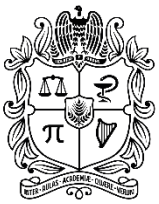

UNIVERSIDAD
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DE COLOMBIA

Study of the interaction between the oligomers from bio-oil heavy fraction and a catalyst in hydrotreatment process

Supplementary material

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Medellín, Colombia

2023

Supplementary Material: Elucidation of biomass derived pyrolytic lignin structures from demethylation reactions through DFT calculations

Oligomer proposal mechanism

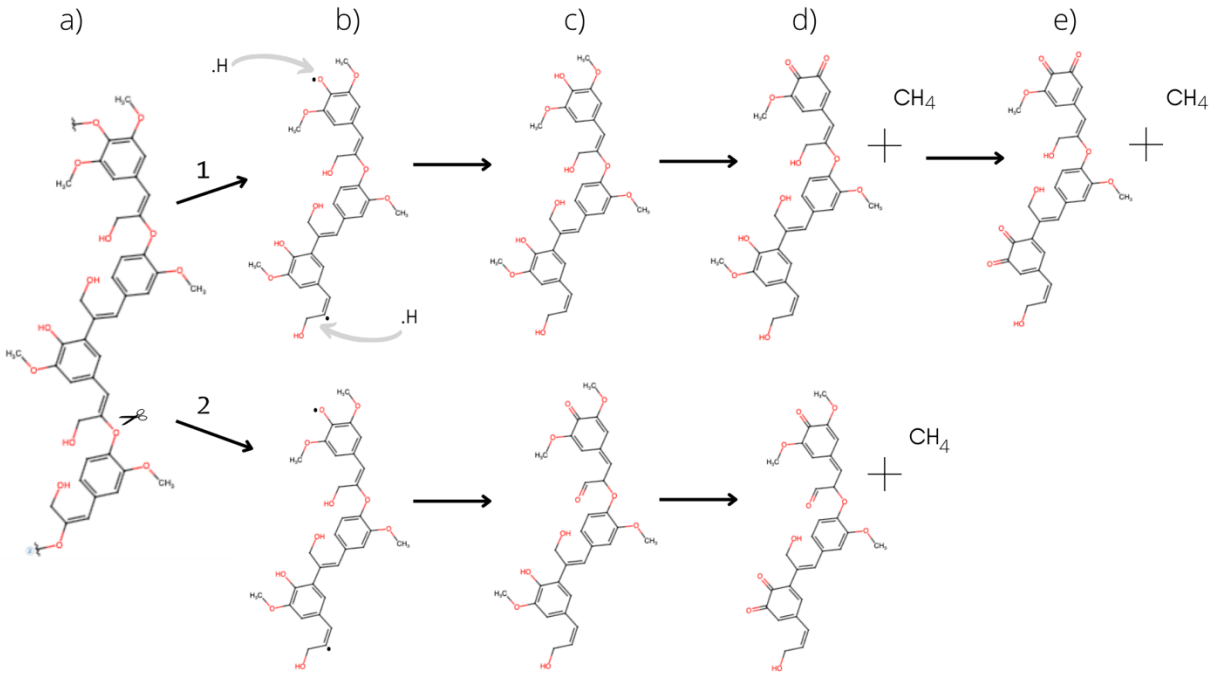


Figure S1. Trimer mechanism proposal.

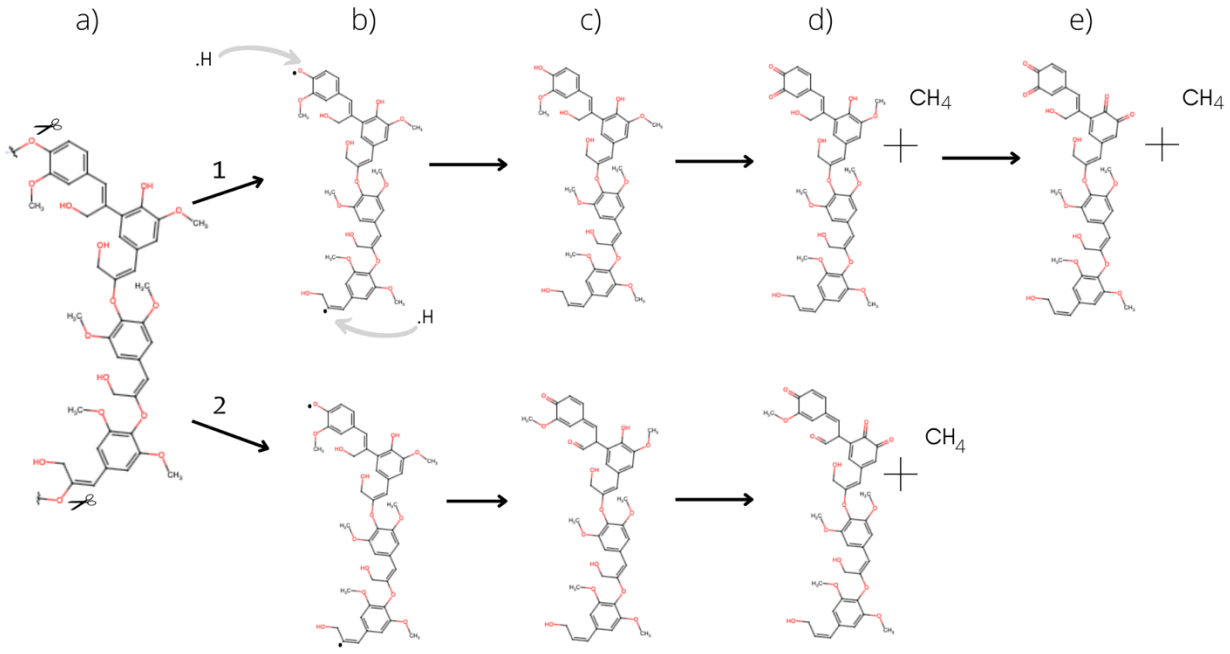
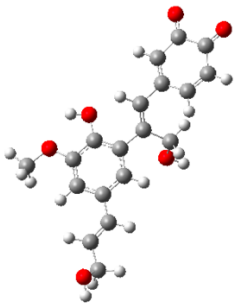


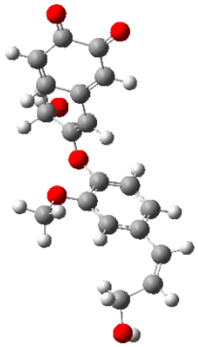
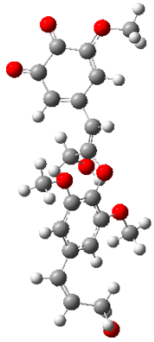
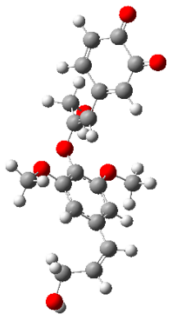
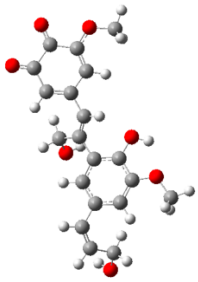
Figure S2. Tetramer mechanism proposal.

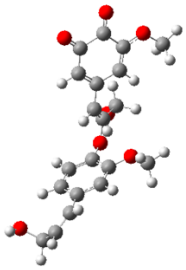
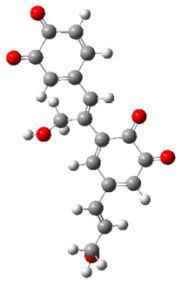
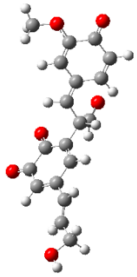
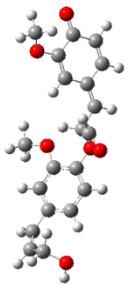
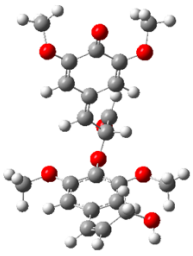
Most probable structures

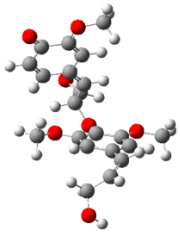
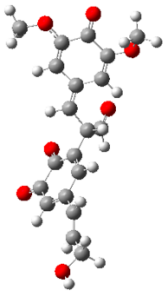
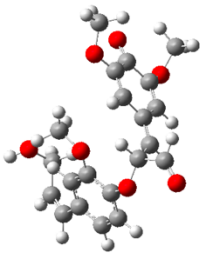
Dimers

Table S1. Most stable dimers per configuration

Label	Product structure	Molecular formula	Molecular weight	ΔG (kJ/mol)	ΔH (kJ/mol)	ΔS (kJ/mol-K)
		Pathway 1				
D1 (GB5G)		$C_{19}H_{18}O_6$	342.8410	-29.513245	86.586365	150.16376

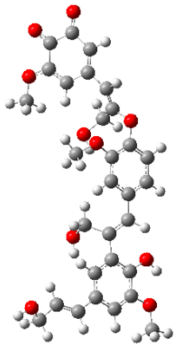
D2 (GBO4G)		$C_{19}H_{18}O_6$	342.8410	-10.777677	108.02357	153.66158
D3 (SBO4S)		$C_{21}H_{22}O_8$	342.8410	-27.142419	86.321189	146.74962
D4 (GBO4S)		$C_{20}H_{20}O_7$	372.6903	-6.206682	107.1099	146.56134
D5 (SB5G)		$C_{20}H_{20}O_7$	372.6903	-21.925551	82.353827	143.32292

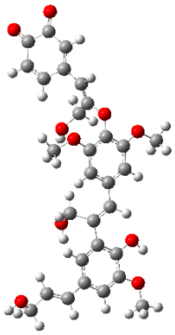
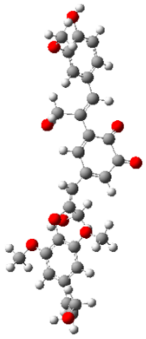
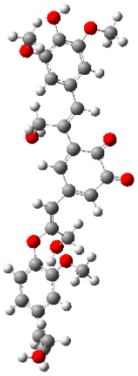
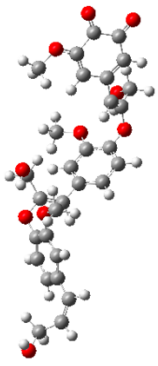
D6 (SBO4G)		$C_{18}H_{14}O_6$	326.688333	-44.625623	176.12642	285.52034
D7 (D-GB5G)		$C_{19}H_{16}O_7$	356.0896	-33.945089	193.65425	294.38206
Pathway 2						
D1* (GB5G-H_2)		$C_{19}H_{16}O_6$	340.01	-4.77	116.83	157.29
D2* (GBO4G-H_2)		$C_{20}H_{20}O_6$	356.13	-3216544.2 (G_P)	-3215538.7 (H_P)	1300.5 (S_P)
D3* (GBO4S-H_2)		$C_{21}H_{22}O_7$	386.14	-3517157.5 (G_P)	-3516074.9 (H_P)	1400.2 (S_P)

