Highly Unsaturated Divanadocene Carbonyls: Interplay between Two-Electron and Four-Electron Donor Carbonyl Groups in Oxophilic Metal Systems

Qian-shu Li* and Xiuhui Zhang
The Institute for Chemical Physics, Beijing Institute of Technology, Beijing 100081, P. R. China

Yaoming Xie, R. Bruce King,* and Henry F. Schaefer III
Department of Chemistry and Center for Computational Chemistry, University of Georgia, Athens, Georgia 30602, USA

Supporting Information

Tables S1-S28. The theoretical harmonic vibrational frequencies for the 28 structures using the BP86 method.

Tables S29-S56. The theoretical Cartesian coordinates for the 28 structures using the BP86 method.

The complete Gaussian reference (reference 27)

Table S1. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5S-1** using the BP86 method (Total energy = –2842.387986 Hartrees)

	a"	a"	a"	a'	a"	a'	a"	a'	a"
Frequencies	19	23	42	51	82	84	91	94	102
IR intensities	0	0	1	1	0	1	1	0	1
	a'	a'	a'	a"	a"	a'	a'	a"	a'
Frequencies	107	112	120	121	149	153	205	301	315
IR intensities	1	1	2	0	1	0	1	5	1
	a"	a'	a'	a'	a"	a'	a"	a'	a"
Frequencies	322	324	334	373	393	417	436	438	449
IR intensities	2	0	0	6	1	0	0	13	2
	a"	a'	a'	a"	a"	a'	a'	a"	a'
Frequencies	462	472	494	520	525	534	556	565	573
IR intensities	3	25	63	2	16	49	56	23	1
	a"	a"	a'	a'	a'	a'	a'	a"	a'
Frequencies	582	583	583	586	600	796	797	801	808
IR intensities	0	0	5	21	6	156	12	5	27
	a"	a'	a'	a"	a'	a"	a'	a"	a'
Frequencies	810	813	814	817	817	818	868	871	880
IR intensities	5	4	7	1	2	0	1	0	2
	a"	a'	a'	a"	a"	a"	a"	a'	a'
Frequencies	884	989	991	1000	1000	1043	1044	1044	1046
IR intensities	0	8	4	7	6	1	0	1	0
	a'	a'	a"	a"	a"	a'	a"	a'	a'
Frequencies	1108	1109	1225	1226	1360	1366	1366	1370	1407
IR intensities	1	0	0	0	0	2	0	1	4
	a'	a"	a"	a"	a'	a"	a'	a'	a"
Frequencies	1410	1416	1418	1836	1865	1891	1926	1966	3165
IR intensities	4	2	2	551	176	927	1129	383	0
	a"	a'	a'	a'	a"	a'	a"	a'	a'
Frequencies	3168	3171	3172	3179	3182	3183	3185	3194	3194
IR intensities	0	0	0	0	0	0	0	0	0

Table S2. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5S-2** using the BP86 method (Total energy = –2842.383803 Hartrees)

	b	b	a	a	b	b	a	a	a
Frequencies	134*i*	33	34	52	59	83	85	91	105
IR intensities		0	0	1	1	1	1	0	0
	b	b	a	b	a	b	a	b	a
Frequencies	106	113	121	128	129	172	209	274	308
IR intensities	1	1	0	1	0	7	0	10	5
	b	a	b	b	a	a	b	b	a
Frequencies	315	318	329	354	358	414	417	437	445
IR intensities	1	0	11	8	0	0	2	27	1
	a	b	b	a	a	b	b	a	a
Frequencies	467	479	500	507	533	546	551	564	577
IR intensities	1	19	73	0	30	83	18	1	1
	b	a	b	a	b	b	a	b	a
Frequencies	579	582	583	588	594	793	794	801	802
IR intensities	5	1	0	3	25	131	6	57	2
	b	a	b	a	a	b	b	a	b
Frequencies	809	809	815	816	818	818	867	868	878
IR intensities	15	2	1	2	0	0	1	0	2
	a	b	a	a	b	a	b	b	a
Frequencies	878	989	990	1000	1001	1043	1044	1044	1045
IR intensities	0	14	0	14	1	1	1	0	0
	b	a	b	a	b	a	b	a	a
Frequencies	1109	1109	1224	1224	1363	1364	1369	1369	1407
IR intensities	1	0	0	0	3	0	3	0	0
	b	a	b	a	b	a	b	a	a
Frequencies	1407	1418	1418	1812	1861	1891	1938	1963	3167
IR intensities	6	4	2	516	273	886	1400	96	0
	b	b	a	a	b	b	a	b	a
Frequencies	3167	3171	3171	3181	3181	3183	3183	3193	3193
IR intensities	0	0	0	0	1	0	0	0	0

Table S3. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5S-3** using the BP86 method (Total energy = –2842.379263 Hartrees).

	a"	a"	a'	a"	a"	a'	a'	a"	a'
Frequencies	27	29	55	57	77	86	93	94	110
IR intensities	0	0	1	0	1	0	3	0	1
	a"	a'	a'	a"	a"	a'	a'	a"	a'
Frequencies	121	122	137	147	168	168	193	312	318
IR intensities	0	0	0	0	0	1	1	5	1
	a"	a'	a'	a'	a"	a"	a'	a"	a'
Frequencies	321	321	350	369	381	407	415	435	439
IR intensities	1	1	1	14	0	0	21	2	25
	a"	a'	a"	a'	a'	a"	a'	a'	a"
Frequencies	444	453	475	480	506	511	547	567	571
IR intensities	0	1	18	44	23	8	72	12	6
	a'	a"	a'	a"	a'	a'	a'	a'	a"
Frequencies	574	580	586	586	590	792	796	799	805
IR intensities	1	0	5	0	1	23	88	44	4
	a'	a'	a"	a"	a'	a"	a"	a'	a'
Frequencies	810	813	815	816	819	819	873	873	879
IR intensities	29	0	5	1	3	1	2	1	2
	a"	a'	a'	a"	a"	a"	a'	a"	a'
Frequencies	885	990	991	1000	1001	1044	1045	1045	1047
IR intensities	0	10	7	1	13	0	0	0	1
	a'	a'	a"	a"	a"	a'	a"	a'	a'
Frequencies	1109	1109	1225	1227	1362	1367	1372	1373	1409
IR intensities	0	2	0	0	1	1	0	1	1
	a'	a"	a"	a"	a'	a'	a"	a'	a'
Frequencies	1411	1417	1418	1812	1846	1902	1925	1977	3164
IR intensities	4	2	3	684	477	280	826	811	1
	a"	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	3168	3174	3174	3178	3182	3186	3187	3191	3197
IR intensities	0	0	0	0	0	0	1	0	0

Table S4. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5S-4** using the BP86 method (Total energy = –2842.3581666 Hartrees).

	b	a	b	a	b	a	b	a	b
Frequencies	202*i*	39	39	52	69	71	90	91	108
IR intensities		0	0	0	2	0	1	0	2
	a	a	a	b	b	a	b	b	a
Frequencies	114	132	138	146	159	172	175	223	311
IR intensities	0	0	0	1	0	0	8	8	1
	b	a	b	a	b	b	a	a	b
Frequencies	316	327	327	344	353	387	399	411	422
IR intensities	5	1	3	3	2	3	2	0	20
	a	b	a	b	b	a	a	b	a
Frequencies	433	451	459	464	518	528	538	552	568
IR intensities	0	58	10	19	77	0	11	63	17
	b	a	b	a	b	b	a	a	b
Frequencies	570	579	581	582	584	792	793	805	806
IR intensities	2	1	0	2	0	80	14	8	3
	a	b	a	b	a	b	a	b	a
Frequencies	809	809	814	814	818	819	865	865	890
IR intensities	6	51	1	5	1	6	0	0	0
	b	a	b	a	b	a	b	a	b
Frequencies	891	989	989	999	999	1043	1044	1046	1046
IR intensities	2	12	3	1	18	1	0	3	1
	a	b	b	a	a	b	b	a	a
Frequencies	1106	1106	1225	1225	1363	1364	1372	1372	1409
IR intensities	0	3	0	0	0	1	2	0	2
	b	a	b	a	a	b	b	a	b
Frequencies	1409	1416	1416	1789	1883	1893	1913	1966	3171
IR intensities	1	0	5	701	170	476	1147	681	0
	a	a	b	a	b	b	a	b	a
Frequencies	3171	3172	3172	3184	3184	3186	3186	3195	3195
IR intensities	0	0	0	0	1	0	1	0	0

Table S5. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5S-5** using the BP86 method (Total energy = –2842.351047 Hartrees).

	b_2	a_2	b_1	a_2	a_2	b_1	a_1	b_2	a_1
Frequencies	61*i*	36*i*	41	45	57	74	81	104	118
IR intensities			0	0	0	1	1	5	0
	b_1	a_2	a_1	b_2	b_1	a_1	b_2	b_2	b_1
Frequencies	126	141	152	171	184	186	248	278	308
IR intensities	0	0	0	0	0	0	3	4	6
	a_2	a1	b_2	a_1	b_2	b_1	a_2	a_1	a_2
Frequencies	311	319	327	355	360	381	391	397	432
IR intensities	0	4	2	1	3	0	0	1	0
	b_1	b_2	a_1	b_1	a_1	a_2	b_2	a_1	b_2
Frequencies	440	440	457	462	523	540	550	560	573
IR intensities	11	77	3	5	1	0	104	40	8
	a_1	b_2	b_1	a_2	b_1	b_2	a_1	b_2	a_1
Frequencies	577	578	579	582	582	801	803	805	806
IR intensities	1	1	28	0	2	135	10	0	32
	a_2	a_1	b_1	b_2	a_2	b_1	b_2	a_1	b_1
Frequencies	813	814	814	814	819	820	882	882	886
IR intensities	0	0	4	1	0	1	3	0	0
	a_2	b_2	a_1	a_2	b_1	a_2	a_1	b_2	b_1
Frequencies	887	992	992	998	998	1045	1045	1046	1046
IR intensities	0	2	10	0	18	0	3	0	2
	b_2	a_1	b_1	a_2	a_2	b_1	b_2	a_1	a_1
Frequencies	1108	1108	1226	1226	1363	1363	1378	1378	1408
IR intensities	2	0	0	0	0	1	2	0	3
	b_2	a_2	b_1	a_1	a_2	b_2	b_1	a_1	b_2
Frequencies	1408	1420	1420	1747	1882	1903	1926	1969	3173
IR intensities	1	0	4	729	0	483	1224	817	0
	a_1	a_2	b_1	a_2	b_1	b_2	a_1	b_2	a_1
Frequencies	3174	3174	3174	3186	3187	3187	3187	3197	3197
IR intensities	0	0	0	0	0	0	1	0	0

Table S6. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5T-1** using the BP86 method (Total energy = –2842.367059 Hartrees).

	a	a	a	a	a	a	a	a	a
Frequencies	35	44	48	49	66	75	84	87	99
IR intensities	1	0	1	0	0	0	1	0	0
	a	a	a	a	a	a	a	a	a
Frequencies	103	107	122	142	157	168	259	288	307
IR intensities	1	0	1	3	0	3	3	2	1
	a	a	a	a	a	a	a	a	a
Frequencies	309	318	326	346	361	401	421	432	439
IR intensities	2	2	7	5	0	7	8	26	6
	a	a	a	a	a	a	a	a	a
Frequencies	450	452	459	480	505	515	531	569	577
IR intensities	13	2	27	20	22	4	8	20	1
	a	a	a	a	a	a	a	a	a
Frequencies	582	583	587	604	623	780	792	796	803
IR intensities	1	1	0	27	28	48	55	58	39
	a	a	a	a	a	a	a	a	a
Frequencies	810	812	815	816	818	818	870	871	878
IR intensities	10	9	1	0	1	1	0	2	3
	a	a	a	a	a	a	a	a	a
Frequencies	881	995	997	998	998	1043	1045	1046	1046
IR intensities	1	7	12	6	9	1	1	0	0
	a	a	a	a	a	a	a	a	a
Frequencies	1110	1112	1225	1226	1362	1366	1368	1370	1412
IR intensities	1	0	0	0	0	1	1	0	4
	a	a	a	a	a	a	a	a	a
Frequencies	1413	1415	1416	1641	1834	1900	1913	1950	3166
IR intensities	3	1	3	291	366	640	2422	1	0
	a	a	a	a	a	a	a	a	a
Frequencies	3167	3170	3170	3181	3181	3181	3182	3192	3193
IR intensities	0	0	0	0	0	0	0	0	0

