	-2.569827	0.924010	-1.422455	-2.569327	0.933344	-1.400138	-2.578783
6	-1.474104	0.000000	-0.160023	-1.462082	0.000000	-0.120766	-1.462399	0.000000	-0.122124	-1.465594	0.000000	-0.112875
8	-2.630342	0.000000	-0.402633	-2.632926	0.000000	-0.283676	-2.630067	0.000000	-0.283435	-2.650069	0.000000	-0.264633
8	0.000000	-1.833576	2.901332	0.000000	-1.903688	2.882109	0.000000	-1.904209	2.883822	0.000000	-1.914203	2.876710
6	0.000000	-1.570872	1.773541	0.000000	-1.619375	1.759587	0.000000	-1.622416	1.764527	0.000000	-1.615642	1.744454
1	-0.924898	-1.364094	-2.529124	-0.926211	-1.414671	-2.569827	-0.924010	-1.422455	-2.569327	-0.933344	-1.400138	-2.578783
6	1.213910	-2.920003	-0.404304	1.220432	-2.966975	-0.426452	1.218600	-2.968706	-0.425127	1.227146	-2.961693	-0.427145
1	1.261047	-3.658192	0.392564	1.267638	-3.706927	0.372261	1.265598	-3.708704	0.371042	1.274663	-3.701509	0.380395
1	2.160541	-2.651595	-0.866431	2.169720	-2.694993	-0.885907	2.166622	-2.701656	-0.885538	2.181058	-2.681030	-0.887445
27	0.000000	-1.253260	0.011383	0.000000	-1.269346	0.003668	0.000000	-1.273818	0.001256	0.000000	-1.258121	0.004561
27	0.000000	1.253260	0.011383	0.000000	1.269346	0.003668	0.000000	1.273818	0.001256	0.000000	1.258121	0.004561

Table S14. Optimized coordinates of the 4S-3 structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	1.955275	-1.602299	0.697909	1.934944	-1.708018	0.805606	1.875406	-1.758056	0.878626	1.973008	-1.685034	0.742189
1	2.008372	-1.943987	1.729371	1.925694	-2.080914	1.829829	1.820455	-2.137654	1.896985	1.995557	-2.053516	1.774583
1	2.647053	-0.806279	0.428359	2.657237	-0.920169	0.594895	2.625919	-0.991079	0.702238	2.679973	-0.883162	0.501169
6	1.507794	-2.505653	-0.322143	1.503145	-2.565370	-0.262853	1.469242	-2.599333	-0.210572	1.503902	-2.551741	-0.312679
6	0.458758	-3.392680	0.073311	0.426581	-3.455184	0.057737	0.360070	-3.462459	0.061313	0.438771	-3.451929	0.049463
1	-0.045815	-3.990086	-0.681712	-0.055490	-4.024174	-0.736687	-0.100571	-4.016517	-0.753543	-0.073740	-4.025570	-0.731448
6	-1.389783	-1.240184	-1.089131	-1.333873	-1.283380	-1.157415	-1.307985	-1.262667	-1.210044	-1.363176	-1.290622	-1.103849
8	-2.319802	-1.218970	-1.787710	-2.222091	-1.296113	-1.907833	-2.161304	-1.270460	-1.994110	-2.290667	-1.310343	-1.826824
8	-1.294315	-1.123607	2.595139	-1.389713	-1.206452	2.556894	-1.469242	-1.181185	2.521485	-1.340408	-1.233629	2.587089
6	-0.773575	-1.176732	1.559259	-0.831221	-1.222864	1.539323	-0.890911	-1.205305	1.519290	-0.788641	-1.234826	1.551356
1	0.448346	-3.790672	1.084837	0.354858	-3.874346	1.060976	0.240832	-3.886743	1.055795	0.402608	-3.868906	1.062594
6	1.294315	-1.868820	-1.589536	1.389713	-1.908289	-1.535397	1.421550	-1.931807	-1.480018	1.340408	-1.894365	-1.588309
1	1.984650	-1.099325	-1.922244	2.110294	-1.141125	-1.809573	2.172276	-1.184607	-1.718630	2.043736	-1.110915	-1.887628
1	0.804185	-2.435396	-2.378371	0.934836	-2.447849	-2.366635	0.993011	-2.455370	-2.332728	0.851364	-2.438899	-2.405308
6	-1.955275	1.602299	0.697909	-1.934944	1.708018	0.805606	-1.875406	1.758056	0.878626	-1.973008	1.685034	0.742189
1	-2.008372	1.943987	1.729371	-1.925694	2.080914	1.829829	-1.820455	2.137654	1.896985	-1.995557	2.053516	1.774583
1	-2.647053	0.806279	0.428359	-2.657237	0.920169	0.594895	-2.625919	0.991079	0.702238	-2.679973	0.883162	0.501169
6	-1.507794	2.505653	-0.322143	-1.503145	2.565370	-0.262853	-1.469242	2.599333	-0.210572	-1.503902	2.551741	-0.312679
6	-0.458758	3.392680	0.073311	-0.426581	3.455184	0.057737	-0.360070	3.462459	0.061313	-0.438771	3.451929	0.049463
1	0.045815	3.990086	-0.681712	0.055490	4.024174	-0.736687	0.100571	4.016517	-0.753543	0.073740	4.025570	-0.731448
6	1.389783	1.240184	-1.089131	1.333873	1.283380	-1.157415	1.307985	1.262667	-1.210044	1.363176	1.290622	-1.103849
8	2.319802	1.218970	-1.787710	2.222091	1.296113	-1.907833	2.161304	1.270460	-1.994110	2.290667	1.310343	-1.826824
8	1.294315	1.123607	2.595139	1.389713	1.206452	2.556894	1.469242	1.181185	2.521485	1.340408	1.233629	2.587089
6	0.773575	1.176732	1.559259	0.831221	1.222864	1.539323	0.890911	1.205305	1.519290	0.788641	1.234826	1.551356
1	-0.448346	3.790672	1.084837	-0.354858	3.874346	1.060976	-0.240832	3.886743	1.055795	-0.402608	3.868906	1.062594
6	-1.294315	1.868820	-1.589536	-1.389713	1.908289	-1.535397	-1.421550	1.931807	-1.480018	-1.340408	1.894365	-1.588309
1	-1.984650	1.099325	-1.922244	-2.110294	1.141125	-1.809573	-2.172276	1.184607	-1.718630	-2.043736	1.110915	-1.887628
1	-0.804185	2.435396	-2.378371	-0.934836	2.447849	-2.366635	-0.993011	2.455370	-2.332728	-0.851364	2.438899	-2.405308
27	-0.015898	1.338771	-0.025840	-0.011876	1.360441	-0.016567	0.001895	1.361289	-0.015581	-0.010907	1.356104	-0.015745
27	0.015898	-1.338771	-0.025840	0.011876	-1.360441	-0.016567	-0.001895	-1.361289	-0.015581	0.010907	-1.356104	-0.015745