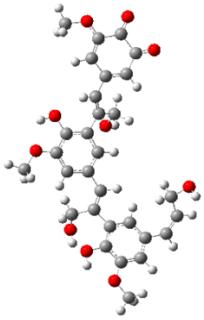
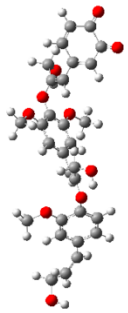
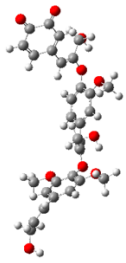
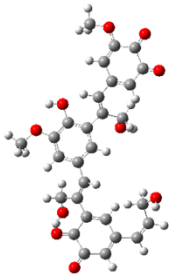
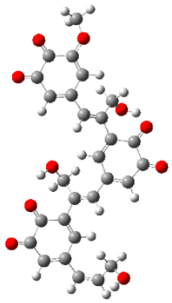
D4* (SB5G-H_2)		$C_{20}H_{18}O_7$	370.10	0.74	116.13	149.25
D5* (SBO4S-H_2)		$C_{22}H_{24}O_8$	416.15	-3817760.1 (G_P)	-3816590.0 (H_P)	1513.4 (S_P)
D6* (SBO4G-H_2)		$C_{21}H_{22}O_7$	386.14	-3517153.9 (G_P)	-3516070.8 (H_P)	1400.9 (S_P)

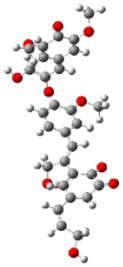
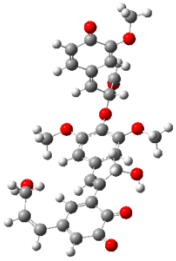
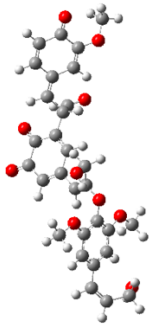
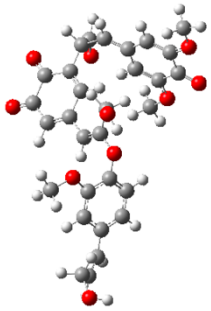
Trimers

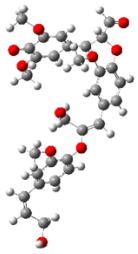
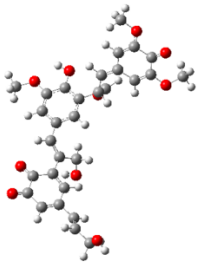
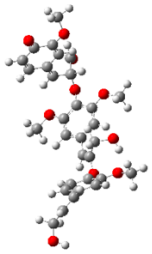
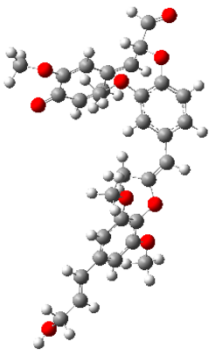
Table S2. Most stable trimers per configuration

Label	**Product structure**	**Molecular formula**	**Molecular weight**	**ΔG (kJ/mol)**	**ΔH (kJ/mol)**	**ΔS (kJ/mol)**
		Pathway 1				
T1 (SBO4GB5G)		$C_{30}H_{30}O_{10}$	550.553	-26.688207	87.211233	147.314456

T2 (GBO4SB5G)		$C_{30}H_{30}O_{10}$	550.553	-35.719928	79.634040	149.20144
T3 (GB5GBO4S)		$C_{30}H_{30}O_{10}$	550.553	-38.206276	60.887970	128.16847 2
T4 (SB5GBO4G)		$C_{30}H_{30}O_{10}$	550.553	-25.829669	115.831809	147.68683 2
T5 (SBO4GBO4G)		$C_{30}H_{30}O_{10}$	550.553	-31.737044	87.471158	154.18458 4

T6 (SB5GB5G)		$C_{30}H_{30}O_{10}$	550.553	-53.3516	5.7078	178.263504
T7 (GBO4SBO4G)		$C_{30}H_{30}O_{10}$	550.553	-45.675073	107.361946	147.979712
T8 (GBO4GBO4S)		$C_{30}H_{30}O_{10}$	550.553	-33.706169	76.391548	142.40244
T9 (D-SB5GB5G)		$C_{29}H_{26}O_{10}$	534.51	-66.37	114.67	344.41
T10 (T-SB5GB5G		$C_{28}H_{22}O_{10}$	518.47	-119.96	325.93	465.03

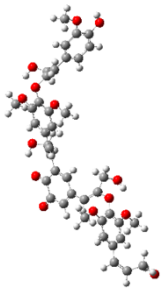
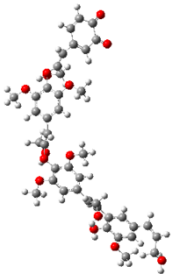
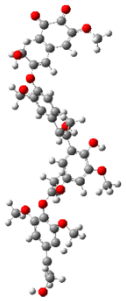
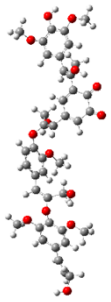
Pathway 2						
T1* (SBO4GB5G-H_2)		$C_{30}H_{28}O_{10}$	548.16	13.51	96.16	141.85
T2* (GBO4SB5G-H_2)		$C_{30}H_{28}O_{10}$	548.16	12.95	107.82	156.21
T3* (GB5GBO4S-H_2)		$C_{30}H_{28}O_{10}$	548.16	11.29	106.81	152.77
T4* (SB5GBO4G-H_2)		$C_{30}H_{28}O_{10}$	548.16	30.67	78.86	141.68

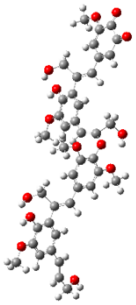
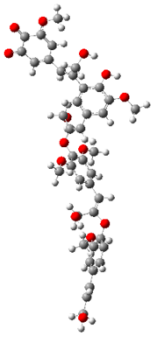
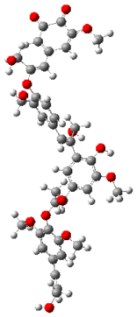
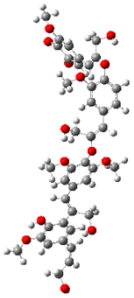
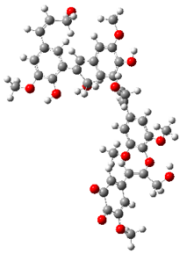
T5* (SBO4GBO4G-H_2)		$C_{31}H_{32}O_{10}$	564.20	-5125409.3 (G_P)	-5123901.5 (H_P)	1950.1 (S_P)
T6* (SB5GB5G-H_2)		$C_{30}H_{28}O_{10}$	548.16	15.33	106.75	157.9
T7* (SBO4SBO4G-H_2)		$C_{31}H_{32}O_{10}$	564.20	-5125405.3 (G_P)	-5123889 (H_P)	1961.23326 (S_P)
T8* (GBO4GBO4S-H_2)		$C_{31}H_{32}O_9$	548.20	-4927941.7 (G_P)	-4926446.4 (H_P)	1933.9 (S_P)

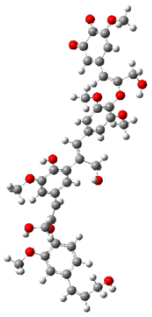
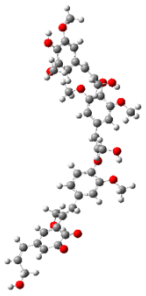
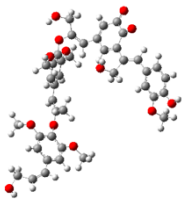
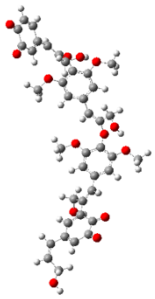
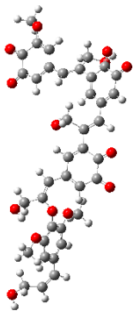
Tetramers

Table S3. Most stable tetramers per configuration

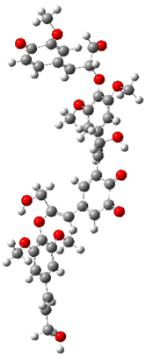
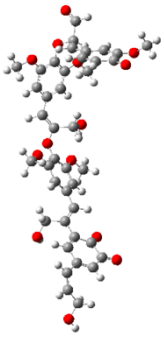
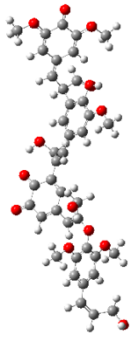
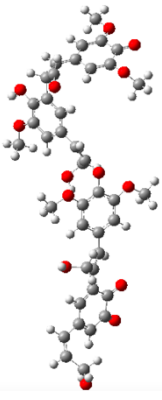
Label	Structure	Molecular formula	Molecular weight	ΔG_{rnx} (kJ/mol)	ΔH_{rxn} (kJ/mol)	ΔS_{rxn}

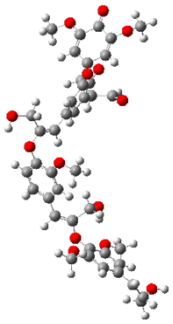
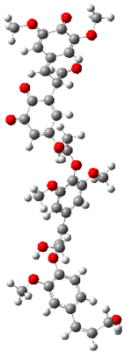
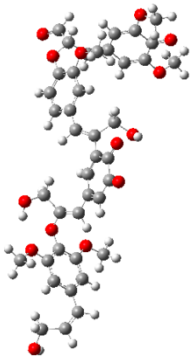
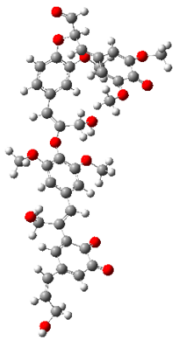
						(kJ/mol-K)
		Pathway 1				
OG1 (GBO4SB5GBO4S)		$C_{41}H_{42}O_{14}$	758.26	-10.26	101.37	144.38
OG2 (GBO4SBO4SB5G		$C_{41}H_{42}O_{14}$	758.26	-29.16	78.67	144.38
OG3 (SB5GB5GBO4S		$C_{41}H_{42}O_{14}$	758.26	-24.93	84.47	145.38
OG4 (SB5GBO4GBO4S		$C_{41}H_{42}O_{14}$	758.26	-17.80	102.63	155.77

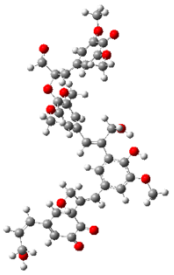
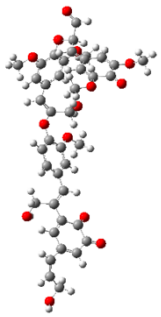
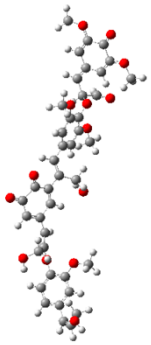
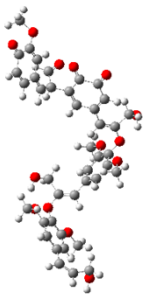
OG5 (SB5GBO4SB5G		$C_{41}H_{42}O_{14}$	758.26	-25.36	94.01	154.41
OG6 (SB5GBO4SBO4G		$C_{41}H_{42}O_{14}$	758.26	-30.14	92.69	158.86
OG7 (SBO4GB5GBO4S		$C_{41}H_{42}O_{14}$	758.26	-29.19	82.13	143.99
OG8 (SBO4GBO4SB5G		$C_{41}H_{42}O_{14}$	758.26	-15.50	96.24	144.53
OG9 (SBO4SB5GB5G		$C_{41}H_{42}O_{14}$	758.26	-23.00	21.69	147.16