Table S7. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **5T-2** using the BP86 method (Total energy = –2842.352210 Hartrees).

	a''	a''	a''	a'	a''	a'	a''	a'	a''
Frequencies	73*i*	26	28	28	50	70	75	80	86
IR intensities		0	0	0	1	0	0	1	0
	a'	a''	a'	a'	a''	a'	a'	a''	a'
Frequencies	98	105	111	113	122	136	172	289	305
IR intensities	0	0	0	2	0	1	0	1	0
	a''	a'	a'	a'	a''	a''	a'	a''	a'
Frequencies	314	322	339	351	366	384	394	417	421
IR intensities	3	1	1	8	2	1	10	11	45
	a'	a''	a''	a'	a'	a'	a''	a'	a''
Frequencies	428	431	463	467	474	502	524	567	575
IR intensities	4	1	1	16	28	26	6	52	16
	a''	a'	a''	a'	a'	a'	a'	a'	a'
Frequencies	578	579	582	583	587	788	792	795	797
IR intensities	0	6	6	33	9	95	82	12	11
	a''	a''	a''	a'	a''	a'	a''	a''	a'
Frequencies	799	800	813	816	816	818	862	871	873
IR intensities	5	4	0	6	1	1	0	0	0
	a'	a'	a'	a''	a''	a''	a'	a''	a'
Frequencies	874	988	993	995	997	1041	1042	1043	1043
IR intensities	2	7	7	8	7	0	0	0	0
	a'	a'	a''	a''	a'	a'	a''	a''	a'
Frequencies	1104	1109	1223	1224	1361	1362	1363	1365	1405
IR intensities	2	1	0	0	0	0	0	0	4
	a'	a''	a''	a''	a'	a''	a'	a'	a'
Frequencies	1410	1411	1415	1806	1831	1920	1927	1955	3163
IR intensities	4	3	3	763	42	619	1576	30	1
	a'	a''	a''	a''	a'	a'	a''	a'	a'
Frequencies	3166	3169	3171	3180	3180	3180	3184	3191	3193
IR intensities	0	0	0	0	0	0	0	0	0

Table S8. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4S-1** using the BP86 method (Total energy = –2729.005377 Hartrees).

	a	a	a	a	a	a	a	a	a
Frequencies	29	43	51	58	78	92	98	103	120
IR Intensities	0	0	1	1	1	0	1	1	0
	a	a	a	a	a	a	a	a	a
Frequencies	132	147	167	189	232	310	315	317	321
IR Intensities	2	0	1	1	0	4	4	0	1
	a	a	a	a	a	a	a	a	a
Frequencies	351	371	398	411	446	456	471	491	503
IR Intensities	3	2	9	3	55	2	15	1	6
	a	a	a	a	a	a	a	a	a
Frequencies	507	539	575	577	583	584	585	600	653
IR Intensities	13	10	2	1	3	3	4	6	42
	a	a	a	a	a	a	a	a	a
Frequencies	780	787	794	797	802	809	813	814	819
IR Intensities	64	49	73	7	7	18	2	0	0
	a	a	a	a	a	a	a	a	a
Frequencies	819	856	867	870	882	993	995	995	1000
IR Intensities	1	1	0	0	1	10	4	8	7
	a	a	a	a	a	a	a	a	a
Frequencies	1043	1045	1046	1048	1106	1109	1224	1228	1359
IR Intensities	0	0	0	2	2	1	0	0	0
	a	a	a	a	a	a	a	a	a
Frequencies	1364	1366	1367	1411	1412	1413	1415	1654	1785
IR Intensities	1	1	2	7	2	3	5	282	407
	a	a	a	a	a	a	a	a	a
Frequencies	1896	1949	3165	3168	3170	3174	3181	3182	3184
IR Intensities	971	661	0	0	0	0	0	0	1
	a	a	a						
Frequencies	3185	3194	3196						
IR Intensities	0	0	0						

Table S9. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4S-2** using the BP86 method (Total energy = –2729.000597 Hartrees).

	a"	a"	a'	a"	a'	a'	a"	a"	a'
Frequencies	18	33	61	64	66	81	88	100	109
IR Intensities	0	0	1	1	0	0	0	0	0
	a"	a"	a'	a'	a'	a"	a'	a"	a'
Frequencies	118	121	129	146	213	304	307	308	310
IR Intensities	0	1	2	0	0	2	2	0	1
	a'	a"	a'	a'	a"	a"	a'	a"	a'
Frequencies	340	369	406	408	439	444	460	470	476
IR Intensities	8	0	8	0	8	0	0	36	41
	a'	a"	a"	a'	a'	a"	a'	a"	a'
Frequencies	496	521	543	545	562	578	580	580	585
IR Intensities	0	0	1	0	8	1	0	0	1
	a'	a'	a"	a'	a'	a"	a'	a"	a'
Frequencies	788	792	799	800	802	806	815	815	817
IR Intensities	84	93	8	16	31	4	0	0	0
	a"	a"	a'	a"	a'	a"	a'	a'	a"
Frequencies	818	867	871	872	873	995	996	999	1000
IR Intensities	0	0	0	0	1	9	12	7	7
	a'	a"	a'	a"	a'	a'	a"	a"	a'
Frequencies	1043	1043	1045	1045	1112	1112	1225	1228	1364
IR Intensities	0	0	0	0	1	1	0	0	1
	a"	a'	a"	a"	a'	a"	a'	a"	a'
Frequencies	1366	1366	1367	1413	1415	1416	1417	1844	1865
IR Intensities	0	1	0	4	2	3	4	2	1237
	a"	a'	a'	a'	a"	a"	a'	a'	a"
Frequencies	1868	1916	3163	3164	3165	3166	3177	3177	3178
IR Intensities	1275	1	0	0	0	0	0	0	0
	a"	a'	a'						
Frequencies	3179	3188	3188						
IR Intensities	0	0	0						

T**able S10.** The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4S-3** using the BP86 method (Total energy = –2729.000939 Hartrees).

	a_u	b_g	b_u	a_u	a_g	b_u	b_g	a_u	a_g
Frequencies	29	30	61	61	65	78	84	99	107
IR Intensities	0	0	1	1	0	0.4	0	0	0
	b_g	a_u	b_u	a_g	a_g	b_u	b_g	a_u	a_g
Frequencies	112	120	129.	145	213	302	303	305	314
IR Intensities	0	1	2	0	0	2	0	2	0
	b_u	b_g	b_u	a_g	a_u	b_g	a_g	a_u	b_u
Frequencies	339	370	400	410	440	446	459	472	477
IR Intensities	7	0	10	0	9	0	0	34	38
	a_g	b_g	a_u	a_g	b_u	a_u	b_g	bu	a_g
Frequencies	495	518	543	547	564	576	576	578	579
IR Intensities	0	0	1	0	7	1	0	2	0
	b_u	a_g	b_u	b_g	a_g	a_u	b_g	a_u	b_u
Frequencies	792	793	800	801	802	803	815	815	817
IR Intensities	188	0	33	0	0	12	0	0	1
	a_g	b_g	b_u	a_g	a_u	b_g	a_u	b_u	a_g
Frequencies	817	870	870	871	871	994	994	1000	1001
IR Intensities	0	0	0	0	0	0	16	14	0
	a_u	b_g	b_u	a_g	b_u	a_g	a_u	b_g	b_g
Frequencies	1043	1044	1045	1046	1111	1111	1225	1225	1365
IR Intensities	1	0	0	0	2	0	0	0	0
	a_u	a_g	b_u	b_g	a_u	b_u	ag	b_g	b_u
Frequencies	1365	1366	1366	1412	1412	1417	1418	1845	1866
IR Intensities	1	0	1	0	7	8	0	0	1250
	a_u	a_g	a_g	b_u	b_g	a_u	b_u	a_g	b_g
Frequencies	1869	1917	3163	3163	3164	3164	3177	3177	3178
IR Intensities	1259	0	0	0	0	0	1	0	0
	a_u	b_u	a_g						
Frequencies	3178	3188	3188						
IR Intensities	0	0	0						

Table S11. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4T-1** using the BP86 method (Total energy = –2729.007233 Hartrees).

	a"	a"	a'	a"	a"	a"	a'	a'	a"
Frequencies	26	44	51	54	77	79	87	102	116
IR Intensities	0	0	0	1	0	0	0	1	0
	a'	a'	a'	a'	a"	a'	a'	a"	a"
Frequencies	118	126	151	188	193	308	312	322	332
IR Intensities	2	0	0	2	1	2	3	3	0
	a'	a'	a"	a"	a'	a'	a"	a'	a'
Frequencies	335	372	379	397	420	442	447	451	469
IR Intensities	2	6	1	0	5	9	0	63	4
	a"	a'	a'	a"	a"	a'	a"	a'	a'
Frequencies	514	515	554	572	579	579	585	585	586
IR Intensities	5	5	65	22	1	1	3	8	21
	a'	a"	a'	a"	a'	a'	a"	a'	a"
Frequencies	781	782	791	794	796	814	816	817	817
IR Intensities	108	2	4	5	82	10	0	1	0
	a'	a"	a'	a"	a'	a'	a'	a"	a"
Frequencies	818	858	864	871	880	993	994	995	997
IR Intensities	2	0	1	0	4	7	8	12	8
	a"	a'	a"	a'	a'	a'	a"	a"	a"
Frequencies	1042	1042	1044	1044	1108	1110	1224	1224	1363
IR Intensities	0	0	0	2	3	1	0	0	0
	a'	a'	a"	a'	a'	a"	a"	a"	a'
Frequencies	1363	1366	1369	1410	1411	1413	1416	1813	1836
IR Intensities	2	3	0	6	2	2	4	1081	110
	a'	a'	a"	a'	a'	a"	a"	a'	a'
Frequencies	1898	1949	3162	3162	3166	3171	3174	3177	3181
IR Intensities	970	494	0	0	0	0	0	0	1
	a"	a'	a'						
Frequencies	3184	3187	3194						
IR Intensities	0	0	0						

Table S12. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4T-2** using the BP86 method (Total energy = –2728.988763 Hartrees).

	a_u	a_g	a_u	a_g	a_u	a_g	a_u	a_u	a_u
Frequencies	11	26	26	45	47	75	83	92	103
IR Intensities	2	0	0	0	0	0	2	1	0
	a_g	a_g	a_u	a_g	a_g	a_u	a_g	a_g	a_u
Frequencies	106	116	122	124	207	305	306	309	310
IR Intensities	0	0	0	0	0	3	0	0	1
	a_u	a_g	a_u	a_g	a_u	a_g	a_u	a_g	a_u
Frequencies	338	338	385	396	403	446	452	457	458
IR Intensities	3	0	32	0	55	0	30	0	9
	a_g	a_u	a_g	a_g	a_u	a_g	a_u	a_u	a_g
Frequencies	471	514	523	552	563	577	577	580	581
IR Intensities	0	37	0	0	22	0	2	0	0
	a_g	a_u	a_u	a_g	a_u	a_g	a_u	a_g	a_u
Frequencies	787	787	793	795	796	797	814	814	817
IR Intensities	0	187	16	0	15	0	0	0	1
	a_g	a_u	a_g	a_u	a_g	a_u	a_g	a_u	a_g
Frequencies	818	864	865	866	866	993	993	999	999
IR Intensities	0	0	0	2	0	19	0	13	0
	a_u	a_g	a_u	a_g	a_u	a_g	a_u	a_g	a_g
Frequencies	1042	1042	1044	1045	1110	1110	1226	1226	1363
IR Intensities	1	0	1	0	3	0	0	0	0
	a_u	a_g	a_u	a_u	a_g	a_u	a_g	a_g	a_u
Frequencies	1363	1366	1366	1411	1411	1416	1416	1840	1845
IR Intensities	1	0	0	6	0	8	0	0	1468
	a_u	a_g	a_g	a_u	a_u	a_g	a_u	a_g	a_u
Frequencies	1883	1920	3163	3163	3166	3167	3177	3177	3181
IR Intensities	1278	0	0	0	1	0	1	0	0
	a_g	a_u	a_g						
Frequencies	3181	3190	3190						
IR Intensities	0	0	0						

Table S13. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **4T-3** using the BP86 method (Total energy = –2728.989586 Hartrees).