Table S15. Optimized coordinates of the 5S structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-2.533457	-1.037957	-1.573216	-2.584515	-1.211542	-1.482365	-2.510479	-1.161649	-1.559233	-3.089909	-0.653199	-1.309351
1	-2.116193	-0.723923	-2.525769	-2.131024	-1.032311	-2.454687	-2.033793	-0.932260	-2.507180	-2.779399	-0.490169	-2.347326
1	-2.763791	-2.096022	-1.471818	-2.852843	-2.243733	-1.256153	-2.770483	-2.205389	-1.393421	-3.624370	-1.587666	-1.101067
6	-3.274870	-0.097977	-0.785301	-3.297886	-0.154707	-0.822331	-3.266963	-0.150064	-0.879966	-3.278652	0.476780	-0.428263
6	-2.764928	1.240069	-0.832309	-2.769200	1.163768	-1.028652	-2.752225	1.183237	-0.999986	-2.398312	1.582693	-0.694897
1	-3.175189	1.980972	-0.150105	-3.179174	1.992435	-0.451142	-3.200823	1.975024	-0.403297	-2.348614	2.419345	0.012272
8	-0.533055	-2.834875	0.919843	-0.690136	-2.745358	1.264175	-0.668721	-2.797231	1.162355	-1.431601	-3.035495	0.908913
6	-0.902683	-1.787502	0.594401	-1.012089	-1.731292	0.809436	-1.002804	-1.770054	0.756627	-1.440301	-1.917388	0.567744
1	-2.355493	1.618762	-1.764951	-2.325478	1.419559	-1.988889	-2.283892	1.493692	-1.929696	-2.094397	1.795221	-1.726621
6	-3.593630	-0.559762	0.531931	-3.677524	-0.444840	0.531542	-3.687969	-0.511514	0.442786	-3.453484	0.158104	0.966794
1	-3.831288	-1.608933	0.686988	-3.947190	-1.463522	0.808677	-3.951656	-1.544420	0.658900	-3.993004	-0.753269	1.249200
1	-4.007164	0.136614	1.256773	-4.087949	0.346713	1.157763	-4.137272	0.240057	1.088062	-3.424177	0.958683	1.714260
6	1.810420	-1.387660	-0.950729	1.871696	-1.516931	-0.682254	1.900205	-1.461340	-0.771899	1.709268	-1.643209	-0.128587
1	1.684165	-2.318816	-0.392071	1.761328	-2.341267	0.029474	1.752121	-2.329940	-0.125527	1.724077	-2.179657	0.833736
1	1.396184	-1.472462	-1.959663	1.447996	-1.784143	-1.657105	1.534098	-1.667540	-1.782179	1.097997	-2.180209	-0.872575
6	3.139016	-0.738316	-0.878560	3.217722	-0.874883	-0.752995	3.251636	-0.826715	-0.730856	3.023531	-1.147105	-0.649566
6	4.285130	-1.261759	-0.400066	4.396378	-1.359584	-0.307630	4.403769	-1.355331	-0.273329	4.269730	-1.573953	-0.327657
1	5.164249	-0.641845	-0.244158	5.290847	-0.735974	-0.285093	5.299420	-0.745971	-0.163943	5.160781	-1.032433	-0.669129
6	1.111212	2.102756	0.319403	1.123976	2.125866	0.025918	1.086371	2.133606	0.139629	1.055692	2.070174	-0.500487
8	1.256804	3.235899	0.507856	1.255440	3.276434	0.036157	1.188434	3.279170	0.236288	1.204502	3.169727	-0.873718
8	1.984699	-0.867559	2.490918	2.048764	-0.380794	2.640180	1.948921	-0.517358	2.612164	2.680127	0.477077	2.438759
6	1.639561	-0.363999	1.509869	1.678104	-0.088685	1.585243	1.613018	-0.171470	1.565611	2.011011	0.424580	1.484967
1	4.359884	-2.316069	-0.146187	4.488347	-2.387905	0.043744	4.472648	-2.406370	0.002279	4.422368	-2.470886	0.285428
6	2.828590	0.684701	-1.087711	2.893629	0.530806	-1.107779	2.952349	0.606286	-0.992147	2.642005	0.123395	-1.332938
1	2.512415	0.952410	-2.099446	2.611370	0.693455	-2.153967	2.745783	0.849965	-2.038522	2.183469	0.010414	-2.327871
1	3.517043	1.418764	-0.662708	3.579846	1.302597	-0.744172	3.620620	1.338853	-0.532090	3.380096	0.940599	-1.300087
27	1.061413	0.349101	-0.075964	1.099775	0.331961	-0.095326	1.101553	0.344542	-0.110338	1.018079	0.344617	-0.027200
27	-1.573541	-0.208874	0.089706	-1.605133	-0.199378	0.107640	-1.613994	-0.214186	0.114584	-1.532197	-0.211699	0.065248
6	-0.010639	0.473154	-1.515303	0.054094	0.234242	-1.543651	0.141058	0.342859	-1.609216	-0.175397	-0.195590	-1.395176
8	-0.277502	0.675001	-2.642468	-0.200317	0.271218	-2.692157	-0.139174	0.431578	-2.741600	-0.225976	-0.419378	-2.568383
6	-1.227507	0.786629	1.537974	-1.301143	0.955908	1.437315	-1.361770	0.891831	1.499860	-0.637411	0.631938	1.432597
8	-1.130280	1.412806	2.508824	-1.235107	1.689202	2.332682	-1.305463	1.593416	2.416377	-0.633336	1.177809	2.483356

Table S16. Optimized coordinates of the 6S structure

	M06-L			B3LYP*			B3LYP			BP86		
	x	y	z	x	y	z	x	y	z	x	y	z
6	-0.897392	1.981735	-1.515517	-0.948352	2.034894	-1.504797	-0.935925	2.010938	-1.511397	-0.969635	2.107342	-1.496544
1	-0.688803	1.368781	-2.397076	-0.729427	1.445244	-2.400533	-0.707244	1.420735	-2.402220	-0.774919	1.519065	-2.406246
1	-1.975179	2.055532	-1.348043	-2.030217	2.075437	-1.337058	-2.018211	2.047195	-1.357298	-2.052309	2.170796	-1.301824
6	-0.146689	3.254844	-1.385830	-0.244892	3.350155	-1.382700	-0.246871	3.334767	-1.396717	-0.217219	3.394443	-1.346101
6	0.533926	3.897216	-2.353207	0.292226	4.090901	-2.372541	0.277807	4.078106	-2.388190	0.371367	4.125251	-2.327052
1	1.172433	4.745780	-2.122413	0.894951	4.973177	-2.154083	0.869382	4.966780	-2.174408	1.009552	4.984763	-2.087876
6	0.898423	1.528829	1.833143	0.903553	1.567863	1.811800	0.899505	1.563347	1.825029	0.887509	1.574736	1.788761
8	1.458348	1.715687	2.827102	1.470980	1.781489	2.796150	1.459016	1.770759	2.810967	1.459283	1.803815	2.782149
8	2.319473	0.848758	-1.538445	2.299745	0.932613	-1.549238	2.326257	0.951713	-1.524202	2.253897	0.895824	-1.595134
6	1.435165	1.033692	-0.817221	1.407030	1.083983	-0.829666	1.427305	1.093456	-0.816257	1.364071	1.062437	-0.855430
1	0.469310	3.582548	-3.391543	0.139198	3.830745	-3.420545	0.126430	3.813372	-3.433373	0.223487	3.879154	-3.385712
6	-0.020015	3.445341	0.070998	-0.003478	3.482485	0.081298	-0.005437	3.474219	0.067609	0.008653	3.504838	0.121768
1	-0.932093	3.757571	0.586105	-0.862171	3.829498	0.667267	-0.862675	3.831334	0.646347	-0.861122	3.826976	0.717208
1	0.855242	3.989927	0.431411	0.917830	3.990964	0.382734	0.912754	3.987614	0.363900	0.936997	3.997828	0.448988
6	0.897392	-1.981735	-1.515517	0.948352	-2.034894	-1.504797	0.935925	-2.010938	-1.511397	0.969635	-2.107342	-1.496544
1	0.688803	-1.368781	-2.397076	0.729427	-1.445244	-2.400533	0.707244	-1.420735	-2.402220	0.774919	-1.519065	-2.406246
1	1.975179	-2.055532	-1.348043	2.030217	-2.075437	-1.337058	2.018211	-2.047195	-1.357298	2.052309	-2.170796	-1.301824
6	0.146689	-3.254844	-1.385830	0.244892	-3.350155	-1.382700	0.246871	-3.334767	-1.396717	0.217219	-3.394443	-1.346101
6	-0.533926	-3.897216	-2.353207	-0.292226	-4.090901	-2.372541	-0.277807	-4.078106	-2.388190	-0.371367	-4.125251	-2.327052
1	-1.172433	-4.745780	-2.122413	-0.894951	-4.973177	-2.154083	-0.869382	-4.966780	-2.174408	-1.009552	-4.984763	-2.087876
6	-0.898423	-1.528829	1.833143	-0.903553	-1.567863	1.811800	-0.899505	-1.563347	1.825029	-0.887509	-1.574736	1.788761
8	-1.458348	-1.715687	2.827102	-1.470980	-1.781489	2.796150	-1.459016	-1.770759	2.810967	-1.459283	-1.803815	2.782149
8	-2.319473	-0.848758	-1.538445	-2.299745	-0.932613	-1.549238	-2.326257	-0.951713	-1.524202	-2.253897	-0.895824	-1.595134
6	-1.435165	-1.033692	-0.817221	-1.407030	-1.083983	-0.829666	-1.427305	-1.093456	-0.816257	-1.364071	-1.062437	-0.855430
1	-0.469310	-3.582548	-3.391543	-0.139198	-3.830745	-3.420545	-0.126430	-3.813372	-3.433373	-0.223487	-3.879154	-3.385712
6	0.020015	-3.445341	0.070998	0.003478	-3.482485	0.081298	0.005437	-3.474219	0.067609	-0.008653	-3.504838	0.121768
1	0.932093	-3.757571	0.586105	0.862171	-3.829498	0.667267	0.862675	-3.831334	0.646347	0.861122	-3.826976	0.717208
1	-0.855242	-3.989927	0.431411	-0.917830	-3.990964	0.382734	-0.912754	-3.987614	0.363900	-0.936997	-3.997828	0.448988
27	-0.020015	-1.384741	0.260160	-0.003478	-1.413108	0.251268	-0.005437	-1.412012	0.250973	0.008653	-1.415693	0.246957
27	0.020015	1.384741	0.260160	0.003478	1.413108	0.251268	0.005437	1.412012	0.250973	-0.008653	1.415693	0.246957
6	1.641275	-1.223093	0.912645	1.640442	-1.291920	0.943716	1.643931	-1.301069	0.941767	1.648842	-1.271545	0.928846
8	2.730674	-1.186797	1.304736	2.714547	-1.295968	1.377504	2.716788	-1.313703	1.369449	2.732509	-1.257200	1.370752
6	-1.641275	1.223093	0.912645	-1.640442	1.291920	0.943716	-1.643931	1.301069	0.941767	-1.648842	1.271545	0.928846
8	-2.730674	1.186797	1.304736	-2.714547	1.295968	1.377504	-2.716788	1.313703	1.369449	-2.732509	1.257200	1.370752