OG10 (SBO4SB5GBO4G		$C_{41}H_{42}O_{14}$	758.26	-29.72	52.78	154.29
OG11 (SBO4SBO4GB5G		$C_{41}H_{42}O_{14}$	758.26	-18.78	99.71	153.25
OG12 (GB5GBO4SBO4S		$C_{41}H_{42}O_{14}$	758.26	-31.00	87.47	149.89
OG13 (D-GBO4SBO4SB5G		$C_{40}H_{38}O_{14}$	742.22	-49.37	42.10	291.70
OG14 (T-SB5GB5GBO4S		$C_{39}H_{34}O_{14}$	726.19	-52.81	76.48	482.24

Pathway 2

OG1*		$C_{41}H_{40}O_{14}$	756.24	24.85	101.43	163.35
OG2*		$C_{41}H_{40}O_{14}$	756.24	21.52	97.63	154.12
OG3*		$C_{41}H_{40}O_{14}$	756.24	17.36	100.54	152.50
OG4*		$C_{41}H_{40}O_{14}$	756.24	17.92	100.32	152.94

OG5*		$C_{41}H_{40}O_{14}$	756.24	16.39	102.32	153.54
OG6*		$C_{41}H_{40}O_{14}$	756.24	16.96	105.58	158.51
OG7*		$C_{41}H_{40}O_{14}$	756.24	24.64	101.37	162.98
OG8*		$C_{41}H_{40}O_{14}$	756.24	11.75	101.71	146.77

OG9*		$C_{41}H_{40}O_{14}$	756.24	13.12	102.87	150.03
OG10*		$C_{41}H_{40}O_{14}$	756.24	12.35	100.07	145.42
OG11*		$C_{41}H_{40}O_{14}$	756.24	19.08	99.87	153.86
OG12*		$C_{41}H_{40}O_{14}$	756.24	20.20	102.44	158.63

Oligomer Characterization

Dimers

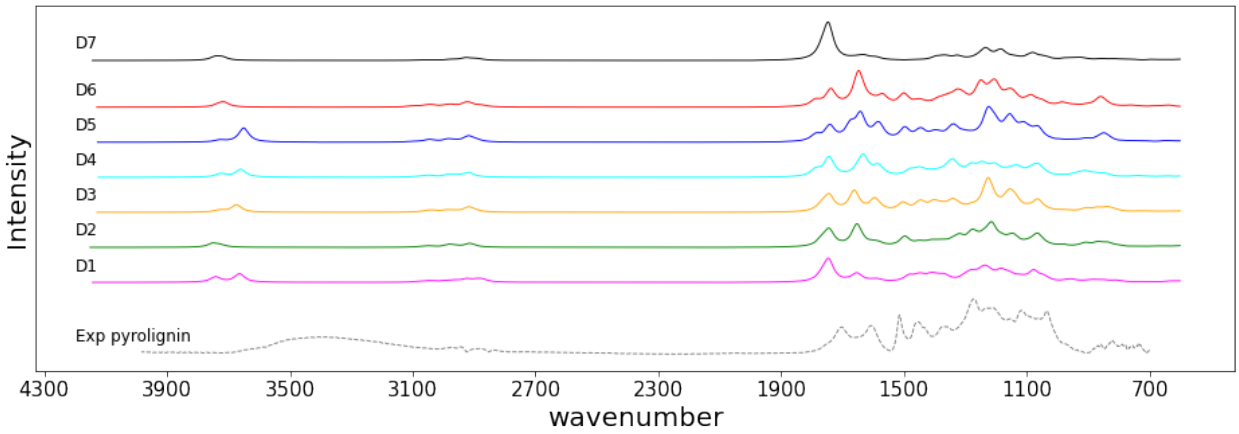


Figure S3. FTIR spectra of the proposed dimers through pathway 1.

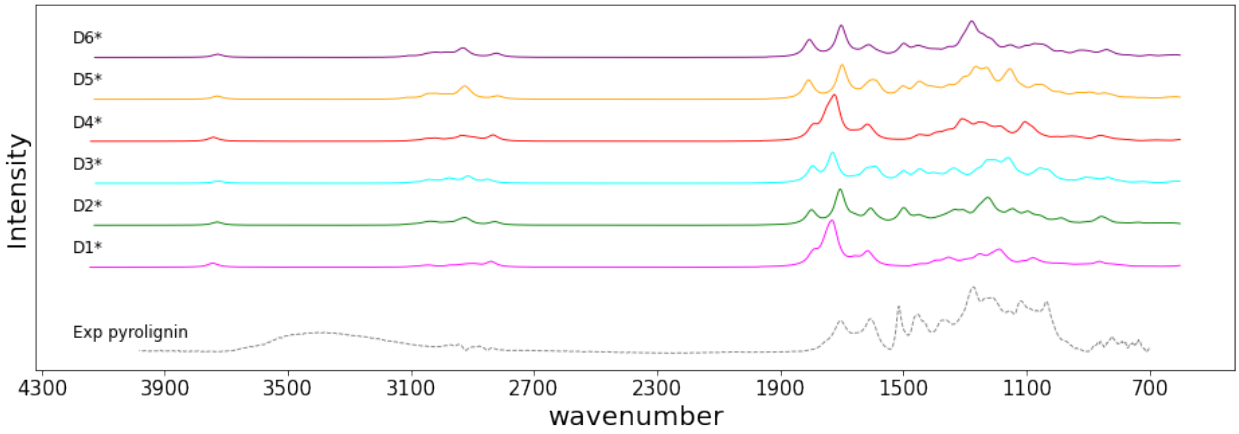


Figure S4. FTIR spectra of the proposed dimers through pathway 2.

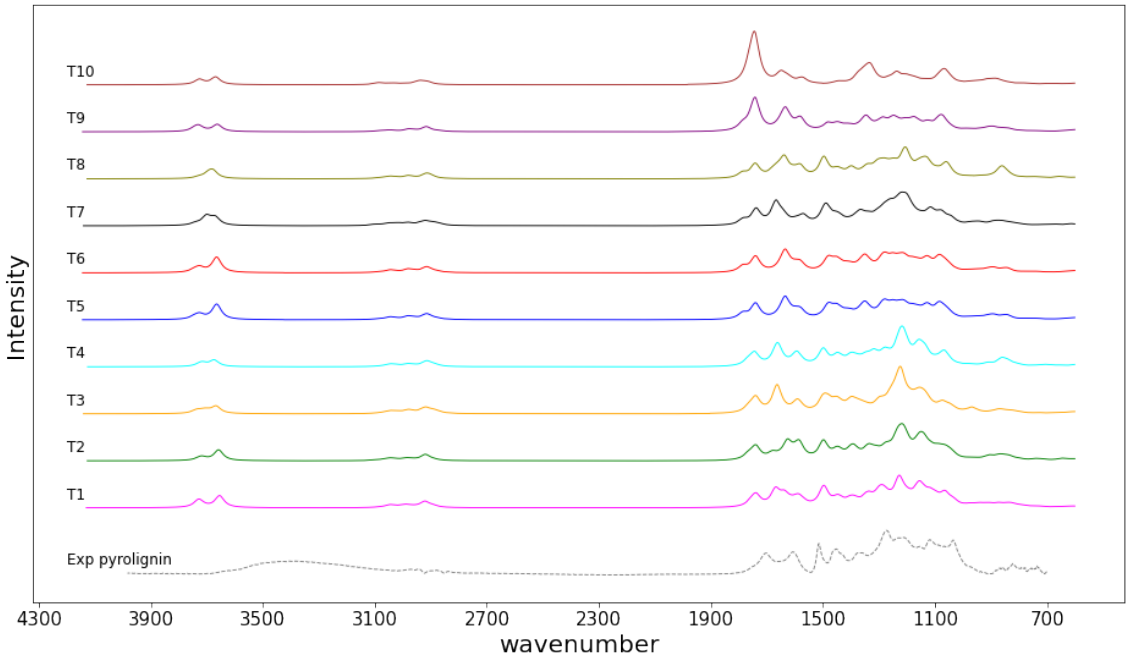


Figure S5. FTIR spectra of the proposed trimers through pathway 1.

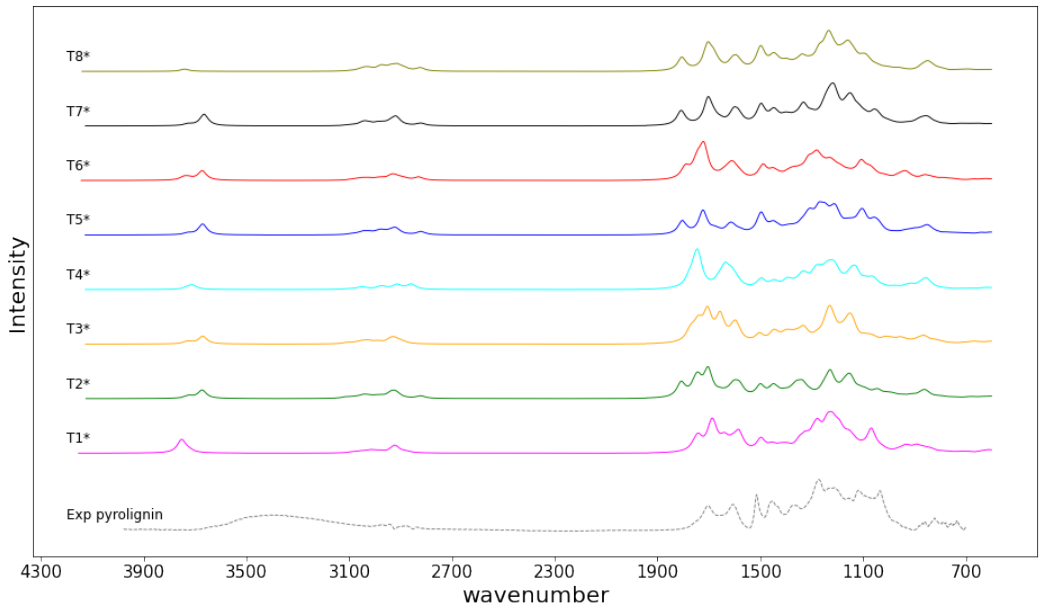


Figure S6. FTIR spectra of the proposed trimers through pathway 2.

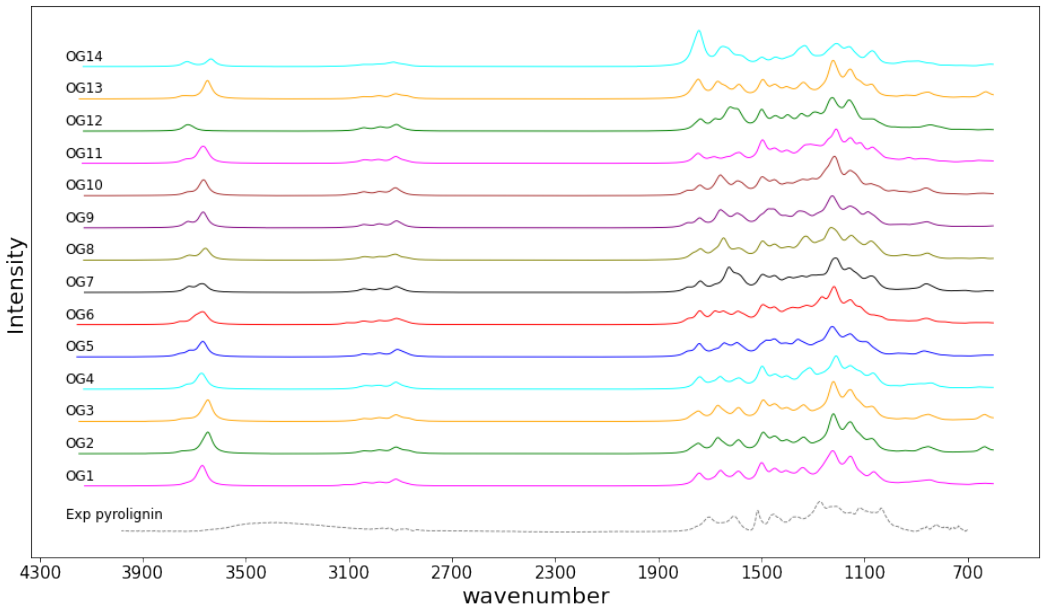


Figure S7. FTIR spectra of the proposed tetramers through pathway 1.