	b	a	b	a	a	b	b	a	a
Frequencies	199*i*	26	30	35	61	62	81	83	96
IR Intensities		0	0	0	0	2	1	1	0
	b	a	b	a	a	b	a	b	a
Frequencies	105	118	127	136	200	301	309	310	310
IR Intensities	0	0	1	0	1	3	3	0	1
	b	b	a	b	a	b	a	a	b
Frequencies	334	358	389	400	417	430	436	451	470
IR Intensities	7	1	0	4	2	3	4	38	9
	b	a	a	a	b	b	a	b	a
Frequencies	475	486	499	539	544	575	575	583	583
IR Intensities	46	0	13	0	11	0	0	1	0
	b	a	b	a	b	a	b	a	b
Frequencies	785	785	795	795	800	802	813	813	815
IR Intensities	122	1	7	5	84	4	0	0	1
	a	b	a	b	a	a	b	b	a
Frequencies	816	860	860	874	874	994	994	998	998
IR Intensities	0	0	0	1	0	17	1	14	1
	b	a	b	a	b	a	a	b	b
Frequencies	1036	1040	1045	1045	1111	1111	1225	1225	1355
IR Intensities	3	1	0	0	2	0	0	0	3
	a	a	b	b	a	b	a	b	a
Frequencies	1358	1371	1371	1411	1411	1417	1417	1823	1845
IR Intensities	1	0	0	0	5	11	0	487	1261
	b	a	b	a	b	a	b	a	b
Frequencies	1861	1910	3163	3163	3165	3165	3177	3177	3178
IR Intensities	973	118	0	0	0	0	1	0	1
	a	b	a						
Frequencies	3178	3189	3189						
IR Intensities	0	0	0						

Table S14. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **3S-1** using the BP86 method (Total energy = –2615.615171 Hartrees).

	a	a	a	a	a	a	a	a	a
Frequencies	35	39	42	82	95	99	115	130	144
IR Intensities	2	0	0	1	0	0	1	0	1
	a	a	a	a	a	a	a	a	a
Frequencies	186	204	272	307	313	314	327	362	367
IR Intensities	0	1	1	4	3	2	2	12	6
	a	a	a	a	a	a	a	a	a
Frequencies	390	432	462	487	499	524	549	572	578
IR Intensities	6	18	10	10	6	8	19	0	1
	a	a	a	a	a	a	a	a	a
Frequencies	580	584	607	690	779	783	785	793	798
IR Intensities	0	0	5	27	55	64	41	11	21
	a	a	a	a	a	a	a	a	a
Frequencies	807	812	816	819	819	856	862	867	878
IR Intensities	8	5	1	0	0	1	0	0	1
	a	a	a	a	a	a	a	a	a
Frequencies	993	993	995	999	1041	1042	1043	1046	1107
IR Intensities	16	3	10	7	1	0	1	1	1
	a	a	a	a	a	a	a	a	a
Frequencies	1108	1223	1227	1356	1358	1365	1370	1411	1411
IR Intensities	4	0	0	4	1	1	2	7	1
	a	a	a	a	a	a	a	a	a
Frequencies	1413	1417	1503	1786	1876	3152	3161	3170	3170
IR Intensities	2	3	311	629	520	0	0	0	0
	a	a	a	a	a	a			
Frequencies	3178	3179	3181	3182	3193	3194			
IR Intensities	1	0	0	0	0	0			

Table S15. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **3S-2** using the BP86 method (Total energy = –2615.615300 Hartrees).

	a	b	b	a	b	a	a	b	a
Frequencies	39	40	53	95	116	121	137	145	173
IR Intensities	0	0	2	1	0	0	0	2	1
	b	a	b	b	a	b	a	b	b
Frequencies	193	213	239	300	310	311	324	365	376
IR Intensities	2	0	3	12	1	2	4	4	6
	a	b	a	a	a	b	b	a	b
Frequencies	425	436	447	459	521	551	555	576	577
IR Intensities	0	5	3	6	1	14	0	0	6
	b	a	b	a	a	b	b	a	b
Frequencies	579	580	642	656	775	775	790	790	808
IR Intensities	1	1	43	3	1	81	51	10	28
	a	a	b	a	b	a	b	a	b
Frequencies	808	817	817	818	819	859	860	876	876
IR Intensities	11	0	4	0	1	1	5	2	0
	a	b	b	a	b	a	a	b	a
Frequencies	992	992	997	997	1043	1043	1045	1045	1107
IR Intensities	6	17	6	13	1	0	1	0	0
	b	a	b	b	a	b	a	a	b
Frequencies	1107	1226	1226	1356	1356	1371	1371	1411	1411
IR Intensities	9	0	0	2	0	7	0	0	4
	b	a	b	a	a	a	b	b	a
Frequencies	1414	1415	1617	1656	1746	3160	3160	3170	3170
IR Intensities	1	5	478	358	355	0	1	0	0
	a	b	b	a	b	a			
Frequencies	3177	3177	3185	3185	3193	3193			
IR Intensities	0	1	0	0	0	0			

Table S16. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **3T-1** using the BP86 method (Total energy = –2615.630904 Hartrees).

	a"	a"	a'	a"	a'	a"	a'	a"	a"
Frequencies	8	29	61	70	95	113	124	126	159
IR Intensities	0	0	2	1	0	0	0	0	0
	a'	a'	a'	a"	a'	a'	a"	a'	a"
Frequencies	160	173	234	312	314	329	340	349	374
IR Intensities	1	0	2	3	4	0	3	5	0
	a'	a"	a'	a"	a'	a'	a'	a'	a"
Frequencies	389	414	427	476	476	546	571	572	576
IR Intensities	8	2	18	13	10	19	9	1	0
	a"	a"	a'	a'	a'	a'	a'	a"	a"
Frequencies	579	584	587	658	779	785	785	789	795
IR Intensities	10	0	0	22	25	150	7	1	5
	a'	a"	a"	a'	a'	a"	a'	a'	a"
Frequencies	800	816	817	818	819	864	866	867	870
IR Intensities	13	0	0	1	4	1	0	2	1
	a'	a'	a"	a"	a"	a"	a'	a'	a'
Frequencies	991	994	997	998	1042	1043	1044	1045	1108
IR Intensities	12	11	9	10	0	1	0	0	4
	a'	a"	a"	a"	a'	a'	a"	a'	a'
Frequencies	1108	1224	1226	1361	1362	1365	1366	1409	1411
IR Intensities	2	0	0	0	1	1	0	2	3
	a"	a"	a'	a"	a'	a'	a'	a"	a"
Frequencies	1412	1416	1608	1804	1845	3161	3162	3166	3168
IR Intensities	1	3	397	1038	108	0	0	0	0
	a"	a'	a'	a"	a'	a'			
Frequencies	3177	3177	3178	3181	3189	3191			
IR Intensities	0	0	0	1	0	0			

Table S17. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-1** using the BP86 method (Total energy = –2502.22341 Hartrees).

	a"	a"	a'	a"	a'	a"	a'	a'	a'
Frequencies	16*i*	60	70	81	104	132	173	211	271
IR Intensities		0	0	0	0	0	1	1	1
	a"	a"	a'	a'	a'	a"	a'	a"	a"
Frequencies	286	303	303	328	341	354	431	446	516
IR Intensities	0	4	0	1	5	1	14	1	0
	a'	a"	a'	a"	a'	a'	a"	a'	a'
Frequencies	524	573	578	579	581	593	653	694	750
IR Intensities	12	0	1	0	1	1	6	7	32
	a"	a'	a'	a"	a'	a'	a"	a'	a"
Frequencies	758	772	773	779	781	814	816	818	818
IR Intensities	1	79	43	2	33	3	2	2	0
	a'	a"	a"	a'	a"	a'	a"	a'	a"
Frequencies	844	847	858	861	989	991	999	1000	1038
IR Intensities	4	0	0	6	20	13	3	11	2
	a'	a"	a'	a'	a'	a"	a"	a"	a'
Frequencies	1043	1044	1051	1103	1111	1222	1229	1352	1360
IR Intensities	1	0	2	5	5	0	0	1	2
	a"	a'	a"	a"	a"	a'	a'	a'	a"
Frequencies	1365	1371	1392	1404	1411	1415	1420	1456	3158
IR Intensities	0	3	227	2	0	3	1	217	0
	a'	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	3161	3162	3167	3172	3176	3179	3179	3186	3192
IR Intensities	0	0	0	2	1	0	0	1	1

Table S18. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-2** using the BP86 method (Total energy = –2502.22251 Hartrees).

	a"	a"	a'	a"	a'	a"	a'	a'	a'
Frequencies	20*i*	31	57	81	97	129	174	212	272
IR Intensities		0	0	0	0	0	1	0	0
	a"	a'	a"	a'	a'	a"	a'	a"	a"
Frequencies	279	299	303	329	343	355	431	448	522
IR Intensities	0	2	4	2	3	0	13	0	0
	a'	a"	a'	a'	a"	a'	a"	a'	a'
Frequencies	524	569	578	579	579	598	653	693	742
IR Intensities	13	0	0	1	1	3	5	7	22
	a'	a"	a"	a'	a'	a"	a'	a'	a"
Frequencies	751	758	773	773	775	814	816	816	818
IR Intensities	40	0	4	48	82	2	2	1	0
	a"	a'	a"	a'	a'	a"	a"	a'	a'
Frequencies	836	837	853	860	988	989	994	997	1035
IR Intensities	1	2	0	7	22	1	24	10	0
	a"	a"	a'	a'	a'	a"	a"	a"	a'
Frequencies	1038	1043	1046	1104	1111	1220	1226	1350	1364
IR Intensities	0	0	1	5	5	0	0	1	2
	a"	a'	a"	a"	a'	a"	a'	a'	a"
Frequencies	1364	1369	1391	1407	1409	1410	1419	1456	3158
IR Intensities	0	2	228	0	2	1	1	208	0
	a'	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	3162	3162	3167	3172	3177	3179	3181	3187	3194
IR Intensities	0	1	0	1	1	0	0	1	1

Tables S19. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-3** using the BP86 method (Total energy = –2502.21366 Hartrees).

	a"	a'	a"	a"	a'	a'	a"	a'	a"
Frequencies	39	53	54	99	116	178	211	216	277
IR Intensities	0	1	0	1	0	5	0	1	1
	a'	a"	a'	a'	a"	a'	a'	a"	a"
Frequencies	285	299	336	338	372	380	407	423	457
IR Intensities	1	0	2	0	0	1	7	5	8
	a'	a"	a"	a'	a'	a'	a"	a'	a"
Frequencies	508	568	576	580	582	595	628	691	766
IR Intensities	7	0	0	0	3	3	1	7	3
	a'	a'	a'	a"	a'	a"	a"	a'	a'
Frequencies	768	770	781	785	786	810	814	818	819
IR Intensities	54	100	26	6	2	0	1	3	1
	a"	a"	a'	a'	a"	a'	a"	a'	a'
Frequencies	844	854	864	871	985	994	995	997	1040
IR Intensities	0	1	0	5	11	13	7	15	0
	a"	a"	a'	a'	a'	a"	a"	a'	a"
Frequencies	1040	1044	1047	1101	1110	1222	1227	1355	1357
IR Intensities	1	0	2	8	5	0	0	0	2
	a'	a"	a"	a"	a'	a"	a'	a'	a'
Frequencies	1365	1367	1409	1410	1410	1412	1420	1444	3144
IR Intensities	2	0	126	23	3	113	0	129	2
	a'	a"	a"	a'	a'	a"	a"	a'	a'
Frequencies	3163	3171	3171	3179	3180	3183	3184	3192	3193
IR Intensities	0	0	0	1	1	0	0	0	0

Table S20. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-4** using the BP86 method (Total energy = –2502.20235 Hartrees).

	a	a	a	a	a	a	a	a	a
Frequencies	28	35	46	90	102	127	151	188	221
IR Intensities	1	1	0	0	2	1	2	0	1
	a	a	a	a	a	a	a	a	a
Frequencies	257	302	306	320	336	369	383	440	450
IR Intensities	3	4	2	2	1	2	1	11	3
	a	a	a	a	a	a	a	a	a
Frequencies	511	518	567	572	577	579	582	708	765
IR Intensities	1	4	6	1	5	1	4	15	23
	a	a	a	a	a	a	a	a	a
Frequencies	772	773	783	785	786	806	809	816	817
IR Intensities	102	19	18	9	3	1	1	1	1
	a	a	a	a	a	a	a	a	a
Frequencies	844	846	862	864	983	986	992	994	1037
IR Intensities	2	0	0	0	12	7	11	13	1
	a	a	a	a	a	a	a	a	a
Frequencies	1038	1039	1041	1099	1101	1221	1223	1347	1355
IR Intensities	1	1	1	10	5	0	0	1	1
	a	a	a	a	a	a	a	a	a
Frequencies	1358	1360	1405	1406	1410	1413	1511	1737	3142
IR Intensities	2	2	2	4	1	1	282	457	2
	a	a	a	a	a	a	a	a	a
Frequencies	3151	3161	3169	3172	3176	3179	3183	3187	3193
IR Intensities	1	0	0	1	1	0	0	0	0