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

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
59(1)	60(0)	60(0)	59(0)	904(10)	891(7)	896(7)	871(6)
64(0)	68(1)	70(1)	60(1)	904(0)	893(1)	900(1)	871(0)
69(1)	72(0)	73(0)	73(1)	928(0)	946(0)	952(0)	914(0)
78(0)	78(0)	78(0)	81(0)	945(0)	948(0)	958(0)	914(0)
110(0)	113(0)	112(0)	113(0)	946(0)	949(0)	959(0)	920(0)
124(0)	135(0)	138(0)	126(1)	962(9)	977(6)	984(5)	946(4)
180(3)	174(2)	175(2)	174(3)	963(1)	979(8)	986(8)	950(9)
212(0)	186(0)	186(0)	191(0)	993(3)	1006(3)	1015(4)	975(2)
234(0)	216(0)	220(0)	208(0)	1028(0)	1019(0)	1028(0)	989(0)
236(2)	226(5)	230(5)	216(3)	1033(2)	1025(7)	1034(7)	996(5)
318(0)	279(0)	279(0)	281(1)	1037(0)	1034(0)	1044(0)	1002(0)
330(1)	285(0)	288(0)	283(0)	1041(2)	1036(0)	1045(0)	1006(1)
367(0)	373(0)	376(0)	360(0)	1351(1)	1354(3)	1363(3)	1317(1)
372(0)	376(15)	378(15)	366(0)	1355(8)	1357(0)	1367(0)	1321(9)
388(15)	380(0)	384(0)	367(14)	1369(0)	1358(4)	1368(2)	1325(0)
389(0)	393(0)	398(0)	376(0)	1375(0)	1363(1)	1372(1)	1331(0)
444(0)	435(1)	436(0)	428(2)	1470(13)	1480(12)	1493(11)	1435(18)
449(10)	447(3)	449(3)	442(3)	1476(24)	1487(33)	1500(33)	1440(29)
451(3)	453(6)	453(3)	445(15)	1477(14)	1492(0)	1505(0)	1447(6)
473(0)	465(0)	468(0)	457(0)	1481(0)	1493(12)	1507(12)	1450(0)
511(31)	502(30)	497(36)	508(19)	1494(0)	1496(8)	1509(7)	1453(1)
517(10)	509(10)	507(12)	511(7)	1497(9)	1497(0)	1511(1)	1454(11)
524(51)	523(0)	517(65)	525(0)	2042(2020)	2031(2013)	2054(2122)	1957(1669)
532(0)	526(50)	520(0)	534(9)	2053(275)	2041(264)	2065(273)	1967(227)
535(2)	533(4)	525(2)	545(35)	3100(74)	3097(0)	3115(0)	3041(0)
544(10)	533(13)	531(7)	551(5)	3101(0)	3099(11)	3117(13)	3042(10)
585(0)	615(1)	621(1)	594(0)	3101(30)	3099(9)	3118(11)	3043(9)
631(0)	626(1)	635(1)	595(2)	3101(24)	3101(25)	3120(25)	3044(32)
638(1)	628(0)	637(0)	600(1)	3134(1)	3129(1)	3148(0)	3065(1)
654(59)	673(51)	680(50)	646(55)	3134(1)	3129(1)	3148(0)	3066(1)
754(1)	774(0)	779(0)	748(1)	3192(0)	3179(0)	3196(0)	3126(0)
766(0)	774(0)	781(1)	753(0)	3193(14)	3181(4)	3198(5)	3127(2)
771(1)	782(1)	789(1)	759(0)	3193(6)	3181(2)	3198(3)	3127(4)
771(0)	782(0)	789(0)	759(1)	3194(19)	3184(9)	3201(10)	3129(8)
789(4)	805(6)	814(5)	775(7)	3217(2)	3205(6)	3224(5)	3143(7)
806(5)	831(9)	842(10)	795(5)	3217(0)	3206(0)	3224(0)	3143(0)

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

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
44(1)	46(1)	47(0)	42(1)	863(41)	866(0)	871(0)	848(6)
58(0)	60(0)	60(0)	51(0)	865(0)	872(9)	878(10)	849(0)
62(0)	62(0)	65(0)	65(0)	892(0)	901(24)	909(25)	882(21)
77(0)	80(0)	80(0)	84(0)	893(0)	903(0)	910(0)	883(0)
102(0)	99(0)	103(0)	118(1)	964(0)	965(0)	974(0)	935(0)
125(1)	117(1)	117(1)	125(0)	965(1)	965(2)	975(2)	935(2)
157(5)	160(4)	161(4)	142(4)	1015(0)	1021(0)	1030(0)	987(0)
160(0)	164(0)	166(0)	147(0)	1018(21)	1024(8)	1033(9)	988(21)
202(0)	193(0)	193(0)	197(0)	1037(3)	1052(8)	1064(8)	1007(12)
220(6)	221(6)	223(5)	215(7)	1041(0)	1053(0)	1065(0)	1010(0)
313(0)	301(0)	302(0)	293(0)	1079(9)	1079(8)	1091(8)	1038(5)
323(2)	313(4)	314(5)	306(4)	1080(0)	1080(0)	1092(0)	1039(0)
345(1)	324(1)	325(1)	321(2)	1351(20)	1338(0)	1347(0)	1310(15)
367(0)	340(0)	340(0)	350(0)	1352(0)	1342(39)	1352(46)	1310(0)
375(0)	363(0)	363(0)	365(0)	1371(0)	1365(5)	1374(4)	1336(0)
389(3)	371(3)	371(4)	373(1)	1372(10)	1368(0)	1377(0)	1338(2)
416(0)	424(0)	425(0)	412(0)	1457(13)	1458(14)	1471(13)	1422(17)
426(11)	427(5)	427(5)	416(15)	1458(0)	1459(0)	1471(0)	1424(0)
454(10)	460(14)	463(22)	440(9)	1493(0)	1499(0)	1511(0)	1456(0)
478(56)	472(0)	473(0)	464(0)	1495(34)	1501(46)	1512(45)	1458(18)
479(0)	490(0)	481(0)	476(0)	1510(0)	1507(0)	1522(0)	1466(0)
484(0)	490(56)	482(54)	495(40)	1510(37)	1507(29)	1522(31)	1468(29)
502(0)	508(0)	512(0)	500(0)	2065(2006)	2056(1886)	2080(1935)	1968(1945)
518(20)	524(39)	524(46)	509(31)	2078(0)	2065(0)	2089(0)	1986(0)
533(0)	528(0)	525(0)	528(21)	3062(97)	3048(46)	3063(50)	3000(47)
535(27)	529(8)	530(4)	532(0)	3063(0)	3048(0)	3063(0)	3000(0)
656(12)	648(8)	651(8)	649(10)	3092(0)	3083(5)	3103(0)	3031(7)
665(0)	656(0)	659(0)	654(0)	3092(22)	3083(0)	3103(6)	3032(0)
679(15)	690(12)	697(10)	671(12)	3116(34)	3105(0)	3120(0)	3060(0)
703(0)	705(0)	709(0)	692(0)	3117(0)	3105(21)	3120(24)	3060(8)
723(22)	726(25)	728(25)	720(3)	3133(0)	3109(7)	3127(9)	3063(0)
723(0)	728(0)	730(0)	725(0)	3133(35)	3110(0)	3127(0)	3063(16)
755(9)	758(8)	765(10)	752(2)	3206(8)	3188(9)	3206(13)	3156(0)
768(0)	770(0)	777(0)	757(0)	3207(0)	3189(0)	3207(0)	3156(8)
846(0)	850(33)	853(33)	837(0)	3218(0)	3207(0)	3225(0)	3158(0)
853(8)	850(0)	854(0)	839(35)	3218(26)	3208(9)	3225(10)	3160(0)