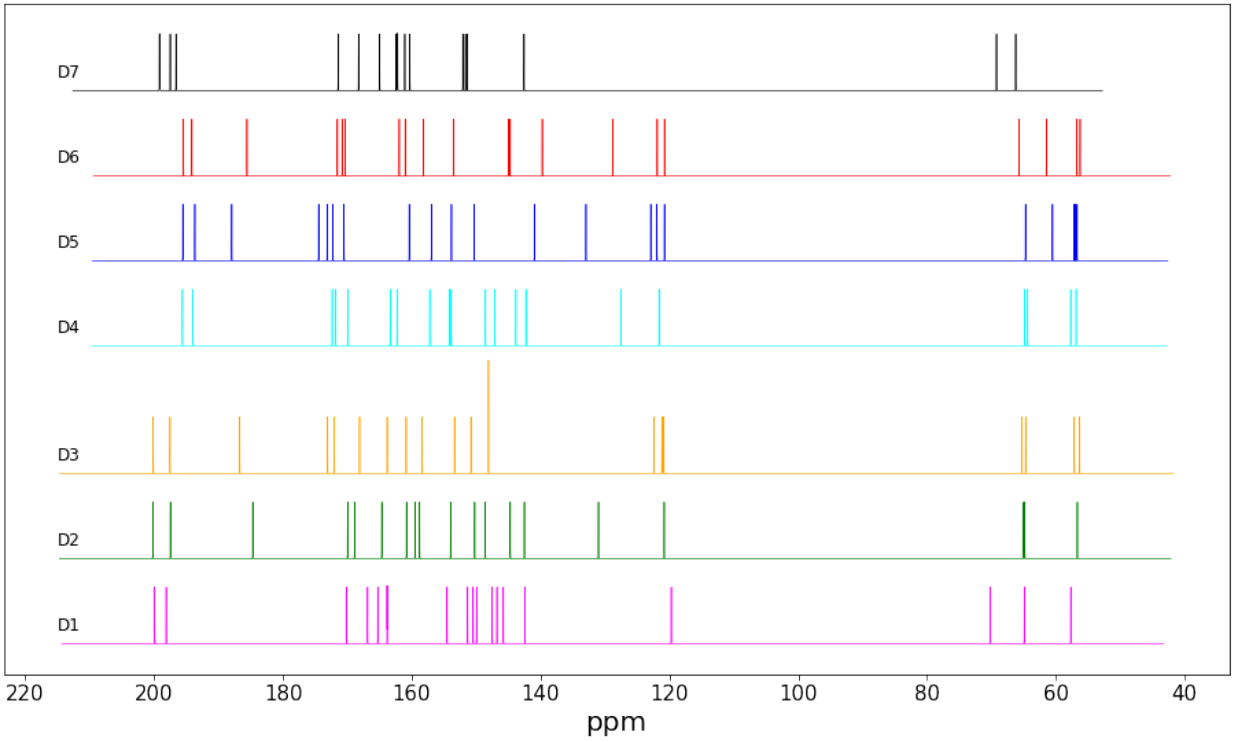


Figure S8. ^{13}C-NMR spectra of the proposed dimers through pathway 1.

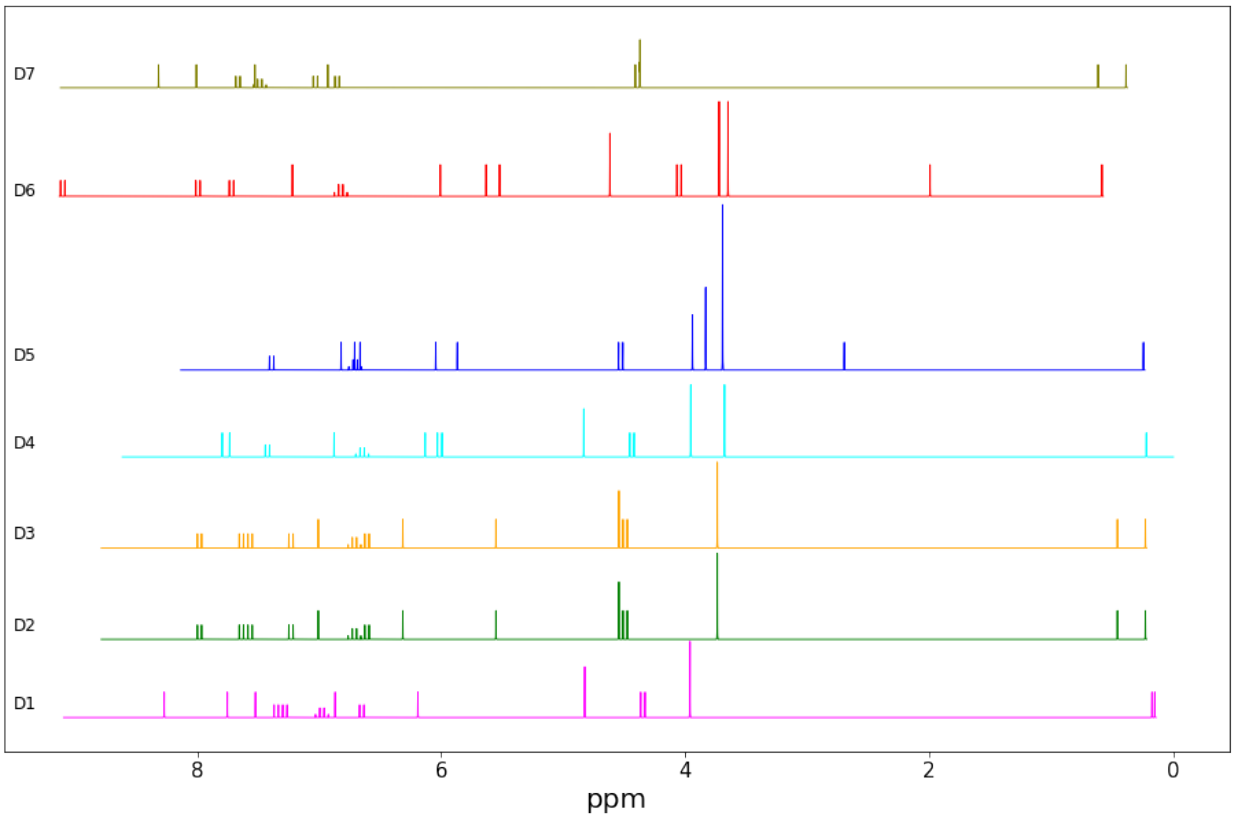


Figure S9. ^{1}H-NMR spectra of the proposed dimers through pathway 1.

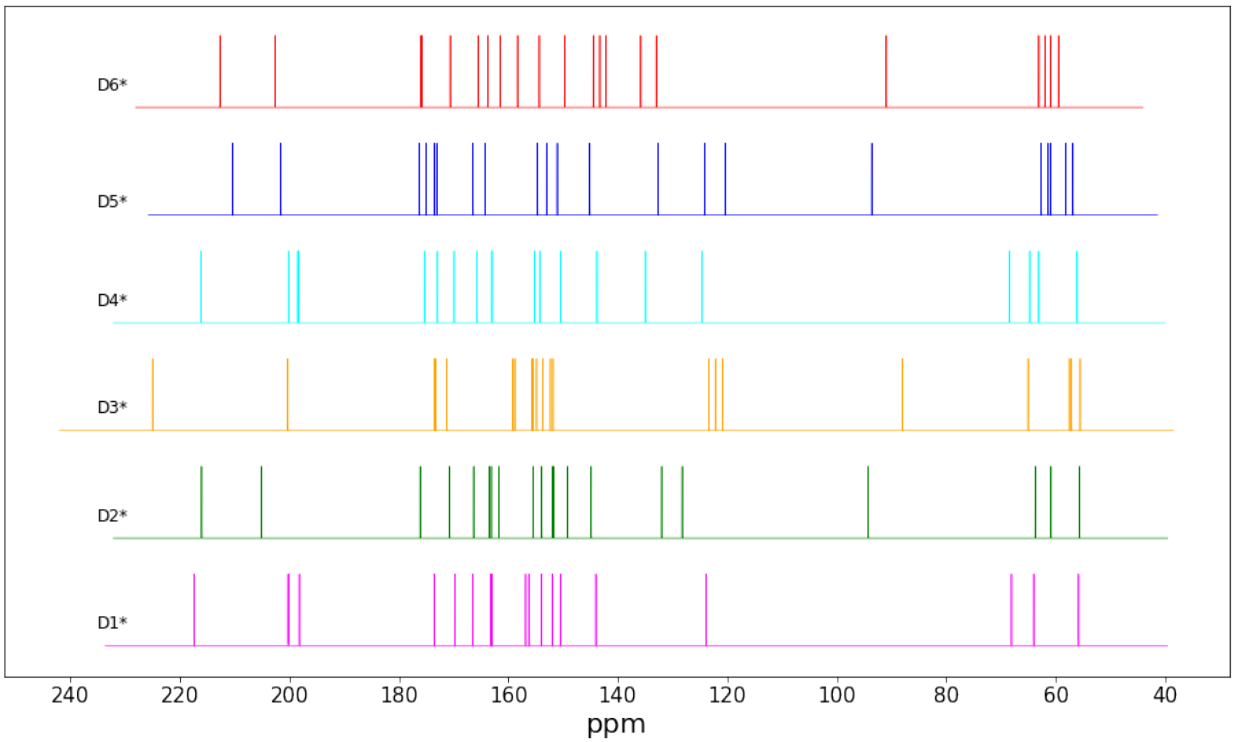


Figure S10. ^{13}C-NMR spectra of the proposed dimers through pathway 2.