Table S21. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-5** using the BP86 method (Total energy = –2502.20013 Hartrees).

	a"	a'	a"	a"	a'	a"	a'	a'	a"
Frequencies	25	64	68	83	101	102	118	171	182
IR Intensities	0	4	0	1	1	0	7	1	0
	a'	a"	a'	a'	a"	a'	a"	a'	a"
Frequencies	227	297	313	324	332	396	398	429	445
IR Intensities	2	1	1	1	0	3	0	5	4
	a'	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	479	523	544	559	560	578	580	589	730
IR Intensities	9	14	8	16	7	5	0	0	8
	a"	a'	a'	a"	a'	a'	a"	a"	a'
Frequencies	743	744	771	776	776	778	804	815	815
IR Intensities	1	26	27	4	70	25	0	0	3
	a'	a"	a"	a'	a"	a'	a'	a"	a"
Frequencies	824	850	853	863	929	968	987	997	1017
IR Intensities	1	0	1	0	7	12	16	8	7
	a'	a'	a"	a'	a'	a"	a"	a"	a'
Frequencies	1039	1040	1043	1073	1106	1195	1222	1279	1333
IR Intensities	2	0	0	15	5	0	0	0	0
	a'	a"	a"	a'	a'	a"	a"	a'	a'
Frequencies	1360	1366	1381	1408	1413	1413	1730	1773	2988
IR Intensities	1	1	2	1	1	3	930	500	1
	a"	a"	a'	a'	a'	a"	a"	a'	a'
Frequencies	3145	3151	3159	3161	3169	3176	3178	3179	3187
IR Intensities	0	0	0	1	1	0	1	0	0

Table S22. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2S-6** using the BP86 method (Total energy = –2502.19556 Hartrees).

	a_u	a_u	a_g	a_u	a_u	a_g	a_g	a_g	a_u
Frequencies	13	30	42	93	103	119	130	148	157
IR Intensities	2	0	0	0	3	0	0	0	3
	a_g	a_u	a_u	a_g	a_g	a_u	a_g	a_g	a_u
Frequencies	227	289	310	310	341	361	375	441	493
IR Intensities	0	2	4	0	0	3	0	0	11
	a_g	a_u	a_g	a_u	a_g	a_u	a_u	a_g	a_u
Frequencies	507	537	552	557	570	572	574	576	759
IR Intensities	0	17	0	4	0	1	8	0	56
	a_g	a_u	a_g	a_u	a_g	a_u	a_g	a_g	a_u
Frequencies	762	771	771	787	787	809	810	815	815
IR Intensities	0	90	0	32	0	0	0	0	7
	a_g	a_u	a_u	a_g	a_u	a_g	a_u	a_g	a_g
Frequencies	849	850	855	856	987	987	992	992	1036
IR Intensities	0	1	1	0	22	0	19	0	0
	a_u	a_g	a_u	a_u	a_g	a_g	a_u	a_g	a_u
Frequencies	1037	1041	1041	1101	1101	1222	1222	1354	1356
IR Intensities	1	0	0	16	0	0	0	0	2
	a_g	a_u	a_g	a_u	a_u	a_g	a_u	a_g	a_u
Frequencies	1359	1362	1405	1405	1409	1410	1740	1755	3142
IR Intensities	0	1	0	2	8	0	1095	0	4
	a_g	a_g	a_u	a_u	a_g	a_u	a_g	a_g	a_u
Frequencies	3142	3167	3167	3174	3174	3181	3182	3190	3190
IR Intensities	0	0	0	2	0	1	0	0	0

Table S23. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2T-1** using the BP86 method (Total energy = –2502.21941 Hartrees).

	a"	a"	a'	a'	a"	a"	a'	a'	a"
Frequencies	11*i*	32	70	85	89	115	127	154	247
IR Intensities		0	0	2	0	0	3	2	1
	a'	a"	a'	a'	a'	a"	a'	a"	a'
Frequencies	255	300	301	310	320	327	382	450	490
IR Intensities	1	2	0	5	0	1	9	1	5
	a"	a'	a"	a"	a'	a'	a"	a'	a'
Frequencies	518	571	575	577	579	580	600	662	754
IR Intensities	0	1	0	0	1	0	7	0	20
	a'	a"	a'	a'	a"	a"	a"	a'	a'
Frequencies	761	763	766	774	776	811	815	816	816
IR Intensities	66	2	42	66	3	0	0	3	0
	a"	a'	a'	a"	a'	a"	a'	a"	a'
Frequencies	841	844	851	858	990	992	993	996	1037
IR Intensities	1	1	1	0	19	0	13	24	1
	a"	a"	a'	a'	a'	a"	a"	a"	a"
Frequencies	1040	1042	1046	1105	1107	1222	1225	1357	1359
IR Intensities	0	0	2	6	4	0	0	0	0
	a'	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	1362	1364	1407	1410	1410	1411	1541	1592	3151
IR Intensities	1	1	2	0	6	0	315	350	0
	a'	a"	a"	a'	a"	a'	a"	a'	a'
Frequencies	3162	3162	3168	3175	3175	3175	3180	3187	3193
IR Intensities	0	0	0	0	1	1	1	1	1

Table S24. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **2T-2** using the BP86 method (Total energy = –2502.21880 Hartrees).

	a"	a"	a'	a"	a'	a"	a'	a'	a"
Frequencies	42*i*	10	62	86	86	111	123	153	243
IR Intensities		0	0	0	4	0	2	2	0
	a'	a"	a'	a'	a'	a"	a'	a"	a'
Frequencies	251	293	301	308	319	326	378	448	494
IR Intensities	1	6	1	4	1	1	8	1	6
	a"	a'	a"	a'	a'	a"	a"	a'	a'
Frequencies	508	568	574	575	579	580	600	658	733
IR Intensities	0	1	0	0	2	0	8	0	37
	a'	a'	a"	a'	a"	a'	a"	a"	a'
Frequencies	758	764	764	767	769	810	814	815	817
IR Intensities	6	74	1	82	2	3	0	0	1
	a'	a"	a"	a'	a'	a"	a'	a"	a"
Frequencies	838	844	846	849	991	991	991	994	1038
IR Intensities	0	1	0	1	15	23	17	2	2
	a'	a'	a"	a'	a'	a"	a"	a"	a'
Frequencies	1038	1041	1041	1106	1107	1221	1223	1358	1360
IR Intensities	0	2	0	6	4	0	0	0	1
	a"	a'	a"	a'	a'	a"	a"	a'	a"
Frequencies	1361	1364	1408	1409	1410	1412	1540	1593	3153
IR Intensities	1	1	2	0	1	2	331	357	0
	a"	a'	a'	a'	a"	a'	a"	a'	a'
Frequencies	3157	3160	3163	3171	3173	3176	3177	3184	3197
IR Intensities	0	0	0	1	0	0	1	0	1

Table S25. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **1Q-1** using the BP86 method (Total energy = –2388.80431 Hartrees).

	a"	a"	a"	a'	a"	a'	a'	a'	a"
Frequencies	3i	61	88	95	117	146	202	243	303
IR Intensities		0	1	0	0	0	2	0	0
	a'	a'	a"	a'	a"	a'	a'	a"	a'
Frequencies	307	316	324	356	377	381	522	544	551
IR Intensities	1	11	2	0	0	9	0	0	2
	a"	a'	a'	a"	a'	a'	a"	a"	a'
Frequencies	575	577	660	680	717	740	753	762	764
IR Intensities	0	0	3	0	6	44	0	0	91
	a'	a'	a'	a"	a"	a'	a"	a'	a"
Frequencies	774	797	813	813	817	826	845	846	956
IR Intensities	4	1	2	0	1	0	0	4	21
	a'	a'	a"	a'	a"	a'	a"	a'	a'
Frequencies	959	988	990	1014	1034	1035	1042	1071	1101
IR Intensities	7	12	19	9	2	0	0	20	9
	a"	a"	a'	a"	a"	a'	a"	a'	a'
Frequencies	1206	1220	1312	1323	1357	1359	1382	1383	1402
IR Intensities	0	0	7	2	0	3	1	27	2
	a"	a'	a"	a'	a"	a'	a'	a"	a'
Frequencies	1409	1412	3103	3114	3146	3157	3158	3165	3172
IR Intensities	0	330	0	2	0	0	1	0	1
	a"	a'	a'						
Frequencies	3173	3177	3191						
IR Intensities	1	0	0						

Table S26. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **1H-1** using the BP86 method (Total energy = –2388.78626 Hartrees).

	a	a	a	a	a	a	a	a
Frequencies	32	38	49	60	89	117	275	284
IR Intensities	0	1	1	1	1	0	2	1
	a	a	a	a	a	a	a	a
Frequencies	309	328	330	356	404	503	557	571
IR Intensities	1	1	1	0	4	6	9	1
	a	a	a	a	a	a	a	a
Frequencies	577	578	747	751	758	760	763	773
IR Intensities	0	1	1	4	51	70	48	0
	a	a	a	a	a	a	a	a
Frequencies	811	812	814	835	843	843	846	984
IR Intensities	0	0	0	1	0	1	0	3
	a	a	a	a	a	a	a	a
Frequencies	992	994	1037	1038	1039	1040	1100	1101
IR Intensities	16	16	1	1	0	0	10	10
	a	a	a	a	a	a	a	a
Frequencies	1221	1354	1355	1358	1358	1400	1401	1411
IR Intensities	0	0	0	2	3	1	1	1
	a	a	a	a	a	a	a	a
Frequencies	1495	3150	3152	3156	3158	3167	3167	3171
IR Intensities	231	0	0	0	0	1	2	1
	a	a						
Frequencies	3181	3184						
IR Intensities	0	0						

Table S27. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **1S-1** using the BP86 method (Total energy = –2388.78348 Hartrees).

	a"	a"	a'	a"	a'	a"	a'	a'	a'
Frequencies	10	37	60	72	88	131	171	240	272
IR Intensities	0	0	1	0	0	0	3	1	0
	a"	a"	a'	a'	a"	a'	a'	a'	a"
Frequencies	283	307	314	344	391	488	543	567	577
IR Intensities	5	0	1	3	2	7	13	3	1
	a"	a'	a'	a"	a"	a'	a'	a'	a'
Frequencies	580	585	612	733	737	751	755	776	780
IR Intensities	0	1	4	0	0	85	80	6	26
	a"	a'	a'	a"	a"	a'	a'	a"	a'
Frequencies	805	812	814	815	839	844	847	848	975
IR Intensities	0	2	1	0	1	4	4	1	13
	a'	a"	a"	a'	a"	a"	a'	a'	a'
Frequencies	985	994	998	1032	1036	1040	1045	1097	1102
IR Intensities	9	33	1	2	0	1	2	6	4
	a"	a"	a'	a"	a"	a'	a'	a'	a"
Frequencies	1219	1223	1342	1344	1362	1363	1396	1399	1411
IR Intensities	0	0	11	1	1	9	1	4	0
	a"	a'	a"	a"	a'	a'	a'	a'	a"
Frequencies	1416	1790	3153	3157	3158	3161	3170	3171	3175
IR Intensities	0	698	0	0	0	0	3	1	1
	a"	a'	a'						
Frequencies	3176	3185	3188						
IR Intensities	0	0	1						

Table S28. The theoretical harmonic vibrational frequencies (in cm^{-1}) and their infrared intensities (in km/mol) for structure **1T-1** using the BP86 method (Total energy = –2388.80031 Hartrees).