Table S19. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **2S-3**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
53(0)	45(0)	42(0)	51(0)	904(0)	918(0)	927(0)	887(0)
58(2)	56(2)	53(0)	55(2)	905(3)	919(2)	927(3)	888(1)
66(0)	60(0)	55(2)	71(0)	918(1)	926(14)	937(15)	893(10)
102(0)	102(0)	101(0)	103(0)	921(8)	927(13)	938(13)	894(10)
124(1)	123(1)	113(11)	121(1)	948(0)	950(0)	960(0)	920(0)
145(2)	135(5)	124(1)	143(2)	948(0)	951(0)	960(0)	921(0)
160(0)	163(0)	166(0)	159(0)	1012(29)	997(14)	1005(16)	971(14)
209(1)	206(2)	189(9)	208(0)	1015(0)	1000(0)	1009(0)	973(0)
230(0)	221(0)	210(1)	222(0)	1037(0)	1030(0)	1040(0)	1002(0)
251(0)	229(16)	220(0)	243(0)	1040(1)	1034(0)	1043(0)	1006(0)
297(13)	239(0)	237(0)	303(4)	1040(0)	1035(0)	1045(0)	1006(0)
341(3)	305(6)	308(7)	311(22)	1041(3)	1036(2)	1046(2)	1007(1)
357(0)	321(0)	315(0)	327(2)	1370(0)	1368(0)	1377(0)	1334(0)
366(0)	326(3)	327(3)	340(0)	1370(0)	1368(0)	1378(0)	1334(1)
366(1)	374(11)	371(14)	365(0)	1374(2)	1370(3)	1379(3)	1337(2)
398(0)	374(1)	376(2)	381(2)	1374(0)	1371(1)	1380(1)	1338(0)
402(1)	390(3)	388(3)	390(1)	1486(0)	1490(2)	1504(2)	1448(3)
407(2)	396(0)	392(0)	392(0)	1488(7)	1492(18)	1505(19)	1450(15)
419(0)	397(0)	400(0)	406(0)	1497(0)	1499(0)	1513(0)	1457(0)
421(0)	410(0)	414(0)	413(0)	1497(9)	1500(14)	1513(15)	1458(12)
425(17)	429(8)	433(9)	414(7)	1500(4)	1508(2)	1521(2)	1467(2)
435(3)	439(1)	443(1)	426(1)	1501(12)	1508(6)	1521(5)	1467(6)
450(0)	452(0)	453(1)	442(0)	1932(1044)	1917(1046)	1942(1108)	1841(871)
495(0)	486(0)	484(0)	492(0)	1950(168)	1934(173)	1960(174)	1858(152)
500(18)	490(18)	484(19)	502(13)	3128(0)	3129(0)	3147(0)	3073(1)
537(9)	534(10)	532(12)	532(6)	3128(35)	3129(6)	3147(7)	3073(7)
694(0)	694(0)	702(0)	669(0)	3128(14)	3129(1)	3148(1)	3074(0)
709(0)	707(0)	714(0)	683(0)	3129(18)	3129(5)	3148(6)	3074(7)
758(2)	756(12)	765(21)	727(0)	3133(6)	3135(0)	3154(0)	3079(0)
760(0)	761(0)	772(0)	731(0)	3133(16)	3135(0)	3154(1)	3079(0)
771(1)	765(1)	773(1)	736(1)	3233(3)	3227(0)	3245(0)	3172(0)
772(3)	765(9)	775(4)	742(12)	3234(0)	3227(0)	3245(0)	3172(1)
785(29)	771(0)	781(0)	742(2)	3234(9)	3230(0)	3248(1)	3175(0)
790(2)	772(3)	782(3)	748(1)	3234(26)	3230(1)	3248(0)	3175(5)
846(0)	855(1)	863(1)	827(0)	3235(0)	3231(6)	3249(8)	3176(1)
854(21)	865(13)	874(15)	839(10)	3236(15)	3231(6)	3249(7)	3176(7)

Table S20. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **2T-4**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
27(1)	32(1)	30(1)	32(0)	869(0)	883(0)	884(15)	852(1)
34(0)	38(0)	44(0)	36(2)	875(30)	885(30)	889(0)	858(25)
44(0)	41(0)	48(0)	43(0)	904(0)	909(8)	916(7)	873(8)
80(0)	89(0)	89(0)	88(0)	910(5)	913(7)	918(17)	881(1)
110(0)	108(1)	108(0)	109(1)	950(0)	950(0)	959(0)	919(0)
143(0)	133(0)	137(0)	122(0)	950(0)	950(0)	959(0)	920(0)
147(0)	148(0)	141(0)	151(0)	1005(44)	986(33)	988(36)	965(14)
204(1)	200(0)	196(0)	206(2)	1010(0)	991(0)	992(0)	969(0)
214(0)	205(0)	199(1)	206(0)	1038(1)	1031(0)	1040(1)	1002(0)
227(0)	234(0)	202(0)	253(0)	1039(3)	1032(1)	1040(1)	1004(0)
304(0)	252(2)	223(2)	270(9)	1040(1)	1033(1)	1041(2)	1005(0)
305(0)	279(0)	275(1)	299(0)	1041(0)	1034(0)	1042(0)	1006(0)
328(5)	285(10)	287(0)	303(0)	1363(5)	1356(6)	1364(21)	1323(2)
356(0)	316(1)	295(7)	331(2)	1365(0)	1358(0)	1368(1)	1325(0)
373(0)	361(0)	334(17)	365(0)	1376(0)	1373(0)	1380(2)	1342(0)
375(0)	368(0)	348(0)	365(0)	1376(0)	1373(0)	1381(0)	1342(0)
393(16)	369(22)	359(0)	388(0)	1486(6)	1488(6)	1500(15)	1446(5)
399(5)	383(1)	382(3)	394(0)	1488(10)	1490(18)	1502(21)	1448(11)
400(2)	403(0)	402(0)	403(0)	1496(5)	1500(0)	1511(43)	1461(0)
425(0)	423(0)	425(0)	413(0)	1496(2)	1500(36)	1511(0)	1462(28)
431(2)	426(15)	426(16)	417(0)	1500(0)	1504(3)	1517(4)	1464(1)
431(0)	427(0)	430(0)	422(1)	1500(30)	1505(1)	1517(1)	1464(1)
433(25)	433(1)	435(1)	452(20)	1906(1013)	1881(997)	1912(1066)	1805(805)
465(10)	454(3)	452(14)	462(3)	1921(11)	1898(5)	1934(0)	1822(31)
465(8)	463(12)	452(2)	477(3)	3122(0)	3124(3)	3141(4)	3069(0)
475(3)	472(7)	470(12)	482(6)	3122(41)	3124(0)	3141(0)	3069(11)
709(2)	704(3)	704(1)	679(4)	3125(28)	3125(1)	3144(1)	3072(4)
712(0)	707(0)	707(0)	679(0)	3125(0)	3125(9)	3145(9)	3072(0)
747(15)	744(14)	747(18)	709(8)	3127(23)	3131(0)	3151(0)	3076(1)
756(0)	748(55)	755(0)	715(24)	3127(3)	3131(0)	3151(1)	3077(1)
756(44)	750(0)	756(77)	716(0)	3228(20)	3225(0)	3242(0)	3169(0)
769(1)	757(0)	762(0)	729(0)	3228(0)	3225(0)	3242(2)	3169(3)
792(30)	770(5)	776(1)	745(5)	3231(0)	3228(0)	3245(0)	3175(0)
795(1)	775(1)	783(2)	749(0)	3231(0)	3228(8)	3245(9)	3175(5)
867(12)	876(0)	870(0)	848(4)	3232(10)	3228(0)	3250(0)	3176(0)
867(0)	880(10)	882(23)	849(0)	3232(27)	3229(7)	3250(8)	3177(7)