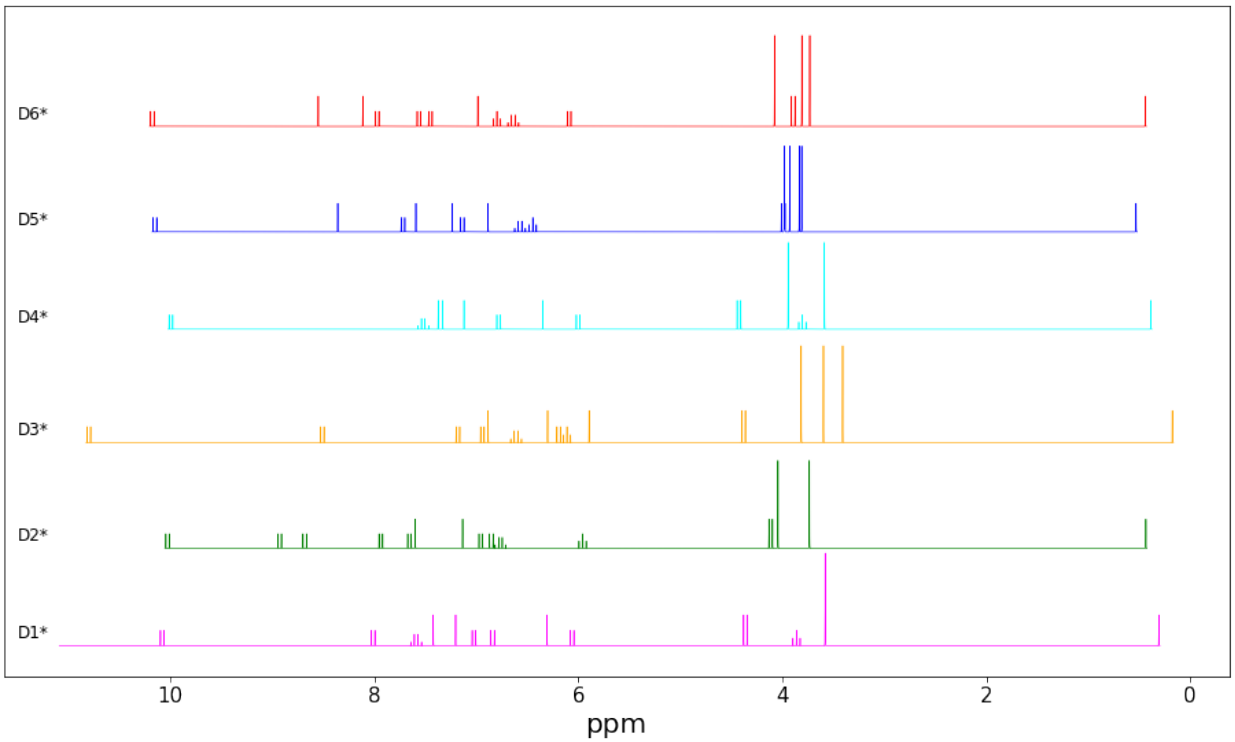


Figure S11. ^{1}H-NMR spectra of the proposed dimers through pathway 2.

Trimers

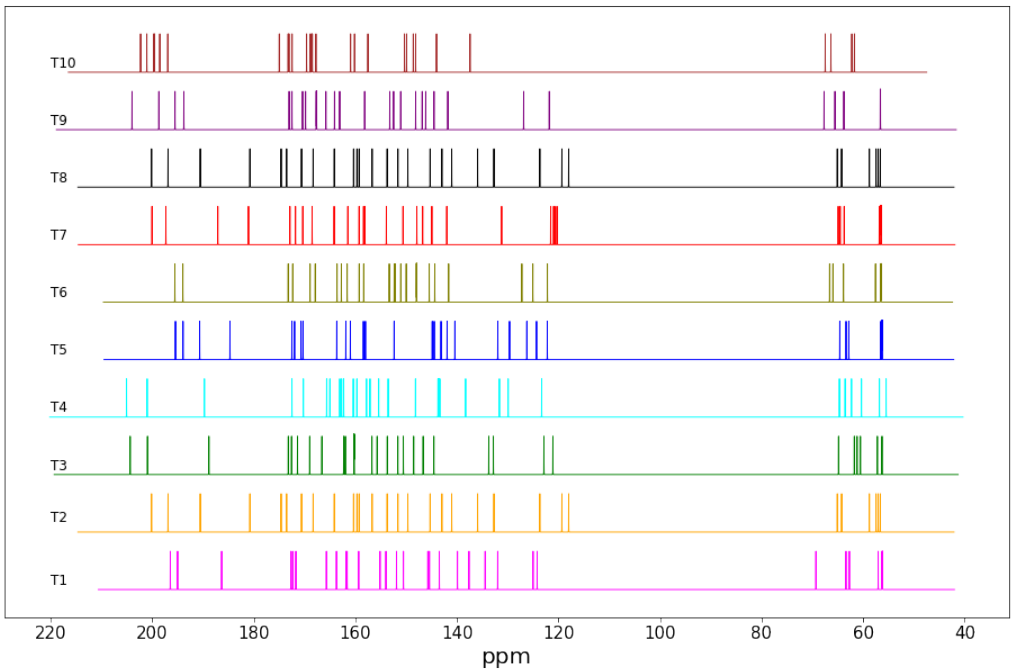


Figure S12. ^{13}C-NMR spectra of the proposed trimers through pathway 1.

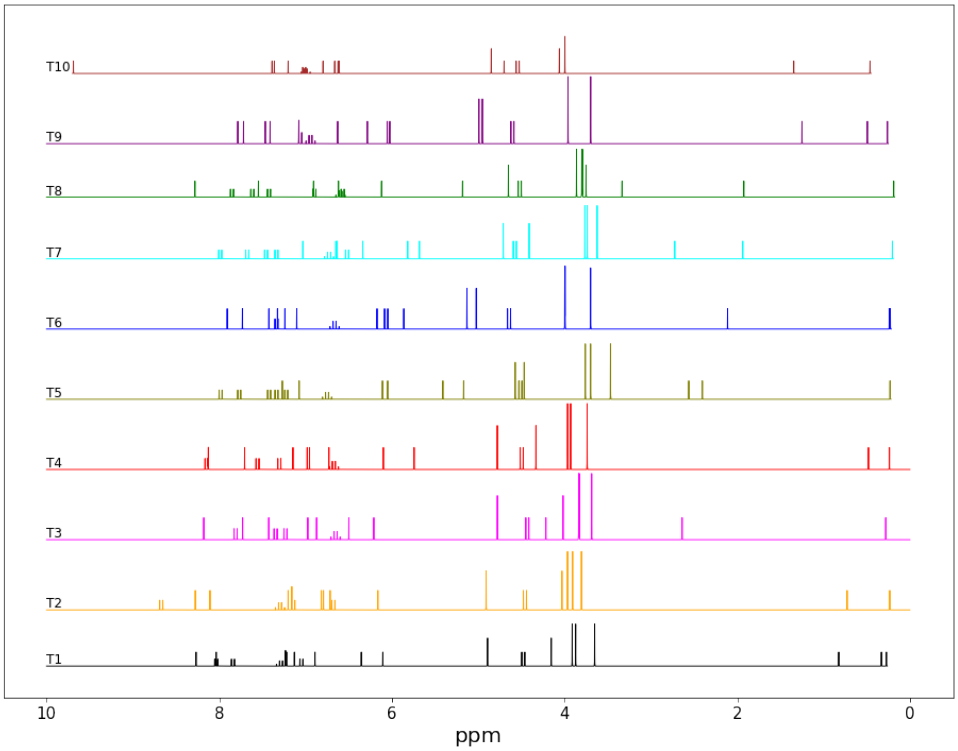


Figure S13. ^{1}H-NMR spectra of the proposed trimers through pathway 1.

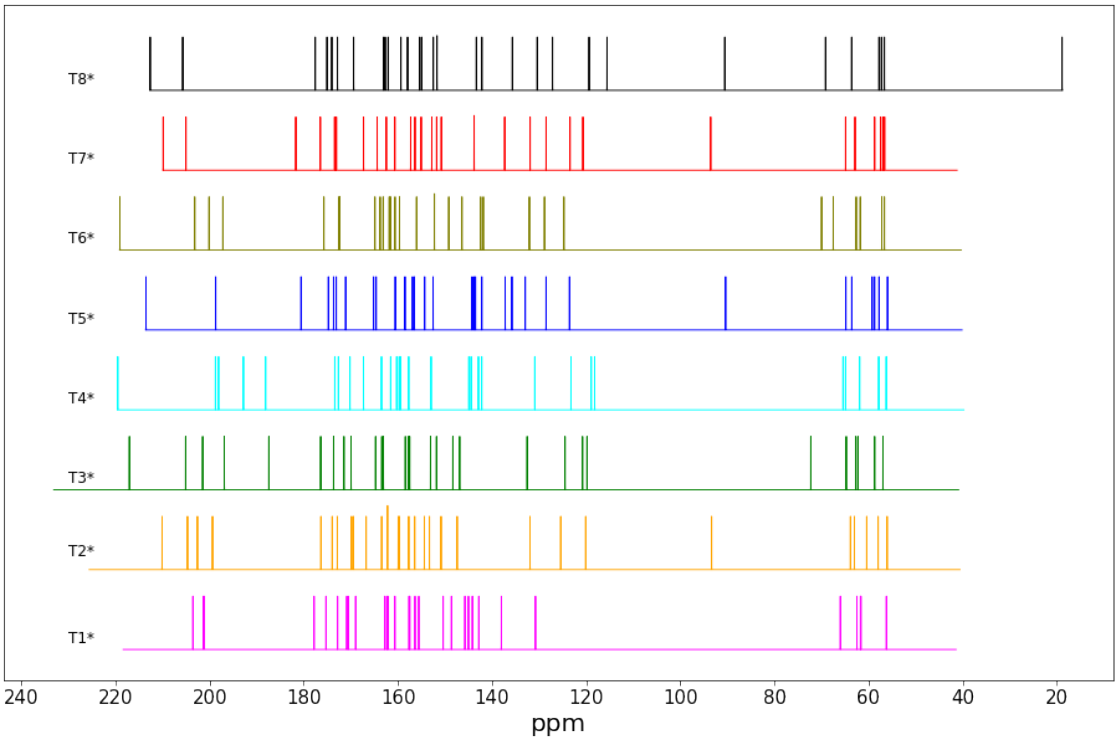


Figure S14. ^{13}C-NMR spectra of the proposed trimers through pathway 2.

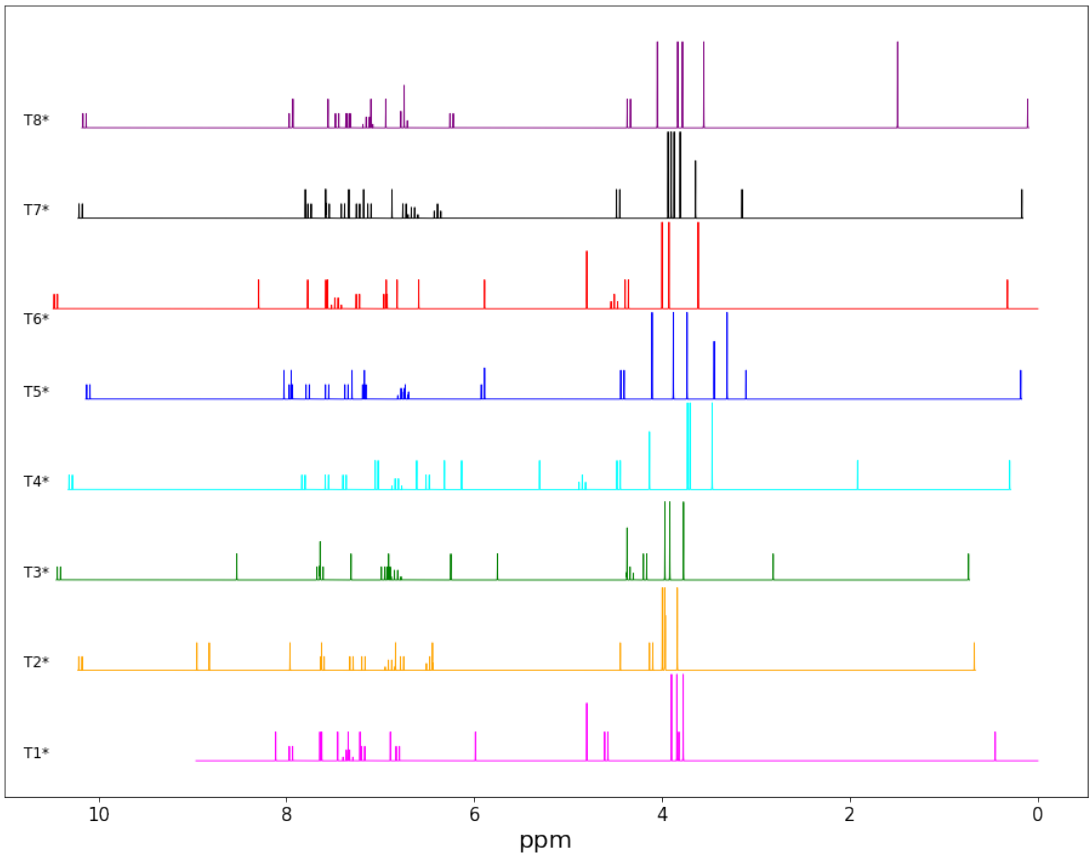


Figure S15. ^{1}H-NMR spectra of the proposed trimers through pathway 2.