	a	a	a	a	a	a	a	a	a
Frequencies	20	40	65	81	95	99	182	261	288
IR Intensities	0	0	1	0	0	1	0	1	1
	a	a	a	a	a	a	a	a	a
Frequencies	296	300	319	341	400	483	561	564	571
IR Intensities	1	1	1	1	4	4	3	1	0
	a	a	a	a	a	a	a	a	a
Frequencies	575	578	717	738	750	755	760	767	772
IR Intensities	3	2	1	10	28	18	62	32	31
	a	a	a	a	a	a	a	a	a
Frequencies	800	806	812	815	826	834	845	850	985
IR Intensities	5	1	1	0	1	2	0	1	17
	a	a	a	a	a	a	a	a	a
Frequencies	985	989	994	1035	1037	1040	1042	1100	1104
IR Intensities	11	22	10	0	0	0	2	10	6
	a	a	a	a	a	a	a	a	a
Frequencies	1220	1221	1352	1356	1358	1359	1363	1402	1404
IR Intensities	0	0	23	49	1	91	103	1	0
	a	a	a	a	a	a	a	a	a
Frequencies	1406	1417	3145	3151	3156	3158	3166	3167	3172
IR Intensities	2	1	1	0	0	1	2	1	2
	a	a	a						
Frequencies	3172	3182	3185						
IR Intensities	1	1	0						

Table S29. The theoretical Cartesian coordinates (in Å) for the structure **5S-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.180820	-1.227476	-0.000000
2	23	0	0.089374	1.209670	0.000000
3	6	0	-1.495497	2.720756	0.716626
4	6	0	-1.495497	2.720756	-0.716626
5	6	0	-0.205679	3.149235	-1.167206
6	6	0	0.597572	3.419024	0.000000
7	6	0	-0.205679	3.149235	1.167206
8	1	0	-2.323171	2.405851	1.358386
9	1	0	-2.323171	2.405851	-1.358386
10	1	0	0.103611	3.268066	-2.208295
11	1	0	1.628325	3.782479	0.000000
12	1	0	0.103611	3.268066	2.208295
13	6	0	0.130725	-3.390255	0.721689
14	6	0	1.240073	-2.600243	1.163409
15	6	0	1.928613	-2.115994	-0.000000
16	6	0	1.240073	-2.600243	-1.163409
17	6	0	0.130725	-3.390255	-0.721689
18	1	0	-0.588166	-3.903205	1.366132
19	1	0	1.513015	-2.395823	2.201837
20	1	0	2.818423	-1.482338	-0.000000
21	1	0	1.513015	-2.395823	-2.201837
22	1	0	-0.588166	-3.903205	-1.366132
23	6	0	-0.780507	-0.349784	1.614690
24	8	0	-1.226116	-0.048548	2.676980
25	6	0	-0.780507	-0.349784	-1.614690
26	8	0	-1.226116	-0.048548	-2.676980
27	6	0	1.502671	0.890087	1.243744
28	8	0	2.398994	0.734626	2.000707
29	6	0	1.502671	0.890087	-1.243744
30	8	0	2.398994	0.734626	-2.000707
31	6	0	-2.081546	-1.624075	-0.000000
32	8	0	-3.236174	-1.841115	-0.000000

Table S30. The theoretical Cartesian coordinates (in Å) for the structure **5S-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.290925	2.760790	0.897472
2	6	0	-1.725705	2.426239	-0.427839
3	6	0	-0.700003	2.820737	-1.355215
4	6	0	0.369652	3.404494	-0.596873
5	6	0	0.000000	3.365799	0.796769
6	1	0	-1.839586	2.570011	1.823620
7	1	0	-2.667552	1.938356	-0.690743
8	1	0	-0.734913	2.703409	-2.440953
9	1	0	1.298983	3.810679	-1.004828
10	1	0	0.600182	3.734459	1.632896
11	6	0	-0.000000	-3.365799	0.796769
12	6	0	1.290925	-2.760790	0.897472
13	6	0	1.725705	-2.426239	-0.427839
14	6	0	0.700003	-2.820737	-1.355215
15	6	0	-0.369652	-3.404494	-0.596873
16	1	0	-0.600182	-3.734459	1.632896
17	1	0	1.839586	-2.570011	1.823620
18	1	0	2.667552	-1.938356	-0.690743
19	1	0	0.734913	-2.703409	-2.440953
20	1	0	-1.298983	-3.810679	-1.004828
21	6	0	-1.253137	-0.535731	-1.431642
22	8	0	-1.968102	-0.271270	-2.342980
23	6	0	1.253137	0.535731	-1.431642
24	8	0	1.968102	0.271270	-2.342980
25	6	0	0.000000	0.000000	1.689447
26	8	0	0.000000	0.000000	2.883648
27	23	0	0.152061	1.198226	-0.024234
28	23	0	-0.152061	-1.198226	-0.024234
29	6	0	-1.876201	-1.286875	0.848888
30	6	0	1.876201	1.286875	0.848888
31	8	0	-2.929463	-1.315992	1.373618
32	8	0	2.929463	1.315992	1.373618

Table S31. The theoretical Cartesian coordinates (in Å) for the structure **5S-3** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.031147	-1.195677	0.000000
2	23	0	-0.088397	1.332573	0.000000
3	6	0	-0.817632	3.172462	1.163198
4	6	0	-1.645616	3.011195	0.000000
5	6	0	-0.817632	3.172462	-1.163198
6	6	0	0.520007	3.421261	-0.722470
7	6	0	0.520007	3.421261	0.722470
8	1	0	-1.153040	3.117335	2.201866
9	1	0	-2.718149	2.796351	0.000000
10	1	0	-1.153040	3.117335	-2.201866
11	1	0	1.387202	3.592749	-1.365292
12	1	0	1.387202	3.592749	1.365292
13	6	0	-1.915854	-2.327115	0.716106
14	6	0	-0.753433	-3.030041	1.166326
15	6	0	-0.026618	-3.469651	0.000000
16	6	0	-0.753433	-3.030041	-1.166326
17	6	0	-1.915854	-2.327115	-0.716106
18	1	0	-2.656081	-1.843587	1.358072
19	1	0	-0.482561	-3.220004	2.207494
20	1	0	0.894590	-4.057442	0.000000
21	1	0	-0.482561	-3.220004	-2.207494
22	1	0	-2.656081	-1.843587	-1.358072
23	6	0	1.348817	-1.325377	1.344294
24	8	0	2.169039	-1.470469	2.176067
25	6	0	1.348817	-1.325377	-1.344294
26	8	0	2.169039	-1.470469	-2.176067
27	6	0	1.831613	1.017881	0.000000
28	8	0	3.011523	1.014767	0.000000
29	6	0	-0.776214	0.414061	-1.556396
30	8	0	-1.289959	0.185583	-2.609508
31	6	0	-0.776214	0.414061	1.556396
32	8	0	-1.289959	0.185583	2.609508

Table S32. The theoretical Cartesian coordinates (in Å) for the structure **5S-4** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.000000	1.281214	0.083045
2	23	0	-0.000000	-1.281214	0.083045
3	6	0	-1.004561	-2.716223	1.522524
4	6	0	0.416572	-2.897142	1.672193
5	6	0	0.935180	-3.373532	0.427182
6	6	0	-0.151558	-3.487422	-0.500961
7	6	0	-1.360544	-3.088328	0.186482
8	1	0	-1.688404	-2.358094	2.296233
9	1	0	0.999207	-2.688886	2.572679
10	1	0	1.981909	-3.608023	0.217566
11	1	0	-0.081614	-3.844327	-1.531017
12	1	0	-2.368020	-3.084391	-0.237446
13	6	0	-0.416572	2.897142	1.672193
14	6	0	-0.935180	3.373532	0.427182
15	6	0	0.151558	3.487422	-0.500961
16	6	0	1.360544	3.088328	0.186482
17	6	0	1.004561	2.716223	1.522524
18	1	0	-0.999207	2.688886	2.572679
19	1	0	-1.981909	3.608023	0.217566
20	1	0	0.081614	3.844327	-1.531017
21	1	0	2.368020	3.084391	-0.237446
22	1	0	1.688404	2.358094	2.296233
23	6	0	-1.804999	1.010216	-0.544978
24	8	0	-2.938601	0.991877	-0.880273
25	6	0	0.862554	1.107545	-1.638509
26	8	0	1.349764	1.159438	-2.711405
27	6	0	-0.862554	-1.107545	-1.638509
28	8	0	-1.349764	-1.159438	-2.711405
29	6	0	1.804999	-1.010216	-0.544978
30	8	0	2.938601	-0.991877	-0.880273
31	6	0	-0.000000	0.000000	1.711582
32	8	0	-0.000000	0.000000	2.906757

Table S33. The theoretical Cartesian coordinates (in Å) for the structure **5S-5** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.000000	1.334722	0.096576
2	23	0	-0.000000	-1.334722	0.096576
3	6	0	-0.718235	-2.779102	1.744723
4	6	0	0.718235	-2.779102	1.744723
5	6	0	1.163010	-3.270543	0.478776
6	6	0	-0.000000	-3.570433	-0.320591
7	6	0	-1.163010	-3.270543	0.478776
8	1	0	-1.355218	-2.436201	2.563386
9	1	0	1.355218	-2.436201	2.563386
10	1	0	2.203208	-3.412220	0.175211
11	1	0	-0.000000	-3.990199	-1.329115
12	1	0	-2.203208	-3.412220	0.175211
13	6	0	-0.718235	2.779102	1.744723
14	6	0	-1.163010	3.270543	0.478776
15	6	0	0.000000	3.570433	-0.320591
16	6	0	1.163010	3.270543	0.478776
17	6	0	0.718235	2.779102	1.744723
18	1	0	-1.355218	2.436201	2.563386
19	1	0	-2.203208	3.412220	0.175211
20	1	0	0.000000	3.990199	-1.329115
21	1	0	2.203208	3.412220	0.175211
22	1	0	1.355218	2.436201	2.563386
23	6	0	-1.406798	1.271548	-1.226867
24	8	0	-2.229969	1.451755	-2.052195
25	6	0	1.406798	1.271548	-1.226867
26	8	0	2.229969	1.451755	-2.052195
27	6	0	-1.406798	-1.271548	-1.226867
28	8	0	-2.229969	-1.451755	-2.052195
29	6	0	1.406798	-1.271548	-1.226867
30	8	0	2.229969	-1.451755	-2.052195
31	6	0	0.000000	0.000000	1.659239
32	8	0	0.000000	0.000000	2.863008

Table S34. The theoretical Cartesian coordinates (in Å) for the structure **5T-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.680244	1.552127	-1.072068
2	6	0	-2.182455	2.033321	0.181179
3	6	0	-2.740835	1.223656	1.226749
4	6	0	-3.598562	0.246778	0.616884
5	6	0	-3.552678	0.445145	-0.806094
6	1	0	-2.434905	1.953743	-2.058646
7	1	0	-1.490839	2.867942	0.317917
8	1	0	-2.540947	1.335178	2.295368
9	1	0	-4.175495	-0.520980	1.139459
10	1	0	-4.092319	-0.140684	-1.554598
11	6	0	3.751319	-0.204892	-0.378933
12	6	0	3.093966	-1.406447	-0.802548
13	6	0	2.314807	-1.908102	0.291445
14	6	0	2.485916	-1.008610	1.396155
15	6	0	3.377216	0.040831	0.989767
16	1	0	4.419574	0.412033	-0.985738
17	1	0	3.138351	-1.837901	-1.806261
18	1	0	1.683609	-2.800206	0.281273
19	1	0	2.018149	-1.108300	2.378952
20	1	0	3.704073	0.879953	1.609557
21	6	0	0.435484	0.936440	1.181827
22	8	0	0.258105	1.537328	2.194913
23	6	0	-0.956301	-1.324348	1.366008
24	8	0	-0.706553	-2.073130	2.244599
25	6	0	-0.218196	-0.274018	-1.475687
26	8	0	0.713881	-0.349163	-2.275747
27	23	0	-1.461909	-0.151773	-0.092121
28	23	0	1.500932	0.174187	-0.300226
29	6	0	1.767070	2.075846	-0.686112
30	6	0	-1.810504	-1.879923	-0.832578
31	8	0	1.985155	3.223258	-0.825997
32	8	0	-2.005938	-2.943681	-1.308928