Table S21. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3S-1**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
52(1)	27(0)	25(0)	35(0)	854(6)	866(10)	874(12)	831(2)
63(0)	47(1)	46(0)	47(1)	858(4)	871(5)	881(3)	842(10)
67(1)	61(1)	61(0)	57(2)	903(5)	918(2)	925(2)	890(3)
90(4)	88(0)	87(0)	81(3)	909(9)	921(11)	928(14)	894(5)
91(0)	89(2)	90(2)	83(0)	920(4)	925(10)	934(10)	896(10)
105(0)	91(0)	93(0)	92(0)	934(11)	937(21)	947(22)	907(16)
118(0)	110(0)	110(0)	109(0)	952(0)	951(0)	960(0)	922(0)
118(0)	111(0)	111(0)	111(0)	957(0)	955(0)	964(0)	927(0)
126(3)	128(0)	128(3)	127(3)	1001(8)	986(2)	993(3)	964(2)
127(0)	128(3)	129(1)	127(0)	1014(8)	1000(3)	1008(4)	975(3)
143(1)	139(1)	138(2)	142(1)	1038(0)	1030(0)	1039(0)	1002(0)
181(1)	170(2)	169(2)	174(1)	1043(1)	1034(0)	1042(0)	1008(0)
326(2)	289(4)	293(4)	277(4)	1045(1)	1039(1)	1047(1)	1010(1)
347(2)	310(3)	311(4)	310(2)	1047(1)	1039(1)	1048(1)	1012(0)
354(3)	328(2)	331(2)	321(2)	1353(0)	1345(0)	1355(0)	1312(0)
363(0)	349(1)	351(1)	341(0)	1370(0)	1366(0)	1375(0)	1336(1)
375(2)	369(4)	372(3)	361(2)	1380(1)	1377(3)	1386(3)	1346(2)
384(3)	386(2)	390(2)	364(5)	1383(0)	1383(1)	1392(1)	1352(0)
418(10)	401(6)	404(6)	394(7)	1480(8)	1484(11)	1498(11)	1442(9)
425(37)	427(31)	429(35)	414(32)	1491(1)	1499(10)	1512(10)	1459(8)
428(6)	428(1)	432(1)	417(1)	1494(5)	1503(0)	1516(1)	1461(0)
434(3)	434(9)	436(9)	420(4)	1495(7)	1504(27)	1517(30)	1464(24)
437(0)	444(1)	448(1)	426(1)	1505(21)	1506(8)	1518(4)	1467(1)
460(3)	459(7)	461(7)	452(6)	1506(7)	1508(0)	1521(0)	1468(11)
481(79)	487(3)	484(4)	483(134)	2017(820)	2014(750)	2035(782)	1938(689)
494(33)	490(119)	488(108)	490(7)	2023(745)	2017(962)	2040(1065)	1946(647)
505(1)	501(13)	500(12)	494(3)	2056(70)	2046(40)	2068(12)	1977(101)
517(22)	535(15)	532(1)	530(33)	3114(20)	3116(4)	3135(5)	3059(5)
524(15)	541(20)	538(22)	541(29)	3115(12)	3119(2)	3138(2)	3062(2)
540(91)	542(61)	541(90)	542(13)	3128(28)	3135(8)	3153(10)	3078(8)
549(29)	553(37)	554(37)	561(18)	3128(14)	3135(3)	3154(3)	3079(3)
730(6)	729(4)	737(4)	700(5)	3133(11)	3137(2)	3155(2)	3082(2)
734(0)	731(0)	738(0)	712(0)	3139(22)	3141(3)	3159(4)	3085(4)
762(19)	750(9)	760(9)	719(12)	3225(1)	3218(0)	3236(0)	3162(0)
768(0)	768(2)	778(0)	740(0)	3225(24)	3221(8)	3240(8)	3165(9)
785(1)	768(0)	778(2)	743(2)	3236(9)	3233(1)	3251(0)	3180(1)
789(7)	772(8)	778(10)	754(6)	3236(7)	3234(0)	3251(2)	3180(2)
798(15)	800(8)	809(8)	770(10)	3238(6)	3237(3)	3254(4)	3182(2)
801(2)	806(1)	814(0)	780(1)	3243(10)	3238(5)	3255(5)	3183(4)

Table S22. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3S-2**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
28(1)	36(1)	37(1)	35(1)	841(8)	856(6)	864(7)	827(5)
56(0)	54(0)	55(0)	49(0)	864(3)	878(2)	887(2)	847(2)
80(0)	72(0)	71(0)	70(0)	884(18)	891(24)	901(25)	859(19)
82(0)	88(0)	87(0)	81(0)	889(8)	897(18)	907(17)	865(19)
92(0)	89(0)	90(0)	88(0)	926(5)	930(7)	938(9)	901(4)
100(1)	96(0)	97(0)	101(1)	944(5)	947(7)	955(8)	920(6)
105(1)	109(1)	111(1)	105(0)	951(0)	952(0)	960(0)	923(0)
116(1)	122(1)	122(2)	122(1)	955(0)	956(0)	964(0)	927(0)
156(1)	155(1)	156(1)	153(1)	1004(5)	991(1)	998(1)	966(1)
211(0)	203(0)	201(0)	206(0)	1017(3)	1000(0)	1007(1)	977(1)
232(1)	233(0)	234(0)	230(1)	1038(2)	1030(1)	1039(1)	1004(0)
246(0)	239(0)	237(0)	243(0)	1040(1)	1036(0)	1045(0)	1008(1)
307(7)	262(11)	266(12)	254(7)	1042(0)	1036(0)	1045(0)	1010(0)
332(2)	293(4)	296(5)	288(3)	1043(0)	1037(0)	1046(0)	1011(0)
351(5)	319(7)	321(8)	314(5)	1354(0)	1346(0)	1355(0)	1317(0)
369(6)	343(8)	346(9)	337(6)	1372(1)	1370(2)	1380(1)	1338(3)
379(0)	380(0)	381(0)	368(1)	1378(0)	1373(1)	1382(1)	1343(0)
400(2)	388(1)	391(2)	379(1)	1385(0)	1383(1)	1393(1)	1352(0)
404(5)	403(12)	405(14)	396(6)	1482(4)	1486(6)	1499(7)	1446(5)
419(0)	419(2)	421(2)	408(2)	1493(0)	1498(28)	1510(27)	1459(26)
425(8)	428(2)	431(2)	416(3)	1496(1)	1502(7)	1515(8)	1462(5)
426(3)	429(1)	432(1)	416(4)	1498(22)	1503(0)	1515(30)	1463(0)
442(6)	437(8)	437(6)	437(14)	1501(4)	1504(29)	1517(0)	1466(23)
461(4)	459(3)	458(2)	459(4)	1506(25)	1508(1)	1521(1)	1468(1)
477(1)	461(7)	462(8)	461(1)	1890(861)	1861(879)	1875(947)	1809(733)
479(19)	473(1)	473(1)	476(2)	1933(52)	1913(52)	1933(51)	1848(52)
488(8)	488(1)	485(7)	485(3)	2079(776)	2063(734)	2086(768)	1993(633)
498(5)	498(14)	497(11)	505(6)	3109(19)	3118(5)	3137(1)	3062(6)
527(15)	518(18)	518(19)	515(13)	3121(10)	3119(1)	3137(6)	3066(1)
543(32)	540(37)	538(37)	541(34)	3122(12)	3126(1)	3144(1)	3071(2)
637(446)	631(479)	628(504)	632(388)	3124(19)	3130(3)	3149(4)	3074(4)
709(16)	703(12)	713(12)	675(14)	3132(16)	3135(2)	3153(3)	3080(3)
734(1)	729(1)	738(1)	702(1)	3134(21)	3140(2)	3158(3)	3084(3)
765(13)	752(14)	762(15)	726(15)	3216(11)	3219(2)	3237(2)	3164(2)
774(3)	761(2)	771(2)	733(2)	3229(6)	3227(3)	3245(3)	3173(2)
791(9)	771(15)	778(15)	752(13)	3232(7)	3229(3)	3247(3)	3175(3)
801(19)	785(3)	793(3)	763(5)	3233(11)	3230(2)	3248(2)	3176(2)
802(2)	793(3)	802(2)	763(3)	3241(13)	3237(1)	3255(1)	3183(0)
804(5)	794(4)	804(4)	769(4)	3241(2)	3239(4)	3257(4)	3185(4)