Tetramers

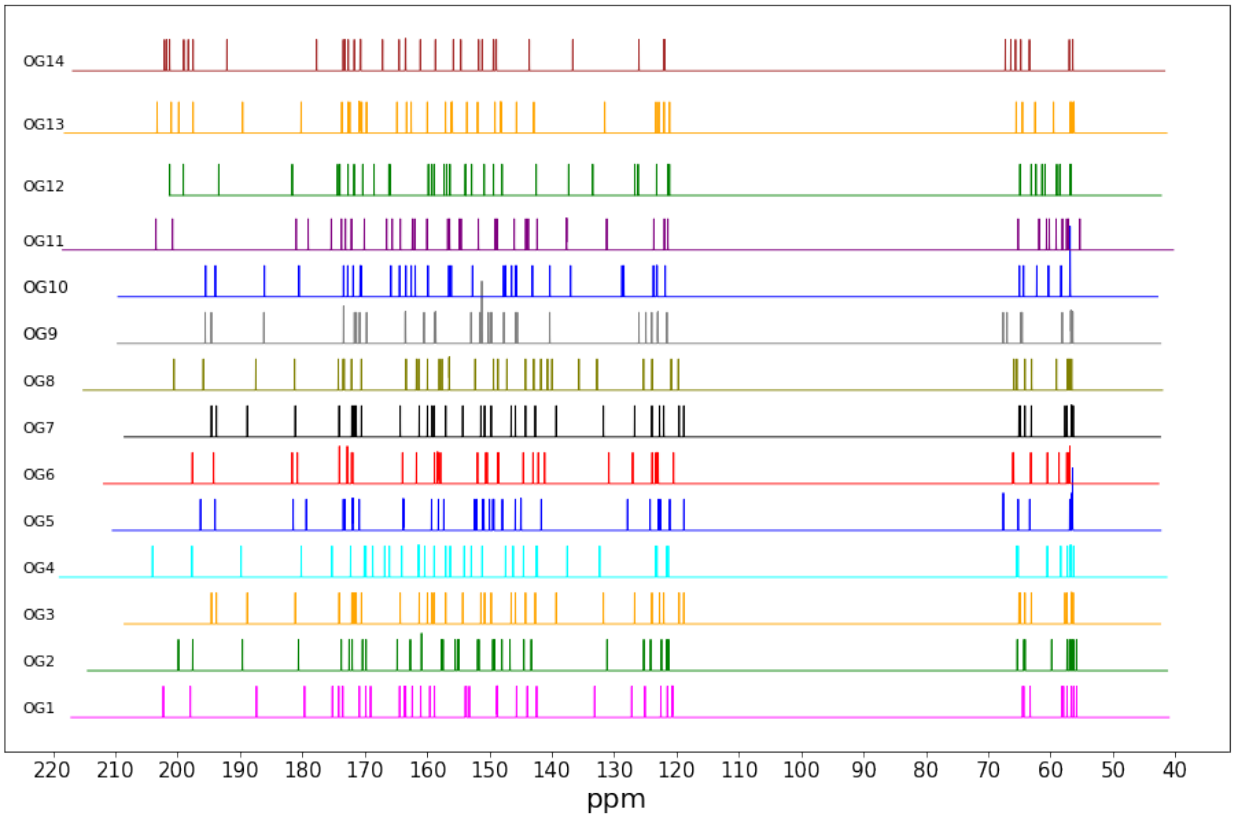


Figure S16. ^{13}C-NMR spectra of the proposed tetramers through pathway 1.

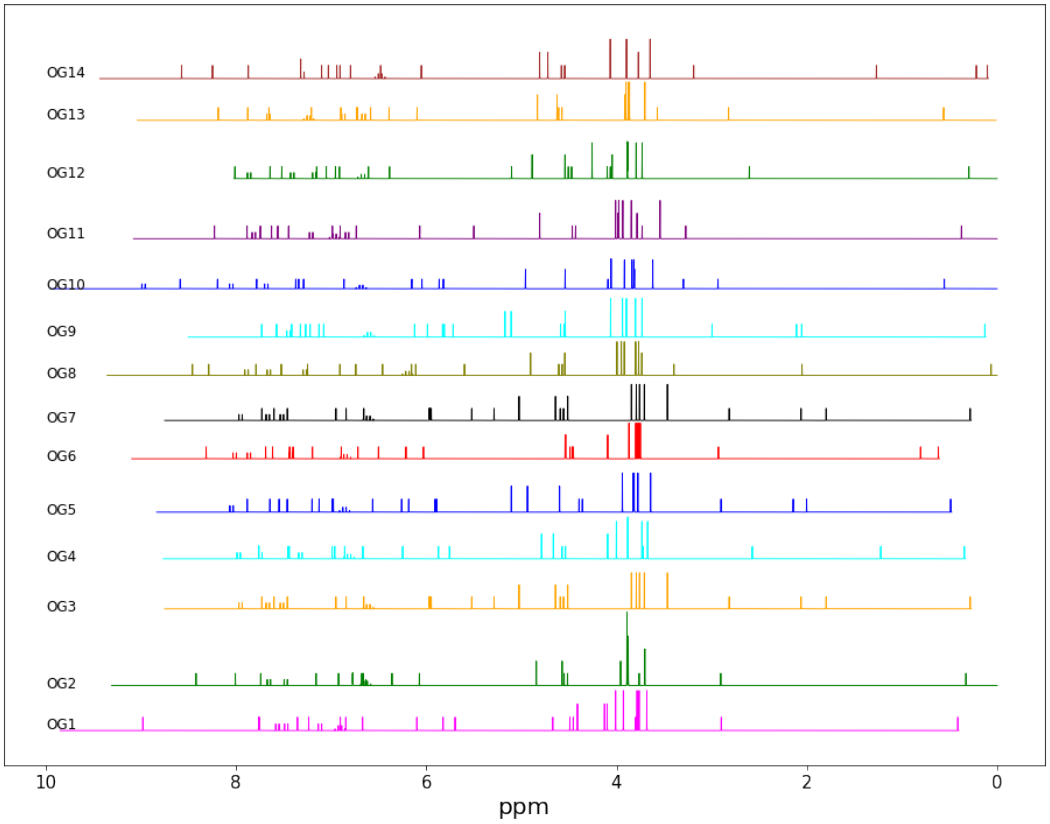


Figure S17. ^{1}H-NMR spectra of the proposed tetramers through pathway 1.

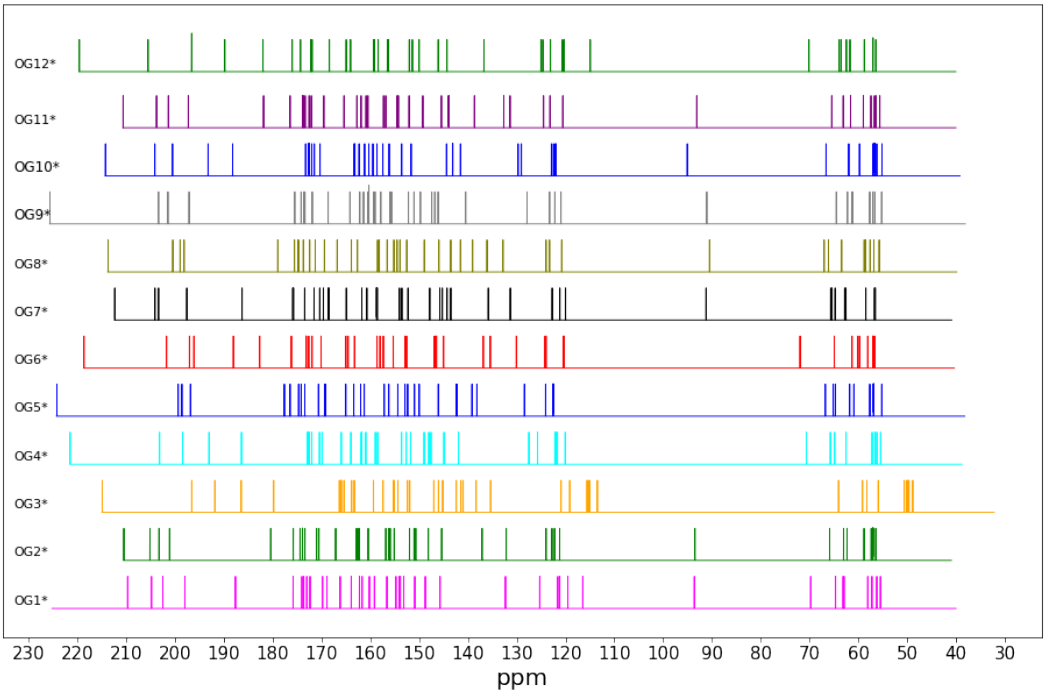


Figure S18. ^{13}C-NMR spectra of the proposed tetramers through pathway 2.

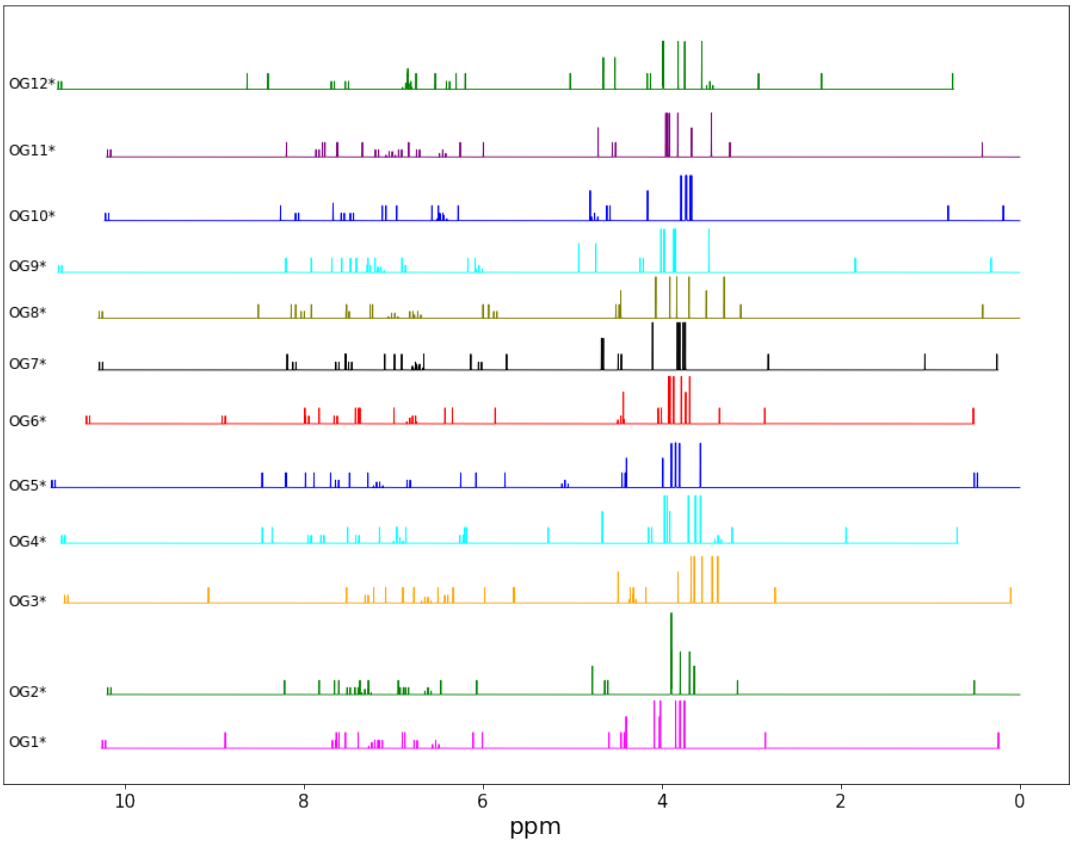


Figure S19. [1]H-NMR spectra of the proposed tetramers through pathway 2.