Table S35. The theoretical Cartesian coordinates (in Å) for the structure **5T-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.178298	1.308722	0.000000
2	23	0	-0.203062	-1.328616	0.000000
3	6	0	1.640993	-2.499513	0.719541
4	6	0	1.640993	-2.499513	-0.719541
5	6	0	0.470565	-3.196290	-1.161787
6	6	0	-0.259483	-3.626206	0.000000
7	6	0	0.470565	-3.196290	1.161787
8	1	0	2.390613	-2.032064	1.363131
9	1	0	2.390613	-2.032064	-1.363131
10	1	0	0.173296	-3.353538	-2.202318
11	1	0	-1.201800	-4.180896	0.000000
12	1	0	0.173296	-3.353538	2.202318
13	6	0	0.333616	3.450363	0.722794
14	6	0	-0.927988	2.926581	1.164641
15	6	0	-1.703079	2.607847	0.000000
16	6	0	-0.927988	2.926581	-1.164641
17	6	0	0.333616	3.450363	-0.722794
18	1	0	1.142343	3.801100	1.368687
19	1	0	-1.243439	2.796512	2.202751
20	1	0	-2.700278	2.157859	0.000000
21	1	0	-1.243439	2.796512	-2.202751
22	1	0	1.142343	3.801100	-1.368687
23	6	0	0.460076	0.386529	1.660643
24	8	0	0.718908	0.026720	2.770366
25	6	0	0.460076	0.386529	-1.660643
26	8	0	0.718908	0.026720	-2.770366
27	6	0	-1.710374	-0.975674	1.235047
28	8	0	-2.645084	-0.809002	1.928722
29	6	0	-1.710374	-0.975674	-1.235047
30	8	0	-2.645084	-0.809002	-1.928722
31	6	0	2.108022	1.279746	0.000000
32	8	0	3.286174	1.237602	0.000000

Table S36. The theoretical Cartesian coordinates (in Å) for the structure **4S-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.277336	-1.882264	0.000809
2	6	0	2.122060	-1.302572	-1.307556
3	6	0	2.899080	-0.094077	-1.352581
4	6	0	3.528769	0.068957	-0.067584
5	6	0	3.149021	-1.035977	0.758546
6	6	0	-3.383119	-0.562547	0.803341
7	6	0	-3.440242	-0.623780	-0.636499
8	6	0	-3.134539	0.678614	-1.148013
9	6	0	-2.879291	1.547310	-0.039703
10	6	0	-3.029584	0.784508	1.169346
11	1	0	1.794437	-2.795300	0.357741
12	1	0	1.525409	-1.713561	-2.125076
13	1	0	3.001930	0.577050	-2.208756
14	1	0	4.188847	0.889753	0.225137
15	1	0	3.422329	-1.175335	1.807821
16	1	0	-3.584025	-1.386525	1.491674
17	1	0	-3.686756	-1.506369	-1.232605
18	1	0	-3.045946	0.950469	-2.203443
19	1	0	-2.584267	2.598386	-0.105680
20	1	0	-2.914831	1.164274	2.187352
21	23	0	-1.299064	-0.121535	0.043662
22	23	0	1.231640	0.133766	0.176836
23	6	0	-0.942864	-1.978541	-0.245631
24	6	0	0.202737	1.019889	-1.184766
25	6	0	-0.291775	-0.242952	1.591983
26	6	0	1.551233	2.022775	0.512288
27	8	0	-0.152297	1.611019	-2.168580
28	8	0	-0.780020	-3.143609	-0.386721
29	8	0	1.744979	3.177326	0.625219
30	8	0	0.644924	-0.179763	2.381397

Table S37. The theoretical Cartesian coordinates (in Å) for the structure **4S-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.196842	-1.134676	-0.000000
2	6	0	-0.803225	-3.250109	0.715733
3	6	0	0.536906	-2.977287	1.160861
4	6	0	1.362483	-2.815591	-0.000000
5	6	0	0.536906	-2.977287	-1.160861
6	6	0	-0.803225	-3.250109	-0.715733
7	1	0	-1.669471	-3.415777	1.361751
8	1	0	0.866257	-2.893620	2.200180
9	1	0	2.430493	-2.579205	-0.000000
10	1	0	0.866257	-2.893620	-2.200180
11	1	0	-1.669471	-3.415777	-1.361751
12	6	0	-1.107930	2.876969	0.718397
13	6	0	-1.107930	2.876969	-0.718397
14	6	0	0.230575	3.144775	-1.160843
15	6	0	1.055461	3.313367	0.000000
16	6	0	0.230575	3.144775	1.160843
17	1	0	-1.971198	2.690397	1.362764
18	1	0	-1.971198	2.690397	-1.362764
19	1	0	0.563924	3.203769	-2.200472
20	1	0	2.133339	3.499219	0.000000
21	1	0	0.563924	3.203769	2.200472
22	6	0	1.289023	0.305702	1.357251
23	8	0	2.046087	-0.037526	2.207153
24	6	0	1.289023	0.305702	-1.357251
25	8	0	2.046087	-0.037526	-2.207153
26	6	0	-1.318155	-0.327476	-1.353994
27	8	0	-2.075522	0.001087	-2.208783
28	23	0	0.192237	1.144934	0.000000
29	6	0	-1.318155	-0.327476	1.353994
30	8	0	-2.075522	0.001087	2.208783

Table S38. The theoretical Cartesian coordinates (in Å) for the structure **4S-3** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.069400	1.151361	0.000000
2	6	0	0.038906	3.348769	0.715869
3	6	0	-1.204321	2.778840	1.160736
4	6	0	-1.971488	2.433396	0.000000
5	6	0	-1.204321	2.778840	-1.160736
6	6	0	0.038906	3.348769	-0.715869
7	1	0	0.845157	3.706294	1.361897
8	1	0	-1.506506	2.622586	2.199983
9	1	0	-2.959377	1.963738	0.000000
10	1	0	-1.506506	2.622586	-2.199983
11	1	0	0.845157	3.706294	-1.361897
12	6	0	1.204321	0.602916	-1.351181
13	8	0	2.022038	0.441367	-2.198308
14	6	0	1.204321	0.602916	1.351181
15	8	0	2.022038	0.441367	2.198308
16	23	0	0.069400	-1.151361	0.000000
17	6	0	-0.038906	-3.348769	-0.715869
18	6	0	1.204321	-2.778840	-1.160736
19	6	0	1.971488	-2.433396	0.000000
20	6	0	1.204321	-2.778840	1.160736
21	6	0	-0.038906	-3.348769	0.715869
22	1	0	-0.845157	-3.706294	-1.361897
23	1	0	1.506506	-2.622586	-2.199983
24	1	0	2.959377	-1.963738	0.000000
25	1	0	1.506506	-2.622586	2.199983
26	1	0	-0.845157	-3.706294	1.361897
27	6	0	-1.204321	-0.602916	1.351181
28	8	0	-2.022038	-0.441367	2.198308
29	6	0	-1.204321	-0.602916	-1.351181
30	8	0	-2.022038	-0.441367	-2.198308

Table S39. The theoretical Cartesian coordinates (in Å) for the structure **4T-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.187162	1.265546	0.000000
2	6	0	-0.200978	3.243313	1.161918
3	6	0	-1.028847	3.410388	0.000000
4	6	0	-0.200978	3.243313	-1.161918
5	6	0	1.138986	2.982155	-0.717707
6	6	0	1.138986	2.982155	0.717707
7	1	0	-0.534588	3.284325	2.202718
8	1	0	-2.101730	3.620916	0.000000
9	1	0	-0.534588	3.284325	-2.202718
10	1	0	1.999887	2.785719	-1.363011
11	1	0	1.999887	2.785719	1.363011
12	6	0	-0.355205	-3.086754	1.165328
13	6	0	0.399870	-3.451672	0.000000
14	6	0	-0.355205	-3.086754	-1.165328
15	6	0	-1.577224	-2.483982	-0.719860
16	6	0	-1.577224	-2.483982	0.719860
17	1	0	-0.048680	-3.235605	2.203719
18	1	0	1.381341	-3.933545	0.000000
19	1	0	-0.048680	-3.235605	-2.203719
20	1	0	-2.370223	-2.090560	-1.360648
21	1	0	-2.370223	-2.090560	1.360648
22	6	0	-2.008809	0.566901	0.000000
23	8	0	-3.160614	0.296298	0.000000
24	6	0	0.503101	-0.199897	-1.638728
25	8	0	0.797235	0.135895	-2.747586
26	6	0	2.059974	-1.198037	0.000000
27	8	0	3.237609	-1.202603	0.000000
28	23	0	0.127100	-1.157829	0.000000
29	6	0	0.503101	-0.199897	1.638728
30	8	0	0.797235	0.135895	2.747586

Table S40. The theoretical Cartesian coordinates (in Å) for the structure **4T-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.009333	1.186745	0.128056
2	6	0	0.106905	3.446972	0.513617
3	6	0	-1.021780	2.927547	1.238467
4	6	0	-1.947876	2.398888	0.281286
5	6	0	-1.399282	2.595781	-1.030560
6	6	0	-0.126377	3.242869	-0.888083
7	1	0	0.998891	3.898763	0.957226
8	1	0	-1.149339	2.931451	2.324064
9	1	0	-2.896877	1.908579	0.514125
10	1	0	-1.857433	2.282483	-1.972486
11	1	0	0.543542	3.530777	-1.702304
12	6	0	1.392369	0.675788	-1.091938
13	8	0	2.302003	0.549577	-1.848749
14	6	0	0.959237	0.648347	1.720304
15	8	0	1.563987	0.417954	2.711080
16	23	0	0.009333	-1.186745	-0.128056
17	6	0	-0.106905	-3.446972	-0.513617
18	6	0	1.021780	-2.927547	-1.238467
19	6	0	1.947876	-2.398888	-0.281286
20	6	0	1.399282	-2.595781	1.030560
21	6	0	0.126377	-3.242869	0.888083
22	1	0	-0.998891	-3.898763	-0.957226
23	1	0	1.149339	-2.931451	-2.324064
24	1	0	2.896877	-1.908579	-0.514125
25	1	0	1.857433	-2.282483	1.972486
26	1	0	-0.543542	-3.530777	1.702304
27	6	0	-1.392369	-0.675788	1.091938
28	8	0	-2.302003	-0.549577	1.848749
29	6	0	-0.959237	-0.648347	-1.720304
30	8	0	-1.563987	-0.417954	-2.711080

Table S41. The theoretical Cartesian coordinates (in Å) for the structure **4T-3** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.056810	1.198322	0.018361
2	6	0	-0.103289	3.292347	-0.983963
3	6	0	1.181564	2.721465	-1.271979
4	6	0	1.877573	2.544076	-0.026858
5	6	0	1.020217	3.011072	1.027219
6	6	0	-0.203152	3.473138	0.430857
7	1	0	-0.876496	3.532076	-1.718725
8	1	0	1.557342	2.446172	-2.261073
9	1	0	2.880352	2.124612	0.094184
10	1	0	1.252111	3.006289	2.096106
11	1	0	-1.068556	3.868514	0.969229
12	6	0	-1.181564	0.740286	1.430215
13	8	0	-1.960425	0.534268	2.300435
14	6	0	-1.361917	0.585167	-1.133673
15	8	0	-2.288033	0.386539	-1.854552
16	23	0	-0.056810	-1.198322	0.018361
17	6	0	0.203152	-3.473138	0.430857
18	6	0	-1.020217	-3.011072	1.027219
19	6	0	-1.877573	-2.544076	-0.026858
20	6	0	-1.181564	-2.721465	-1.271979
21	6	0	0.103289	-3.292347	-0.983963
22	1	0	1.068556	-3.868514	0.969229
23	1	0	-1.252111	-3.006289	2.096106
24	1	0	-2.880352	-2.124612	0.094184
25	1	0	-1.557342	-2.446172	-2.261073
26	1	0	0.876496	-3.532076	-1.718725
27	6	0	1.361917	-0.585167	-1.133673
28	8	0	2.288033	-0.386539	-1.854552
29	6	0	1.181564	-0.740286	1.430215
30	8	0	1.960425	-0.534268	2.300435