Table S23. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **3T-3**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
72(1)	56(0)	4(0)	62(0)	864(0)	879(0)	891(0)	848(0)
72(1)	56(0)	4(0)	68(0)	864(0)	879(0)	891(0)	848(0)
75(0)	72(1)	74(1)	71(1)	870(18)	885(16)	897(21)	853(9)
82(0)	72(1)	74(1)	71(1)	870(18)	885(16)	897(21)	853(9)
82(0)	81(0)	93(0)	99(0)	898(0)	904(6)	918(4)	869(11)
83(0)	82(0)	95(0)	99(0)	899(0)	905(0)	918(0)	870(0)
98(0)	102(0)	105(0)	100(0)	956(0)	955(0)	963(0)	926(0)
98(0)	102(0)	105(0)	100(0)	956(0)	955(0)	963(0)	926(0)
146(0)	136(0)	136(0)	150(0)	1002(43)	984(27)	991(39)	963(15)
146(0)	136(0)	137(0)	150(0)	1005(0)	987(0)	994(0)	965(0)
174(1)	173(1)	170(1)	177(1)	1043(0)	1035(0)	1043(0)	1009(0)
238(0)	226(0)	226(0)	227(0)	1043(0)	1035(0)	1043(0)	1009(0)
319(0)	290(0)	296(0)	284(0)	1045(1)	1036(0)	1045(1)	1010(0)
319(0)	290(0)	296(0)	284(0)	1045(1)	1036(0)	1045(1)	1010(0)
335(2)	298(7)	307(7)	287(6)	1374(0)	1369(0)	1378(1)	1340(0)
335(2)	298(7)	307(7)	287(6)	1374(0)	1369(0)	1378(1)	1340(0)
354(0)	338(0)	339(0)	341(0)	1374(0)	1369(0)	1378(0)	1340(0)
354(0)	338(0)	339(0)	341(0)	1374(0)	1369(0)	1378(0)	1340(0)
390(0)	368(9)	370(0)	352(3)	1495(1)	1496(0)	1509(0)	1459(0)
393(16)	379(0)	379(15)	389(0)	1495(0)	1496(0)	1509(0)	1459(0)
417(0)	413(6)	412(8)	407(2)	1497(0)	1497(34)	1509(35)	1460(32)
417(5)	413(6)	412(8)	407(2)	1497(0)	1497(34)	1509(35)	1460(32)
417(5)	415(0)	415(0)	409(0)	1497(29)	1505(1)	1519(1)	1465(0)
420(0)	425(0)	429(0)	413(0)	1497(29)	1505(0)	1519(0)	1465(0)
421(0)	425(0)	429(0)	413(0)	1965(850)	1938(835)	1960(897)	1868(703)
445(4)	441(4)	441(76)	445(4)	1965(849)	1938(835)	1960(897)	1868(703)
445(4)	441(4)	443(3)	445(4)	1995(0)	1965(0)	1982(0)	1900(0)
481(0)	459(87)	443(3)	476(0)	3126(0)	3129(0)	3148(0)	3076(0)
482(94)	466(0)	465(0)	497(105)	3126(0)	3129(0)	3148(0)	3076(0)
516(27)	513(25)	509(26)	517(22)	3126(39)	3130(7)	3148(8)	3076(9)
516(27)	513(25)	509(26)	517(22)	3126(39)	3130(7)	3148(8)	3076(9)
718(0)	716(0)	731(0)	687(0)	3128(24)	3135(0)	3154(1)	3080(1)
722(0)	717(0)	732(0)	689(0)	3129(0)	3135(0)	3155(0)	3081(0)
772(0)	766(0)	774(47)	736(0)	3234(0)	3229(0)	3247(0)	3177(0)
772(0)	766(0)	780(0)	736(0)	3234(0)	3229(0)	3247(0)	3177(0)
773(4)	767(33)	781(0)	736(4)	3234(25)	3232(0)	3251(0)	3180(0)
773(4)	767(5)	781(0)	736(4)	3234(25)	3232(0)	3251(0)	3180(0)
791(57)	767(5)	782(5)	746(22)	3234(0)	3233(7)	3251(8)	3180(7)
796(0)	771(0)	782(5)	750(0)	3234(0)	3233(7)	3251(8)	3180(7)

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

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
48(1)	48(1)	48(1)	48(1)	806(18)	797(6)	806(5)	774(9)
54(0)	52(0)	52(0)	51(1)	807(0)	798(0)	807(0)	774(0)
70(0)	76(0)	76(0)	73(0)	874(7)	887(4)	896(5)	859(3)
83(0)	82(0)	83(0)	78(0)	877(0)	889(0)	898(0)	861(0)
83(0)	84(0)	86(0)	79(0)	894(0)	903(0)	912(0)	873(0)
84(0)	87(0)	88(0)	86(0)	896(9)	904(22)	913(21)	874(21)
86(0)	89(0)	90(0)	87(0)	921(0)	924(0)	932(0)	896(0)
117(0)	114(0)	108(0)	119(1)	924(23)	926(35)	935(36)	899(31)
120(1)	121(1)	122(1)	128(1)	954(0)	954(0)	963(0)	926(0)
123(0)	131(0)	132(0)	128(0)	955(0)	954(0)	963(0)	926(0)
150(0)	154(0)	155(0)	151(0)	1009(6)	993(0)	1001(0)	970(1)
220(0)	214(0)	213(0)	215(0)	1009(0)	994(0)	1001(0)	970(0)
229(0)	234(0)	234(0)	231(0)	1043(0)	1036(0)	1045(0)	1009(0)
243(0)	239(0)	236(0)	245(0)	1044(0)	1037(0)	1046(0)	1010(0)
337(9)	299(14)	303(15)	292(10)	1044(3)	1038(1)	1046(1)	1011(1)
347(0)	309(0)	309(0)	305(8)	1044(0)	1038(0)	1046(0)	1011(0)
350(7)	310(9)	312(9)	310(0)	1375(2)	1372(1)	1381(2)	1342(0)
354(0)	317(0)	319(0)	312(0)	1376(0)	1373(0)	1381(0)	1343(0)
373(0)	366(0)	366(0)	367(0)	1378(0)	1374(3)	1383(3)	1343(5)
394(1)	382(2)	385(2)	373(3)	1378(0)	1375(0)	1384(0)	1343(0)
395(0)	392(0)	392(2)	386(0)	1498(2)	1500(46)	1512(46)	1461(42)
400(0)	394(1)	393(0)	392(0)	1498(0)	1500(0)	1512(0)	1462(0)
423(0)	422(0)	422(0)	413(4)	1501(36)	1505(10)	1518(12)	1466(7)
423(6)	427(4)	430(5)	414(0)	1501(0)	1506(0)	1518(0)	1466(0)
424(0)	429(0)	433(0)	414(0)	1506(4)	1510(0)	1523(0)	1470(1)
433(0)	431(0)	433(0)	430(0)	1507(0)	1510(1)	1523(1)	1470(0)
440(0)	443(0)	445(0)	438(0)	1910(914)	1875(933)	1888(1008)	1826(768)
460(14)	461(10)	456(15)	470(1)	1949(0)	1925(0)	1945(0)	1862(0)
481(0)	484(0)	482(0)	481(0)	2077(1395)	2064(1363)	2087(1402)	1990(1220)
491(0)	490(0)	485(0)	504(31)	2089(0)	2074(0)	2097(0)	2002(0)
501(42)	499(35)	497(32)	507(0)	3120(23)	3128(5)	3146(6)	3075(5)
518(0)	511(0)	510(0)	514(54)	3120(0)	3128(0)	3146(0)	3075(0)
520(62)	515(62)	514(65)	515(0)	3134(0)	3135(5)	3153(7)	3081(6)
543(34)	544(42)	543(41)	544(42)	3134(35)	3135(0)	3153(0)	3081(0)
557(0)	552(0)	552(0)	550(0)	3136(38)	3140(3)	3158(5)	3084(4)
618(491)	613(530)	611(542)	619(480)	3136(0)	3140(0)	3158(0)	3085(0)
742(0)	734(1)	742(1)	711(0)	3226(0)	3227(3)	3245(3)	3176(3)
743(0)	736(0)	744(0)	712(0)	3226(16)	3227(0)	3245(0)	3176(0)
790(0)	769(0)	775(0)	750(0)	3241(27)	3236(0)	3253(0)	3183(0)
792(15)	770(18)	777(20)	752(15)	3241(0)	3236(1)	3253(2)	3183(1)
799(0)	791(0)	801(0)	764(0)	3241(0)	3238(8)	3255(9)	3184(8)
801(7)	792(5)	802(5)	764(7)	3241(4)	3238(0)	3255(0)	3184(0)

Table S25. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-2**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
49(0)	49(0)	49(0)	47(0)	806(0)	799(4)	808(3)	775(6)
58(1)	52(1)	52(1)	51(1)	809(9)	800(1)	809(1)	776(1)
75(0)	78(0)	79(0)	76(0)	874(7)	889(4)	897(5)	860(3)
78(0)	83(0)	84(0)	77(0)	877(0)	891(0)	900(0)	863(0)
88(0)	87(0)	88(0)	83(0)	894(1)	903(0)	911(0)	873(0)
89(0)	87(0)	88(0)	86(0)	897(11)	906(18)	915(20)	875(15)
99(0)	91(0)	94(0)	86(0)	916(21)	916(36)	926(36)	884(34)
107(0)	113(0)	106(0)	119(1)	934(3)	933(4)	941(3)	903(6)
117(1)	121(1)	123(1)	128(0)	953(0)	954(0)	962(0)	925(0)
126(0)	131(0)	132(0)	129(0)	958(0)	957(0)	966(0)	929(0)
158(0)	159(0)	160(0)	154(1)	1006(6)	991(0)	999(0)	968(1)
214(0)	209(0)	208(0)	212(0)	1009(0)	995(0)	1003(0)	971(0)
231(0)	236(0)	237(0)	233(0)	1040(0)	1035(0)	1043(0)	1008(0)
244(0)	241(0)	238(0)	247(0)	1043(1)	1038(0)	1046(0)	1011(0)
336(8)	301(13)	305(15)	295(9)	1045(1)	1039(1)	1048(1)	1012(0)
346(0)	308(0)	309(0)	306(2)	1049(0)	1041(0)	1049(0)	1015(0)
351(4)	312(4)	314(4)	309(0)	1373(3)	1372(0)	1380(0)	1341(5)
355(2)	318(6)	321(5)	313(6)	1375(0)	1372(1)	1381(2)	1342(0)
382(0)	373(0)	373(0)	373(0)	1376(0)	1373(3)	1383(3)	1343(0)
394(1)	382(0)	385(1)	374(0)	1377(0)	1375(0)	1385(0)	1343(0)
397(1)	394(0)	392(1)	390(3)	1496(1)	1499(0)	1511(0)	1460(0)
399(0)	395(1)	396(0)	393(0)	1497(1)	1499(50)	1511(50)	1461(46)
423(2)	425(1)	425(1)	413(2)	1498(0)	1504(3)	1517(4)	1465(2)
424(0)	427(1)	430(0)	416(1)	1498(42)	1506(6)	1518(7)	1466(5)
425(5)	431(3)	433(5)	417(0)	1503(2)	1507(0)	1521(0)	1466(0)
435(3)	431(0)	435(0)	429(3)	1507(5)	1512(3)	1525(3)	1471(2)
436(0)	437(3)	439(3)	431(0)	1905(875)	1873(911)	1886(985)	1823(751)
468(14)	471(3)	467(5)	470(12)	1946(57)	1924(26)	1944(23)	1860(32)
472(6)	473(17)	474(19)	479(0)	2069(168)	2058(160)	2080(153)	1987(176)
475(31)	482(33)	475(30)	492(18)	2104(1219)	2088(1225)	2111(1281)	2017(1047)
501(5)	494(2)	494(4)	505(15)	3119(1)	3129(2)	3147(2)	3073(2)
515(15)	507(7)	506(7)	510(4)	3121(25)	3131(5)	3150(5)	3076(6)
528(0)	521(0)	520(0)	523(0)	3132(0)	3134(5)	3152(6)	3080(0)
540(35)	542(46)	541(46)	543(41)	3133(34)	3134(0)	3152(0)	3080(6)
551(49)	544(45)	544(46)	544(40)	3134(37)	3139(3)	3158(4)	3084(4)
620(490)	615(531)	612(542)	620(481)	3134(1)	3139(0)	3158(0)	3084(0)
742(0)	737(0)	745(0)	712(0)	3225(0)	3228(0)	3246(0)	3175(0)
744(1)	738(1)	746(1)	714(1)	3228(16)	3231(3)	3249(3)	3177(4)
790(17)	766(18)	772(20)	747(15)	3240(9)	3236(0)	3253(0)	3182(0)
796(3)	773(1)	780(1)	754(2)	3241(16)	3236(2)	3254(3)	3182(1)
797(0)	785(0)	795(0)	755(0)	3241(0)	3238(3)	3255(4)	3184(3)
804(15)	797(7)	807(6)	768(9)	3241(4)	3238(4)	3255(5)	3184(4)

Table S26. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **4S-3**

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
28(0)	17(0)	11(0)	22(1)	815(20)	804(13)	812(13)	778(11)
49(0)	50(0)	50(0)	44(0)	820(0)	809(0)	817(0)	782(0)
70(0)	71(0)	72(0)	67(0)	878(11)	888(15)	896(17)	863(11)
74(0)	72(0)	73(0)	71(0)	879(1)	888(1)	896(1)	863(1)
83(0)	79(0)	79(0)	79(0)	903(3)	912(3)	920(4)	884(2)
90(0)	89(0)	90(0)	87(0)	904(1)	913(4)	921(3)	885(5)
93(0)	91(0)	92(0)	89(0)	932(0)	931(0)	939(1)	903(0)
106(0)	98(0)	100(0)	94(0)	934(12)	932(23)	940(23)	904(21)
117(1)	118(0)	119(0)	113(0)	954(0)	953(0)	962(0)	925(0)
118(0)	122(1)	123(1)	119(1)	954(0)	953(0)	962(0)	925(0)
128(5)	129(4)	130(0)	127(3)	1006(15)	991(8)	999(9)	968(7)
145(0)	131(0)	131(5)	129(0)	1008(0)	993(0)	1000(0)	969(0)
153(1)	144(1)	145(1)	140(1)	1042(2)	1035(0)	1043(0)	1008(1)
170(0)	162(0)	164(0)	158(0)	1042(0)	1035(1)	1043(1)	1009(0)
351(5)	315(8)	316(10)	315(5)	1043(0)	1036(1)	1045(1)	1009(0)
357(1)	324(3)	326(4)	320(1)	1043(2)	1036(0)	1045(0)	1009(1)
364(1)	324(1)	326(1)	320(4)	1373(1)	1371(0)	1380(0)	1340(1)
366(0)	326(1)	328(0)	323(0)	1374(0)	1371(0)	1380(0)	1340(0)
385(0)	369(0)	371(0)	364(0)	1377(7)	1373(12)	1383(11)	1342(12)
389(3)	375(5)	377(5)	368(8)	1378(0)	1375(0)	1384(0)	1344(0)
398(2)	398(1)	397(1)	393(1)	1496(0)	1501(5)	1514(6)	1462(6)
417(2)	417(1)	419(2)	407(0)	1496(3)	1501(8)	1514(7)	1462(3)
422(9)	424(6)	426(6)	412(7)	1502(0)	1504(14)	1516(14)	1464(17)
423(1)	425(0)	427(0)	413(0)	1502(8)	1504(8)	1517(7)	1465(7)
448(0)	444(0)	445(0)	436(0)	1505(15)	1509(3)	1522(2)	1468(2)
459(8)	457(10)	457(8)	454(12)	1506(5)	1509(0)	1522(0)	1468(1)
463(1)	462(1)	463(1)	458(1)	2038(152)	2028(176)	2051(195)	1959(119)
475(2)	467(4)	467(6)	462(2)	2050(999)	2038(1085)	2057(1094)	1968(940)
485(48)	488(85)	480(90)	504(80)	2055(997)	2039(1043)	2061(1186)	1978(882)
495(7)	502(2)	496(2)	513(0)	2094(261)	2077(191)	2097(142)	2011(194)
519(6)	530(1)	524(1)	535(95)	3125(10)	3134(1)	3152(6)	3080(0)
524(41)	532(41)	527(42)	540(4)	3125(22)	3134(6)	3152(2)	3080(9)
541(153)	534(134)	533(145)	543(6)	3136(37)	3137(1)	3155(1)	3082(0)
550(0)	540(1)	538(0)	544(30)	3136(3)	3137(6)	3155(6)	3082(9)
564(56)	555(0)	553(0)	559(1)	3139(13)	3142(4)	3161(5)	3086(5)
564(1)	562(61)	561(64)	563(48)	3140(30)	3143(4)	3161(4)	3086(3)
745(3)	739(0)	746(0)	718(1)	3228(10)	3231(1)	3248(1)	3180(3)
745(0)	739(1)	746(1)	718(0)	3229(10)	3232(4)	3248(4)	3180(0)
793(19)	772(0)	778(0)	755(0)	3241(2)	3235(7)	3253(8)	3182(8)
796(1)	773(24)	778(29)	757(16)	3241(18)	3235(0)	3253(0)	3182(2)
798(2)	789(17)	798(18)	763(18)	3251(7)	3245(4)	3262(5)	3188(3)
798(21)	794(1)	803(1)	768(2)	3251(1)	3245(1)	3262(1)	3188(1)