Table S42. The theoretical Cartesian coordinates (in Å) for the structure **3S-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.164202	-0.110121	0.087918
2	23	0	1.271580	0.213503	0.424702
3	6	0	2.331824	-0.215471	-1.500667
4	6	0	2.669138	-1.221650	-0.527711
5	6	0	3.426377	-0.584388	0.522170
6	6	0	3.535530	0.802776	0.204955
7	6	0	2.849588	1.042725	-1.029969
8	1	0	1.775704	-0.377662	-2.426498
9	1	0	2.407391	-2.281453	-0.585147
10	1	0	3.808277	-1.073847	1.422441
11	1	0	3.998020	1.570310	0.834318
12	1	0	2.750596	2.009587	-1.529975
13	6	0	-2.931340	0.842059	-1.083916
14	6	0	-2.943791	1.346566	0.257590
15	6	0	-3.145374	0.237474	1.144861
16	6	0	-3.256089	-0.958504	0.349506
17	6	0	-3.126299	-0.576079	-1.032827
18	1	0	-2.754277	1.435771	-1.985703
19	1	0	-2.792856	2.389360	0.548209
20	1	0	-3.199681	0.289200	2.235110
21	1	0	-3.420406	-1.971724	0.723459
22	1	0	-3.164935	-1.252073	-1.891095
23	6	0	-0.469868	-1.673358	-0.728933
24	8	0	-0.132315	-2.699532	-1.227331
25	6	0	-0.211641	-0.553793	1.615770
26	8	0	0.848291	-0.565166	2.294561
27	6	0	0.176353	1.677656	-0.231225
28	8	0	-0.128972	2.750781	-0.678856

Table S43. The theoretical Cartesian coordinates (in Å) for the structure **3S-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.638473	2.797761	1.313686
2	6	0	-0.000000	3.238173	0.106619
3	6	0	0.977509	3.209742	-0.958496
4	6	0	2.217428	2.766442	-0.389774
5	6	0	2.010365	2.510857	1.004365
6	1	0	0.167979	2.682729	2.292788
7	1	0	-1.044865	3.542807	0.008385
8	1	0	0.804996	3.490309	-2.000258
9	1	0	3.146018	2.591676	-0.941101
10	1	0	2.750466	2.112689	1.705049
11	6	0	-2.010365	-2.510857	1.004365
12	6	0	-0.638473	-2.797761	1.313686
13	6	0	-0.000000	-3.238173	0.106619
14	6	0	-0.977509	-3.209742	-0.958496
15	6	0	-2.217428	-2.766442	-0.389774
16	1	0	-2.750466	-2.112689	1.705049
17	1	0	-0.167979	-2.682729	2.292788
18	1	0	1.044865	-3.542807	0.008385
19	1	0	-0.804996	-3.490309	-2.000258
20	1	0	-3.146018	-2.591676	-0.941101
21	6	0	0.000000	0.000000	1.403177
22	8	0	0.000000	0.000000	2.613714
23	6	0	0.991751	-0.796729	-1.047043
24	6	0	-0.991751	0.796729	-1.047043
25	8	0	2.047362	-0.274719	-1.401504
26	8	0	-2.047362	0.274719	-1.401504
27	23	0	-0.650707	-1.101412	-0.204059
28	23	0	0.650707	1.101412	-0.204059

Table S44. The theoretical Cartesian coordinates (in Å) for the structure **3T-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.091595	1.242072	-0.000000
2	23	0	-0.278539	-1.283319	0.000000
3	6	0	-0.005455	-3.233732	1.162866
4	6	0	1.278167	-2.764883	0.718529
5	1	0	-0.330835	-3.323485	2.203352
6	1	0	2.096493	-2.435849	1.364331
7	6	0	1.317398	3.068268	-0.000000
8	6	0	0.476661	3.144923	1.162729
9	6	0	-0.880429	3.263313	0.720843
10	1	0	2.405713	2.958122	-0.000000
11	1	0	0.814691	3.118076	2.201897
12	1	0	-1.761675	3.329996	1.363771
13	6	0	-1.697534	0.268500	-0.000000
14	8	0	-2.421515	-0.732412	0.000000
15	6	0	0.550135	0.279116	1.549974
16	8	0	0.980768	-0.050206	2.615954
17	6	0	-0.005455	-3.233732	-1.162866
18	6	0	1.278167	-2.764883	-0.718529
19	1	0	-0.330835	-3.323485	-2.203352
20	1	0	2.096493	-2.435849	-1.364331
21	6	0	0.476661	3.144923	-1.162729
22	6	0	-0.880429	3.263313	-0.720843
23	1	0	0.814691	3.118076	-2.201897
24	1	0	-1.761675	3.329996	-1.363771
25	6	0	0.550135	0.279116	-1.549974
26	8	0	0.980768	-0.050206	-2.615954
27	6	0	-0.793611	-3.525743	0.000000
28	1	0	-1.836583	-3.855304	0.000000

Table S45. The theoretical Cartesian coordinates (in Å) for the structure **2S-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.470800	1.207060	0.000000
2	23	0	0.433170	-1.206595	0.000000
3	6	0	-1.691946	-1.532588	0.718867
4	6	0	-0.922240	-2.663163	1.156601
5	6	0	-0.440442	-3.357981	0.000000
6	6	0	-0.922240	-2.663163	-1.156601
7	6	0	-1.691946	-1.532588	-0.718867
8	1	0	-2.193515	-0.807873	1.364329
9	1	0	-0.687604	-2.912784	2.195293
10	1	0	0.207951	-4.238516	0.000000
11	1	0	-0.687604	-2.912784	-2.195293
12	1	0	-2.193515	-0.807873	-1.364329
13	6	0	-1.655143	1.987355	0.000000
14	6	0	-1.005867	2.529735	-1.165751
15	6	0	0.038428	3.409886	-0.713440
16	6	0	0.038428	3.409886	0.713440
17	6	0	-1.005867	2.529735	1.165751
18	1	0	-2.519881	1.318705	0.000000
19	1	0	-1.264686	2.325711	-2.208082
20	1	0	0.745134	3.945139	-1.354552
21	1	0	0.745134	3.945139	1.354552
22	1	0	-1.264686	2.325711	2.208082
23	6	0	1.440970	0.155237	1.201649
24	8	0	1.661458	-1.047299	1.557455
25	6	0	1.440970	0.155237	-1.201649
26	8	0	1.661458	-1.047299	-1.557455

Table S46. The theoretical Cartesian coordinates (in Å) for the structure **2S-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.473535	1.211968	0.000000
2	23	0	0.429075	-1.210830	0.000000
3	6	0	-1.699641	-1.546157	0.718537
4	6	0	-0.920795	-2.670338	1.156820
5	6	0	-0.434371	-3.361904	0.000000
6	6	0	-0.920795	-2.670338	-1.156820
7	6	0	-1.699641	-1.546157	-0.718537
8	1	0	-2.210829	-0.826768	1.361662
9	1	0	-0.684931	-2.919022	2.195454
10	1	0	0.219857	-4.238167	0.000000
11	1	0	-0.684931	-2.919022	-2.195454
12	1	0	-2.210829	-0.826768	-1.361662
13	6	0	-1.519967	2.210328	0.717255
14	6	0	-1.519967	2.210328	-0.717255
15	6	0	-0.409692	3.000754	-1.164081
16	6	0	0.286197	3.485621	0.000000
17	6	0	-0.409692	3.000754	1.164081
18	1	0	-2.240716	1.699423	1.361825
19	1	0	-2.240716	1.699423	-1.361825
20	1	0	-0.129927	3.185258	-2.204733
21	1	0	1.180980	4.114232	0.000000
22	1	0	-0.129927	3.185258	2.204733
23	6	0	1.439364	0.156439	1.196240
24	8	0	1.661861	-1.045914	1.552267
25	6	0	1.439364	0.156439	-1.196240
26	8	0	1.661861	-1.045914	-1.552267

Table S47. The theoretical Cartesian coordinates (in Å) for the structure **2S-3** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.373893	1.284683	0.000000
2	23	0	-0.392197	-1.232501	-0.000000
3	6	0	-0.486132	-3.601880	-0.000000
4	6	0	0.224936	-3.148260	1.155620
5	6	0	1.369531	-2.398260	0.722699
6	6	0	1.369531	-2.398260	-0.722699
7	6	0	0.224936	-3.148260	-1.155620
8	1	0	-1.423783	-4.165393	-0.000000
9	1	0	-0.094181	-3.273259	2.193230
10	1	0	2.109815	-1.923571	1.370966
11	1	0	2.109815	-1.923571	-1.370966
12	1	0	-0.094181	-3.273259	-2.193230
13	6	0	-0.981008	2.885270	0.720292
14	6	0	-0.981008	2.885270	-0.720292
15	6	0	0.337581	3.275822	-1.163133
16	6	0	1.135630	3.511639	0.000000
17	6	0	0.337581	3.275822	1.163133
18	1	0	-1.830547	2.658860	1.368769
19	1	0	-1.830547	2.658860	-1.368769
20	1	0	0.669038	3.355582	-2.201271
21	1	0	2.199583	3.774539	0.000000
22	1	0	0.669038	3.355582	2.201271
23	6	0	-0.175199	0.178062	1.400980
24	8	0	-0.954383	-0.713421	1.884400
25	6	0	-0.175199	0.178062	-1.400980
26	8	0	-0.954383	-0.713421	-1.884400

Table S48. The theoretical Cartesian coordinates (in Å) for the structure **2S-4** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.105669	-0.168175	0.297825
2	23	0	1.240208	-0.153094	-0.437073
3	6	0	2.109551	0.724949	1.420904
4	6	0	2.792709	1.342791	0.306768
5	6	0	3.526140	0.319463	-0.377178
6	6	0	3.288938	-0.928468	0.275154
7	6	0	2.406230	-0.684204	1.389107
8	1	0	1.522493	1.250935	2.178562
9	1	0	2.767366	2.403629	0.046902
10	1	0	4.116302	0.460927	-1.288731
11	1	0	3.667739	-1.905241	-0.037665
12	1	0	2.041762	-1.438639	2.091948
13	6	0	-3.002566	1.150791	0.509830
14	6	0	-3.222850	-0.014285	1.314333
15	6	0	-3.157352	-1.171247	0.476665
16	6	0	-2.893877	-0.716940	-0.875736
17	6	0	-2.801947	0.721211	-0.848587
18	1	0	-2.957744	2.184373	0.864988
19	1	0	-3.365601	-0.021374	2.401017
20	1	0	-3.288677	-2.208832	0.792860
21	1	0	-2.824237	-1.353161	-1.760939
22	1	0	-2.611837	1.379039	-1.699703
23	6	0	0.123813	1.383092	-0.702257
24	8	0	-0.223791	2.537055	-0.835265
25	6	0	-0.181968	-1.589757	-0.377881
26	8	0	0.713429	-2.110412	-1.096395

Table S49. The theoretical Cartesian coordinates (in Å) for the structure **2S-5** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.035237	-0.835314	0.000000
2	23	0	-0.602429	1.399295	-0.000000
3	6	0	1.426774	1.193687	-0.000000
4	6	0	1.097636	2.008284	1.184943
5	6	0	0.589754	3.270301	0.711315
6	6	0	0.589754	3.270301	-0.711315
7	6	0	1.097636	2.008284	-1.184943
8	1	0	2.071740	0.291178	-0.000000
9	1	0	1.280766	1.727534	2.224858
10	1	0	0.190990	4.071593	1.342253
11	1	0	0.190990	4.071593	-1.342253
12	1	0	1.280766	1.727534	-2.224858
13	6	0	1.533972	-2.403137	0.723156
14	6	0	1.533972	-2.403137	-0.723156
15	6	0	0.237382	-2.822991	-1.162476
16	6	0	-0.566527	-3.074220	0.000000
17	6	0	0.237382	-2.822991	1.162476
18	1	0	2.379593	-2.152158	1.370941
19	1	0	2.379593	-2.152158	-1.370941
20	1	0	-0.089249	-2.922522	-2.200922
21	1	0	-1.615845	-3.381463	0.000000
22	1	0	-0.089249	-2.922522	2.200922
23	6	0	-1.053090	-0.162133	1.420444
24	8	0	-1.810250	0.079322	2.335913
25	6	0	-1.053090	-0.162133	-1.420444
26	8	0	-1.810250	0.079322	-2.335913

Table S50. The theoretical Cartesian coordinates (in Å) for the structure **2S-6** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.433480	1.086156	0.031831
2	23	0	0.433480	-1.086156	-0.031831
3	6	0	1.029335	-3.331833	-0.062807
4	6	0	0.319597	-3.036597	-1.275758
5	6	0	-0.998334	-2.597815	-0.911035
6	6	0	-1.098365	-2.622081	0.524026
7	6	0	0.164960	-3.088705	1.051387
8	1	0	2.074407	-3.655395	0.001825
9	1	0	0.711885	-3.105575	-2.294192
10	1	0	-1.780492	-2.286255	-1.607820
11	1	0	-1.982109	-2.371438	1.116127
12	1	0	0.408611	-3.227596	2.107370
13	6	0	1.098365	2.622081	-0.524026
14	6	0	0.998334	2.597815	0.911035
15	6	0	-0.319597	3.036597	1.275758
16	6	0	-1.029335	3.331833	0.062807
17	6	0	-0.164960	3.088705	-1.051387
18	1	0	1.982109	2.371438	-1.116127
19	1	0	1.780492	2.286255	1.607820
20	1	0	-0.711885	3.105575	2.294192
21	1	0	-2.074407	3.655395	-0.001825
22	1	0	-0.408611	3.227596	-2.107370
23	6	0	-0.267548	0.264636	-1.643126
24	8	0	-0.157959	-0.021141	-2.816412
25	6	0	0.267548	-0.264636	1.643126
26	8	0	0.157959	0.021141	2.816412

Table S51. The theoretical Cartesian coordinates (in Å) for the structure **2T-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.609935	1.408262	0.000000
2	23	0	0.328855	-1.160512	0.000000
3	6	0	-1.753476	-1.814257	0.719286
4	6	0	-0.797496	-2.787545	1.160826
5	6	0	-0.203452	-3.391591	0.000000
6	6	0	-0.797496	-2.787545	-1.160826
7	6	0	-1.753476	-1.814257	-0.719286
8	1	0	-2.372236	-1.186168	1.365615
9	1	0	-0.534162	-3.000866	2.200668
10	1	0	0.580601	-4.153765	0.000000
11	1	0	-0.534162	-3.000866	-2.200668
12	1	0	-2.372236	-1.186168	-1.365615
13	6	0	-1.518172	1.967886	0.717673
14	6	0	-1.518172	1.967886	-0.717673
15	6	0	-0.609126	2.987155	-1.163886
16	6	0	-0.046465	3.612571	0.000000
17	6	0	-0.609126	2.987155	1.163886
18	1	0	-2.116150	1.322182	1.364735
19	1	0	-2.116150	1.322182	-1.364735
20	1	0	-0.379856	3.234622	-2.203988
21	1	0	0.700686	4.412958	0.000000
22	1	0	-0.379856	3.234622	2.203988
23	6	0	1.423146	0.210317	1.191308
24	8	0	1.780770	-0.924096	1.556534
25	6	0	1.423146	0.210317	-1.191308
26	8	0	1.780770	-0.924096	-1.556534

Table S52. The theoretical Cartesian coordinates (in Å) for the structure **2T-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.609676	1.410990	0.000000
2	23	0	0.341267	-1.180290	0.000000
3	6	0	-1.751372	-1.792557	0.719467
4	6	0	-0.815963	-2.785646	1.160729
5	6	0	-0.234461	-3.401812	0.000000
6	6	0	-0.815963	-2.785646	-1.160729
7	6	0	-1.751372	-1.792557	-0.719467
8	1	0	-2.350116	-1.148227	1.369259
9	1	0	-0.558422	-3.005001	2.200838
10	1	0	0.531848	-4.181858	0.000000
11	1	0	-0.558422	-3.005001	-2.200838
12	1	0	-2.350116	-1.148227	-1.369259
13	6	0	-1.668426	1.788453	0.000000
14	6	0	-1.114508	2.423911	-1.163110
15	6	0	-0.210696	3.446305	-0.718262
16	6	0	-0.210696	3.446305	0.718262
17	6	0	-1.114508	2.423911	1.163110
18	1	0	-2.409330	0.987469	0.000000
19	1	0	-1.330252	2.167602	-2.203700
20	1	0	0.389174	4.095683	-1.363461
21	1	0	0.389174	4.095683	1.363461
22	1	0	-1.330252	2.167602	2.203700
23	6	0	1.423084	0.210555	1.186272
24	8	0	1.797237	-0.917655	1.553844
25	6	0	1.423084	0.210555	-1.186272
26	8	0	1.797237	-0.917655	-1.553844

Table S53. The theoretical Cartesian coordinates (in Å) for the structure **1Q-1** using the BP86 method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	23	0	-0.753389	-1.584324	0.000000
2	23	0	-0.075338	0.851003	0.000000
3	6	0	-0.009886	2.818118	1.166022
4	6	0	-0.833347	2.993670	0.000000
5	6	0	-0.009886	2.818118	-1.166022
6	6	0	1.326779	2.540623	-0.718924
7	6	0	1.326779	2.540623	0.718924
8	1	0	-0.344281	2.884281	2.204997
9	1	0	-1.906331	3.197885	0.000000
10	1	0	-0.344281	2.884281	-2.204997
11	1	0	2.196236	2.364353	-1.360316
12	1	0	2.196236	2.364353	1.360316
13	6	0	0.970605	-2.437473	1.159075
14	6	0	1.326779	-1.092213	0.725381
15	6	0	1.326779	-1.092213	-0.725381
16	6	0	0.970605	-2.437473	-1.159075
17	6	0	0.840726	-3.270671	0.000000
18	1	0	0.897354	-2.757661	2.202562
19	1	0	1.698537	-0.298260	1.387751
20	1	0	1.698537	-0.298260	-1.387751
21	1	0	0.897354	-2.757661	-2.202562
22	1	0	0.599038	-4.337128	0.000000
23	6	0	-1.785053	0.063567	0.000000
24	8	0	-2.654121	-0.880982	0.000000

Table S54. The theoretical Cartesian coordinates (in Å) for the structure **1H-1** using the BP86 method.

Standard orientation:

Center Number	atomic Number	atomic Type	Coordinates (angstroms) X	Y	Z
1	23	0	1.503191	0.400517	0.074787
2	23	0	-1.448121	0.180198	-0.178353
3	6	0	-3.513711	-0.234668	-1.074268
4	6	0	-3.653377	0.710525	-0.002172
5	6	0	-3.238068	0.064181	1.213256
6	6	0	-2.861191	-1.289661	0.894756
7	6	0	-3.030993	-1.472919	-0.514631
8	1	0	-3.742021	-0.049504	-2.128139
9	1	0	-3.985295	1.747849	-0.096910
10	1	0	-3.208623	0.523255	2.205644
11	1	0	-2.496567	-2.038688	1.603773
12	1	0	-2.814655	-2.388586	-1.073812
13	6	0	3.698411	0.127870	-0.608537
14	6	0	2.851894	-0.855985	-1.237560
15	6	0	2.308251	-1.704996	-0.210835
16	6	0	2.779169	-1.215648	1.053750
17	6	0	3.647310	-0.091871	0.802279
18	1	0	4.254325	0.919239	-1.119719
19	1	0	2.670709	-0.952732	-2.312478
20	1	0	1.632530	-2.550694	-0.364634
21	1	0	2.531833	-1.629420	2.035969
22	1	0	4.150881	0.510125	1.565228
23	6	0	-0.192297	1.632817	-0.041733
24	8	0	0.870983	2.316855	0.052657

Tables S55. The theoretical Cartesian coordinates (in Å) for the structure **1S-1** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.229112	0.914972	0.000000
2	6	0	0.821823	2.604432	1.170822
3	6	0	0.172237	3.142790	0.000000
4	6	0	1.846983	1.712806	0.719121
5	1	0	0.566986	2.830390	2.209839
6	1	0	-0.669350	3.842037	0.000000
7	1	0	2.516312	1.131385	1.359522
8	6	0	-2.147021	0.598807	0.000000
9	8	0	-3.244552	0.109936	0.000000
10	6	0	0.821823	2.604432	-1.170822
11	6	0	1.846983	1.712806	-0.719121
12	1	0	0.566986	2.830390	-2.209839
13	1	0	2.516312	1.131385	-1.359522
14	23	0	-0.504183	-0.866686	0.000000
15	6	0	0.821823	-2.336015	1.168987
16	6	0	1.542488	-1.906120	0.000000
17	6	0	-0.368098	-2.998152	0.728019
18	1	0	1.120718	-2.168514	2.207196
19	1	0	2.491178	-1.364043	0.000000
20	1	0	-1.142137	-3.432154	1.368596
21	6	0	0.821823	-2.336015	-1.168987
22	6	0	-0.368098	-2.998152	-0.728019
23	1	0	1.120718	-2.168514	-2.207196
24	1	0	-1.142137	-3.432154	-1.368596

Tables S56. The theoretical Cartesian coordinates (in Å) for the structure **1T-1** using the BP86 method.

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-1.080742	0.494910	0.138947
2	23	0	1.212348	0.460428	-0.569487
3	6	0	3.023541	-1.045681	-0.704845
4	6	0	1.976812	-1.680821	0.033958
5	6	0	1.692156	-0.880718	1.194683
6	6	0	2.587912	0.250387	1.175330
7	6	0	3.404241	0.150337	-0.007878
8	1	0	3.443698	-1.396489	-1.653462
9	1	0	1.469641	-2.609424	-0.244618
10	1	0	0.996352	-1.132797	1.998638
11	1	0	2.638753	1.041441	1.927512
12	1	0	4.176622	0.860850	-0.317182
13	6	0	-2.528385	-0.537043	-1.259659
14	6	0	-3.332566	-0.028362	-0.176898
15	6	0	-2.924101	-0.688892	1.018923
16	6	0	-1.876454	-1.616880	0.685969
17	6	0	-1.644740	-1.542936	-0.728992
18	1	0	-2.598764	-0.233487	-2.308479
19	1	0	-4.082583	0.764186	-0.253058
20	1	0	-3.311290	-0.495649	2.024367
21	1	0	-1.361168	-2.278301	1.388730
22	1	0	-0.949979	-2.157928	-1.306087
23	6	0	0.233475	1.959134	-0.147949
24	8	0	-0.889945	2.454210	0.268777

Tables S53. The theoretical Cartesian coordinates (in Å) for the structure **1S-2** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	-0.606742	-0.805760	0.000000
2	23	0	-0.125532	0.935038	0.000000
3	6	0	1.107723	2.498928	1.170784
4	6	0	0.521949	3.105574	0.000000
5	6	0	1.107723	2.498928	-1.170784
6	6	0	2.027373	1.498723	-0.719250
7	6	0	2.027373	1.498723	0.719250
8	1	0	0.879041	2.752621	2.209498
9	1	0	-0.237489	3.893243	0.000000
10	1	0	0.879041	2.752621	-2.209498
11	1	0	2.635244	0.851879	-1.358102
12	1	0	2.635244	0.851879	1.358102
13	6	0	-0.132971	-2.702540	1.173501
14	6	0	1.107723	-2.145920	0.720286
15	6	0	1.107723	-2.145920	-0.720286
16	6	0	-0.132971	-2.702540	-1.173501
17	6	0	-0.910848	-3.027357	0.000000
18	1	0	-0.438531	-2.848079	2.213203
19	1	0	1.917483	-1.783622	1.358745
20	1	0	1.917483	-1.783622	-1.358745
21	1	0	-0.438531	-2.848079	-2.213203
22	1	0	-1.921188	-3.450243	0.000000
23	6	0	-2.063940	0.827283	0.000000
24	8	0	-3.198330	0.426838	0.000000

Table S54. The theoretical Cartesian coordinates (in Å) for the structure **1S-3** using the BP86 method.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	23	0	0.575227	-0.824682	0.000000
2	23	0	0.128981	0.924735	0.000000
3	6	0	-1.575979	2.013894	1.166527
4	6	0	-2.168519	1.420930	0.000000
5	6	0	-1.575979	2.013894	-1.166527
6	6	0	-0.594175	2.957541	-0.726844
7	6	0	-0.594175	2.957541	0.726844
8	1	0	-1.821963	1.777084	2.205630
9	1	0	-2.961174	0.667941	0.000000
10	1	0	-1.821963	1.777084	-2.205630
11	1	0	0.044117	3.574955	-1.365363
12	1	0	0.044117	3.574955	1.365363
13	6	0	-0.594175	-2.419904	1.169419
14	6	0	0.655417	-2.960422	0.727906
15	6	0	0.655417	-2.960422	-0.727906
16	6	0	-0.594175	-2.419904	-1.169419
17	6	0	-1.354075	-2.064790	0.000000
18	1	0	-0.908748	-2.281837	2.207298
19	1	0	1.469522	-3.314612	1.368053
20	1	0	1.469522	-3.314612	-1.368053
21	1	0	-0.908748	-2.281837	-2.207298
22	1	0	-2.353001	-1.623291	0.000000
23	6	0	2.064909	0.790209	0.000000
24	8	0	3.200573	0.396442	0.000000

Complete Gaussian 03 reference (Reference 27)

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