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

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
26(0)	22(0)	25(0)	20(0)	795(12)	780(4)	781(3)	764(8)
56(0)	46(1)	36(3)	52(0)	799(18)	796(14)	802(15)	773(1)
58(0)	56(0)	56(0)	59(1)	809(67)	811(3)	818(4)	775(10)
64(1)	64(1)	61(1)	72(3)	813(4)	817(8)	824(10)	784(4)
77(0)	79(0)	78(0)	75(0)	824(9)	861(75)	870(69)	830(66)
80(0)	81(0)	83(0)	79(0)	895(6)	878(2)	882(7)	859(1)
87(0)	83(0)	84(0)	82(0)	897(2)	910(6)	917(7)	872(4)
96(0)	89(0)	87(0)	90(0)	924(4)	936(5)	941(6)	900(7)
100(1)	97(1)	96(1)	93(1)	940(5)	941(11)	948(11)	907(11)
103(0)	103(0)	105(0)	99(0)	957(0)	955(0)	962(0)	926(0)
113(0)	114(0)	113(0)	109(0)	958(1)	957(0)	965(0)	926(0)
120(0)	123(2)	121(4)	129(0)	1000(9)	1000(1)	1009(3)	976(1)
132(1)	127(3)	125(0)	141(0)	1013(9)	1002(4)	1011(4)	977(2)
134(4)	132(3)	129(3)	155(0)	1031(30)	1039(0)	1047(0)	1007(17)
153(0)	150(1)	146(1)	186(9)	1045(1)	1040(1)	1048(1)	1010(0)
163(0)	155(0)	156(0)	200(0)	1047(0)	1045(36)	1054(39)	1012(0)
199(0)	194(0)	185(0)	253(1)	1048(10)	1060(10)	1074(10)	1028(19)
326(3)	319(10)	324(11)	299(5)	1094(5)	1092(4)	1103(5)	1064(3)
352(7)	324(1)	326(0)	303(8)	1308(1)	1289(1)	1296(1)	1258(1)
361(2)	330(3)	331(3)	320(4)	1377(3)	1373(5)	1381(5)	1342(1)
365(1)	358(3)	359(4)	343(1)	1378(2)	1376(1)	1385(0)	1345(3)
374(12)	375(15)	377(11)	361(8)	1410(1)	1416(2)	1428(2)	1378(3)
391(1)	381(2)	387(6)	380(4)	1442(2)	1446(2)	1459(2)	1401(2)
404(6)	408(10)	405(17)	394(3)	1466(1)	1468(1)	1481(1)	1423(2)
410(6)	411(4)	413(3)	414(3)	1496(8)	1500(18)	1513(17)	1462(20)
429(12)	431(4)	433(1)	416(1)	1503(9)	1506(9)	1518(10)	1468(5)
433(1)	433(5)	436(8)	420(3)	1504(6)	1510(1)	1523(1)	1471(0)
440(9)	442(16)	443(21)	423(2)	1685(48)	1673(51)	1687(60)	1640(44)
445(3)	446(4)	450(2)	440(6)	1961(560)	1935(561)	1978(636)	1830(526)
451(7)	451(9)	454(6)	446(1)	2059(216)	2048(219)	2069(241)	1896(196)
464(31)	463(34)	461(49)	449(13)	2073(139)	2061(227)	2082(127)	1991(694)
475(12)	475(21)	478(21)	468(7)	2082(1219)	2069(1151)	2091(1278)	2010(629)
483(7)	485(16)	484(8)	483(14)	2122(639)	2106(672)	2128(701)	2032(412)
488(8)	491(5)	490(5)	490(6)	3066(27)	3065(15)	3083(18)	3008(12)
502(12)	513(52)	510(13)	496(13)	3072(27)	3069(8)	3086(8)	3017(9)
505(22)	514(10)	517(67)	509(8)	3135(20)	3126(5)	3144(5)	3071(6)
534(17)	534(18)	535(76)	526(58)	3137(11)	3137(1)	3156(1)	3078(2)
541(159)	535(86)	538(21)	530(52)	3138(35)	3139(4)	3157(6)	3081(2)
543(36)	545(35)	546(45)	542(62)	3138(6)	3141(6)	3158(5)	3084(6)
550(44)	552(76)	554(76)	553(12)	3154(13)	3143(1)	3161(9)	3085(1)
570(77)	577(76)	576(62)	585(19)	3161(16)	3146(8)	3162(2)	3100(5)
608(13)	606(20)	611(25)	604(336)	3236(19)	3220(8)	3237(8)	3166(7)
660(1)	651(1)	657(0)	625(11)	3244(9)	3237(1)	3254(1)	3180(1)
765(0)	762(0)	768(0)	727(0)	3246(3)	3243(2)	3261(2)	3184(0)
776(6)	775(15)	780(19)	754(12)	3249(3)	3246(1)	3266(1)	3186(2)

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

M06-L	B3LYP*	B3LYP	BP86	M06-L	B3LYP*	B3LYP	BP86
29(0)	27(0)	28(0)	27(0)	655(0)	645(0)	651(0)	625(0)
37(0)	38(0)	39(0)	35(0)	655(1)	645(1)	651(0)	625(1)
53(0)	52(0)	53(0)	48(0)	758(4)	766(6)	771(8)	747(2)
62(0)	59(2)	60(2)	57(1)	759(3)	766(2)	772(3)	747(1)
64(1)	61(0)	61(0)	61(0)	789(9)	793(13)	797(15)	775(8)
68(0)	64(0)	64(0)	62(0)	790(3)	795(6)	799(7)	777(3)
75(0)	69(0)	70(0)	67(1)	828(137)	868(61)	872(41)	835(164)
82(0)	81(0)	81(0)	82(0)	828(9)	868(2)	873(2)	835(3)
87(0)	86(0)	86(0)	84(0)	892(1)	882(0)	891(1)	860(0)
89(0)	86(0)	87(0)	85(0)	892(2)	882(98)	891(115)	861(1)
98(0)	92(1)	92(1)	91(0)	955(0)	953(0)	960(0)	928(1)
99(0)	101(0)	102(0)	97(0)	955(0)	953(0)	961(0)	929(0)
103(1)	106(1)	109(1)	99(0)	998(32)	997(3)	1007(3)	969(6)
112(0)	109(0)	110(0)	105(0)	999(0)	998(0)	1009(1)	970(0)
118(0)	115(0)	118(0)	109(0)	1015(79)	1040(103)	1051(102)	1004(97)
118(0)	118(0)	118(1)	114(0)	1017(3)	1042(1)	1053(1)	1008(1)
125(2)	126(2)	128(2)	120(2)	1049(37)	1068(27)	1079(32)	1032(21)
140(0)	135(0)	137(0)	131(0)	1052(6)	1071(7)	1083(9)	1035(3)
151(0)	151(2)	153(2)	145(0)	1088(4)	1090(2)	1102(2)	1055(2)
151(1)	151(0)	154(0)	145(1)	1088(1)	1090(1)	1102(1)	1056(0)
316(3)	314(2)	317(2)	305(2)	1303(0)	1284(0)	1291(0)	1259(0)
319(0)	317(0)	320(0)	308(0)	1304(0)	1284(1)	1292(0)	1259(1)
355(3)	350(4)	352(6)	342(1)	1410(2)	1416(3)	1428(3)	1379(5)
357(0)	353(0)	355(0)	344(0)	1410(1)	1417(2)	1428(2)	1379(3)
392(42)	395(41)	393(70)	390(0)	1440(2)	1446(2)	1458(2)	1406(3)
394(1)	397(0)	398(0)	391(13)	1441(1)	1446(3)	1458(2)	1406(2)
409(29)	414(60)	409(30)	416(0)	1464(1)	1467(1)	1479(1)	1429(1)
418(1)	425(1)	420(4)	418(4)	1464(1)	1467(1)	1479(1)	1429(1)
427(2)	427(1)	428(0)	424(62)	1687(41)	1677(40)	1691(44)	1630(26)
427(0)	429(1)	429(4)	436(1)	1687(26)	1677(36)	1691(44)	1630(13)
440(23)	440(18)	441(25)	441(1)	2054(103)	2043(138)	2066(137)	1971(147)
442(0)	449(0)	451(0)	443(1)	2069(888)	2053(802)	2072(722)	1986(804)
458(2)	457(0)	458(1)	447(6)	2079(32)	2064(278)	2086(471)	1999(180)
460(1)	459(2)	460(1)	450(2)	2087(975)	2073(941)	2096(954)	2001(863)
466(0)	465(1)	467(2)	458(1)	2091(1161)	2075(1090)	2097(1084)	2005(901)
476(15)	481(15)	484(9)	468(19)	2139(421)	2122(385)	2144(414)	2053(317)
491(5)	490(6)	491(6)	497(13)	3069(18)	3069(8)	3085(11)	3018(6)
493(13)	491(10)	493(12)	499(2)	3070(23)	3069(16)	3085(18)	3018(15)
500(25)	521(16)	520(23)	519(4)	3076(29)	3073(0)	3089(0)	3022(0)
504(27)	522(14)	521(23)	520(7)	3076(19)	3073(11)	3089(12)	3023(10)
535(13)	539(20)	538(15)	536(189)	3140(28)	3128(5)	3145(5)	3075(8)
536(72)	540(129)	539(101)	540(44)	3140(17)	3128(2)	3146(3)	3075(3)
551(249)	548(231)	549(279)	542(18)	3151(9)	3142(5)	3157(6)	3096(4)
554(55)	553(39)	557(36)	548(92)	3152(13)	3142(4)	3157(4)	3096(4)
557(37)	559(47)	561(35)	552(75)	3162(0)	3145(0)	3160(0)	3099(0)
576(20)	573(35)	574(37)	568(37)	3162(29)	3145(13)	3160(15)	3099(11)
606(25)	604(40)	608(43)	590(28)	3238(18)	3222(7)	3239(7)	3170(7)
611(8)	610(12)	614(12)	593(11)	3238(13)	3222(5)	3239(5)	3170(5)