Thermophysical properties

Dimers – pathway 1

Table S4. Thermophysical properties of proposed lignin dimers through pathway 1.

Physical property	Symbol	Author	D1	D2	D3	D4	D5	D6	D7
Normal boiling point, K	T_b	Satou et al.	748.6	748.6	770.4	770.4	790.0	770.4	736.1
		Yuan et al.	636.4	636.4	647.6	647.6	658.3	647.6	624.6
		Stein and Brown	713.7	704.3	772.2	749.3	782.1	729.0	552.5
Critical temperature, K	T_c	Joeback and Reid	4715.9	4622.0	4734.2	4679.0	4764.6	4764.5	3754.9
		Lydersen	936.6	933.9	955.1	955.1	981.8	979.4	918.5
	V_c	Joeback and Reid	1116	1159	1325	1242	1190	1190	1115

Critical volume, m^3K/mol		Lydersen	1325	624	836	730	1293	730	828.0
Critical pressure, MPa	P_c	Lydersen	19.7	19.7	24.1	13.2	15.9	19.3	21.8
Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	22.1	21.7	21.1	21.1	21.1	28.0	25.1
	δ_h		19.9	21.7	23.4	21.8	21.3	33.4	25.7
	δ_{hb}		31.3	23.9	24.4	24.0	38.6	24.7	27.5
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	166.5	174.9	196.2	181.4	181.3	181.4	158.2
Solid heat capacity at 293.15 K, J/mol.K	$C_{p,s}$	Hurst and Harrinson	423.5	423.5	462.9	462.9	502.4	687.7	382.4
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	272.5	272.5	299.2	299.2	326.0	299.2	247.5
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-2791	-2417	-4163	-3290	-3478	-3104	-2367
Gas standard Gibbs free energy, kJ/mol	$\Delta G^{\circ}_{f,G}$	Joback	-1150	-763	-2010	-1386	-1594	-1208	-757
Gas heat capacity at constant volume, J/mol.K	C_v	DFT calculation	720.2	719.5	785.3	785.8	851.6	784.8	646.9
Dipole moment, Debye	μ	DFT calculation	9.1	6.7	7.3	9.1	7.9	10.1	8.0

Dimers – pathway 2

Table S5. Thermophysical properties of proposed dimers through pathway 2.

Physical property	**Symbol**	**Author**	**D1***	**D2***	**D3***	**D4***	**D5***	**D6***
Normal boiling point, K	T_b	Satou et al.	747.1	759.1	779.8	769.0	798.6	779.8
		Yuan et al.	636.4	647.6	658.3	647.6	668.4	658.3

		Stein and Brown	632.3	709.7	799.7	754.7	676.6	754.7
Critical temperature, K	T_c	Joeback and Reid	4925.1	4831.3	4940.6	4887.5	5058.5	4887.5
		Lydersen	928.4	899.4	917.7	917.7	918.7	917.7
Critical volume, m^3K/mol	V_c	Joeback and Reid	1095.5	1159.5	1307.5	1233.5	1233.5	1233.5
		Lydersen	631.0	657.0	869.0	763.0	737.0	763
Critical pressure, MPa	P_c	Lydersen	19.2	15.9	11.1	14.2	19.8	14.8
Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	24.8	21.5	20.9	20.9	24.9	21.5
	δ_h		25.5	21.5	23.3	21.7	27.2	23.1
	δ_{hb}		21.3	17.7	18.3	17.8	21.8	18.1
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	161.1	189.6	199.2	184.4	175.9	184.4
Solid heat capacity at 293.15 K, J/mol.K	$C_{p,s}$	Hurst and Harrinson	255	268.4	281.8	268.4	295.2	281.8
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	262.8	287.8	314.6	289.6	341.3	314.6
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-2731	-2578	-3953	-3265	-3030	-3265
Gas standard Gibbs free energy, kJ/mol	$\Delta G^{\circ}_{f,G}$	Joback	-1278	-1011	-1900	-1455	-1270	-1455
Gas heat capacity at constant volume, J/mol.K	C_v	DFT calculation	692.1	761.9	896.9	829.9	758.7	829.9
Dipole moment, Debye	μ	DFT calculation	9.9	3.8	3.3	6.4	9.7	2.9

Trimers- pathway 1

Table S6. Thermophysical properties of proposed trimers through pathway 1

Physical property	Symbol	Author	T1	T2	T3	T4	T5	T6	T7	T8	T9	T10
Normal boiling point, K	T_b	Satou et al.	908.6	908.6	908.6	908.6	908.6	908.6	908.6	908.6	900.8	893.1
		Yuan et al.	736.2	736.2	736.2	736.2	736.2	736.2	736.2	736.2	728.8	721.1
		Stein and Brown	950.0	968.0	968.6	917.6	950.0	949.9	959.3	957.4	881.2	795.3
Critical temperature, K	T_c	Joback and Reid	5084.5	5172.9	5319.7	5034.2	5084.5	5084.5	5207.4	5241.3	5172.2	4783.4
		Lydersen	1116.7	1118.4	1116.9	1120.4	1120.2	970.9	1121.2	118.4	1110.5	1064.0
Critical volume, m^3K/mol	V_c	Joback and Reid	1666	1623	1626	1621	1666	1666	1646	1678	1602	1499
		Lydersen	1099	2045	2756	2991	1068	1054	2045	2045	1042	1292
Critical pressure, MPa	P_c	Lydersen	10.7	11.3	11.3	11.9	10.6	10.6	11.3	11.3	11.9	13.7
Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	22.2	23.2	23.6	22.5	22.2	22.8	23.7	23.7	25.6	29.6
	δ_h		28.4	28.1	26.4	24.2	28.4	29.8	29.2	29.2	32.4	37.9
	δ_{hb}		30.4	38.0	45.4	31.5	30.4	30.7	45.0	45.0	34.1	38.0
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	262.3	267.6	267.3	259.9	262.3	257.7	249.2	246.3	251.6	243.2
Solid heat capacity at 293.15 K, J/mol.K	$C_{p,s}$	Hurst and Harrinson	687.7	687.7	687.7	687.7	687.7	687.7	687.7	687.7	646.6	605.4
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	438.6	438.6	438.6	438.6	438.6	438.6	438.6	438.6	413.6	388.6
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-4930	-4742	-4936	-5316	-4942	-3650	-4942	-4507	-5095	-3247
Gas standard Gibbs free	$\Delta G^{\circ}_{f,G}$	Joback	-1817	-2044	-2229	-2634	-2248	-1190	-2248	-1818	-2515	-662

energy, kJ/mol												
Gas heat capacity at constant volume,	C_v	DFT calculation	1179.4	1176.5	1179.9	1179.9	1178.8	1179.4	1179.5	1178.4	1106.9	1033.9
Dipole moment, Debye	μ	DFT calculation	16.7	10.6	3.8	2.4	10.2	11.8	16.1	11.4	4.5	8.8

Trimers – pathway 2

Table S7. Thermophysical properties of proposed trimers through pathway 2

Physical property	Symbol	**Author**	**T1***	**T2***	**T3***	**T4***	**T5***	**T6***	**T7***	**T8***
Normal boiling point, K	T_b	Satou et al.	907.6	907.6	907.67	907.6	915.3	907.6	915.3	907.6
		Yuan et al.	736.2	736.2	736.2	736.2	743.4	736.2	743.3	743.4
		Stein and Brown	894.4	894.4	881.5	886.5	973.2	973.2	973.2	1017.5
Critical temperature, K	T_c	Joeback and Reid	5473.3	5473.3	5508.4	5473.3	5367.6	5560.0	5367.0	5367.6
		Lydersen	875.6	875.6	880.8	875.6	880.6	876.6	884.2	877.5
Critical volume, m^3K/mol	V_c	Joeback and Reid	1657	1657	1689	1657	1712	1605	1712	1712
		Lydersen	1061	1061	1087	1061	1104	1859	1090	1165
Critical pressure, MPa	P_c	Lydersen	11.2	11.2	11.4	11.2	10.1	12.8	10.2	8.9
Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	29.4	27.9	26.0	26.0	22.6	26.4	22.6	22.6
	δ_h		35.5	36.4	33.7	33.7	29.7	32.0	29.7	29.7
	δ_{hb}		24.2	28.1	28.2	28.2	24.5	35.5	24.5	24.5
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	232.7	232.7	249.8	249.8	260.6	252.1	255.9	255.9
Solid heat capacity at	$C_{p,s}$	Hurst and Harrinson	402.6	402.6	402.6	402.6	416.0	402.6	416.0	416.0

293.15 K, J/mol.K										
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	428.9	428.9	428.9	428.9	453.9	428.9	453.9	442.6
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-4682	-4682	-4488	-4682	-4343	-4871	-4343	-4343
Gas standard Gibbs free energy, kJ/mol	$\Delta G^{\circ}_{f,G}$	Joback	-2132	-2132	-1906	-2132	-1686	-2340	-1686	-1686
Gas heat capacity at constant volume,	C_v	DFT calculation	1153.9	1150.0	1151.2	1150.3	1222.8	1152.4	1122.4	1202.7
Dipole moment, Debye	μ	DFT calculation	3.7	9.1	11.2	3.9	5.0	1.9	5.5	6.2

Tetramers pathway 1

Table S8. Thermophysical properties of proposed tetramers through pathway 1

Physical property	Symbol	Author	OG1	OG2	OG3	OG4	OG5	OG6	OG7	OG8	OG9	OG10	OG11	OG12	OG13	OG14
Normal boiling point, K	T_b	Satou et al.	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1068.6	1056.7	1045.5
		Yuan et al.	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	799.1	793.5
		Stein and Brown	1204.9	1204.9	1185.35	1194.5	1171.5	1193.8	1204.9	1261.4	1208.3	1204.9	1204.9	1204.9	118.2	1040.9
Critical temperature, K	T_c	Joeback and Reid	5620.2	5653.6	5523.6	5653.5	5767.5	5686.8	5686.8	5686.8	5759.8	5653.6	5686.8	5719.5	5625.4	5765.9
		Lydersen	971.8	1005.4	1028.9	1026.4	1013.6	1020.7	1020.7	1028.9	1028.9	1028.9	1020.6	1026.4	968.1	1009.8
Critical volume, m^3K/mol	V_c	Joeback and Reid	2112.0	2144.0	2188.0	2144.0	2124.0	2176.0	2176.0	2176.0	2119.0	2144.0	2176.0	2208.0	2091.0	2100.0
		Lydersen	2569.0	2765.0	1612.0	2748.0	3756.0	2779.0	2779.0	2779.0	4001.0	4001.0	2779.0	2748.0	1294.0	1394.0
Critical pressure, MPa	P_c	Lydersen	9.6	7.9	7.2	8.2	8.3	7.9	7.9	7.9	8.2	8.2	7.9	8.2	9.8	8.7

Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	25.5	23.1	22.7	22.5	24.1	22.5	22.5	22.5	24.1	23.8	23.8	23.8	26.1	28.9
	δ_h		34.3	33.4	34.2	32.8	33.1	32.8	32.8	32.8	33.1	34.9	34.9	34.9	39.2	42.6
	δ_{hb}		44.2	44.3	37.9	44.5	52	44.5	44.5	44.5	52.0	44.6	44.6	44.6	40.6	44.5
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	340.1	348.8	363.1	348.8	348.7	348.8	348.8	348.8	348.7	345.9	345.9	348.8	340.4	329.0
Solid heat capacity at 293.15 K, J/mol.K	$C_{p,s}$	Hurst and Harrinson	951.9	951.9	951.9	951.9	951.9	951.9	951.9	951.9	951.9	951.9	951.9	951.9	910.8	869.6
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	604.8	604.8	604.8	604.8	604.8	604.8	604.8	604.8	604.8	604.8	604.8	604.8	579.8	554.8
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-7470	-7276	-7610	-7276	-7271	-7082	-7082	-7082	-8204	-7276	-7082	-6888	-7250	-7200
Gas standard Gibbs free energy, kJ/mol	$\Delta G^{\circ}_{f,G}$	Joback	-3761	-3535	-3785	-3535	-3517	-3309	-3309	-3309	-4361	-3535	-3309	-3083	-3642	-3636
Gas heat capacity at constant volume,	C_v	DFT calculation	391.5	391.8	391.8	391.8	391.8	391.8	391.7	391.7	391.9	391.5	391.7	391.7	357.2	357.2
Dipole moment, Debye	μ	DFT calculation	11.4	11.7	11.7	6.8	18.9	19.2	15.7	8	11.1	13.5	5.8	10.2	8.2	8.2

Tetramers pathway 2

Table S9. Thermophysical properties of proposed tetramers through pathway 2.

Physical property	Symbol	Author	OG1*	OG2*	OG3*	OG4*	OG5*	OG6*	OG7*	OG8*	OG9*	OG10*	OG11*	OG12*
Normal boiling point, K	T_b	Satou et al.	1046.8	1047.5	1048.2	1048.9	1049.6	1050.3	1051	1051.7	1052.4	1053.1	1053.8	1054.6
		Yuan et al.	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4	804.4
		Stein and Brown	1123.6	1123.6	1089.8	1123.6	1132.9	1123.6	1123.6	1123.6	1132.9	1123.6	1123.6	1089.8
Critical temperature, K	T_c	Joeback and Reid	5990.1	5990.1	6079.6	5990.1	6078.2	5990.1	5990.1	5090.5	6078.2	5990.5	5990.1	5966.4
		Lydersen	899.4	906.3	902.9	906.3	887.5	906.3	906.3	906.3	924.8	906.3	906.3	898.7
	V_c	Joeback and Reid	2219.5	2219.5	2176.5	2219.5	2167.5	2219.5	2219.5	2228.5	2167.5	228.5	2219.5	2201.5

Critical volume, m^3K/mol		Lydersen	1550.0	1519.0	2634.0	1519.0	1475.0	1519.0	1519.0	1519.0	1548.0	1519.0	1519.0	1499.0
Critical pressure, MPa	P_c	Lydersen	7.6	7.5	7.9	7.6	8.3	7.6	7.6	7.6	7.9	7.6	7.6	7.9
Hansen solubility parameters, $MPa^{1/2}$	δ_d	Stefanis and Panayiotou	26.5	25.3	25.7	25.9	26.3	26.4	25.9	26.5	27.6	25.9	25.9	25.2
	δ_h		37.2	37.6	35.9	39.0	37.3	40.1	39.0	40.4	39.4	39.0	39.0	34.2
	δ_{hb}		33.9	34.2	41.5	34.4	41.8	41.4	34.4	34.7	41.9	34.4	24.4	34.1
Liquid heat capacity at 293.15 K, J/mol.K	$C_{p,l}$	Chueh and Swanson	340.9	343.3	343.2	334.9	343.2	340.9	340.9	340.9	340.3	340.9	343.3	324.1
Solid heat capacity at 293.15 K, J/mol.K	$C_{p,s}$	Hurst and Harrinson	550.2	550.2	550.2	936.8	936.8	936.8	936.8	936.8	936.8	936.8	936.8	936.8
Gas heat capacity at constant pressure at 300 K, kJ/mol.K	$C_{p,g}$	Harrison and Seaton	595.1	595.1	595.1	595.1	595.1	595.1	595.1	595.1	595.1	595.1	595.1	595.1
Gas standard enthalpy of formation, KJ/mol	$\Delta H^{\circ}_{f,G}$	Joback	-6634	-6634	-7008	-6634	-6822	-6634	-6634	-6819	-6822	-6819	-6634	-6080
Gas standard Gibbs free energy, kJ/mol	$\Delta G^{\circ}_{f,G}$	Joback	-2985	-2985	-3372	-2985	-3193	-2985	-2985	-3164	-3193	-3164	-2985	-2546
Gas heat capacity at constant volume,	C_v	DFT calculation	1610.4	1611.0	1609.8	1610.2	1611.3	1609.9	1611.3	1610.2	1611.2	1610.8	1610.9	1610.7
Dipole moment, Debye	μ	DFT calculation	13.1	7.6	13.3	16.1	8.1	15.2	8.1	7.4	9.2	11.0	7.4	17.9

Coordinates to the most stable structures in their ground states

D1-GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.349466
3	6	0	1.278848	0.000000	2.093682

4	6	0	2.475979	-0.068451	1.499332
5	6	0	2.578926	-0.146694	0.028188
6	6	0	1.247184	-0.085231	-0.772923
7	1	0	-0.923474	0.035241	-0.567645
8	1	0	1.217731	0.097686	3.172285
9	1	0	3.405610	-0.049943	2.055856
10	8	0	1.276822	-0.117820	-1.976679
11	8	0	3.628802	-0.239936	-0.550861
12	6	0	-1.272117	0.089825	2.087836
13	1	0	-2.005080	0.758780	1.653388
14	6	0	-1.606478	-0.585644	3.198695
15	6	0	-0.694313	-1.616922	3.830551
16	1	0	0.067932	-1.922316	3.109586
17	1	0	-0.183216	-1.185858	4.704711
18	8	0	-1.481641	-2.728631	4.217276
19	1	0	-0.898166	-3.423671	4.529872
20	6	0	-2.905956	-0.364281	3.879843
21	6	0	-2.972742	-0.422981	5.281180
22	6	0	-4.083535	-0.101622	3.184335
23	6	0	-4.145210	-0.199444	5.986297
24	1	0	-2.070605	-0.650827	5.836380
25	6	0	-5.286309	0.102277	3.890094
26	6	0	-5.324866	0.058369	5.266805
27	1	0	-6.258809	0.204791	5.791779
28	6	0	-4.117963	-0.246421	7.455813
29	1	0	-3.186230	-0.611157	7.884424
30	6	0	-5.093408	0.117480	8.287860
31	1	0	-6.030223	0.527329	7.919835
32	6	0	-4.995897	0.001709	9.774177
33	1	0	-3.986856	-0.319434	10.058253
34	1	0	-5.707721	-0.755609	10.129254
35	8	0	-4.116784	-0.058571	1.830331

36	1	0	-5.036989	0.064534	1.564083
37	8	0	-6.358382	0.322602	3.072439
38	6	0	-7.622306	0.507915	3.680446
39	1	0	-7.906755	-0.374890	4.259880
40	1	0	-7.615131	1.388746	4.328559
41	1	0	-8.330813	0.657117	2.869379
42	8	0	-5.311777	1.267280	10.339489
43	1	0	-5.416037	1.165715	11.288117

D5 – SBO4S -CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.243871	0.675714	-0.872066
2	6	0	3.128285	-0.077807	-0.279925
3	6	0	3.324160	-1.067009	0.622346
4	6	0	4.664226	-1.407591	1.087402
5	6	0	5.853478	-0.587441	0.505882
6	6	0	5.524790	0.461175	-0.515354
7	1	0	3.985882	1.437560	-1.596515
8	1	0	2.505896	-1.670107	0.996069
9	8	0	6.974245	-0.798195	0.868835
10	8	0	6.606211	1.096391	-0.969901
11	8	0	4.905670	-2.285716	1.878076
12	6	0	1.796925	0.280694	-0.774478
13	1	0	1.700538	0.471697	-1.839819
14	6	0	0.691593	0.428146	-0.040284
15	6	0	0.543177	0.381572	1.456283
16	1	0	-0.134616	-0.438263	1.732913
17	1	0	1.510373	0.193035	1.915818
18	6	0	6.402547	2.113508	-1.933400

19	1	0	7.388247	2.503734	-2.171564
20	1	0	5.937179	1.703786	-2.834871
21	1	0	5.774935	2.911208	-1.525218
22	8	0	0.077655	1.614582	1.963595
23	1	0	-0.636359	1.953150	1.408597
24	8	0	-0.448706	0.831815	-0.713630
25	6	0	-1.643321	0.251165	-0.358705
26	6	0	-1.869072	-1.112749	-0.575584
27	6	0	-2.656082	1.048249	0.174149
28	6	0	-3.110852	-1.666122	-0.275634
29	6	0	-3.903762	0.496655	0.461520
30	6	0	-4.137905	-0.857506	0.220059
31	1	0	-3.300902	-2.718045	-0.441678
32	1	0	-4.677150	1.096925	0.918548
33	8	0	-2.315874	2.342708	0.407387
34	8	0	-0.813608	-1.797126	-1.068757
35	6	0	-5.447993	-1.471812	0.508756
36	1	0	-5.410139	-2.485231	0.899555
37	6	0	-6.649467	-0.918564	0.321288
38	1	0	-7.531097	-1.490157	0.600924
39	6	0	-6.964247	0.414882	-0.297491
40	1	0	-7.171984	1.160276	0.475919
41	1	0	-6.120604	0.778303	-0.894131
42	6	0	-0.968443	-3.188109	-1.282109
43	1	0	-0.011564	-3.539404	-1.660070
44	1	0	-1.204713	-3.704093	-0.347147
45	1	0	-1.749905	-3.386318	-2.021144
46	6	0	-3.307696	3.201846	0.946930
47	1	0	-4.171434	3.261875	0.279379
48	1	0	-3.623085	2.861431	1.936839
49	1	0	-2.840311	4.179843	1.028457
50	8	0	-8.147380	0.347790	-1.075572

51	1	0	-8.010152	-0.292565	-1.778647

D7 – D-GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.349675
3	6	0	1.269206	0.000000	2.108817
4	6	0	2.471343	-0.050518	1.523945
5	6	0	2.586721	-0.093896	0.052225
6	6	0	1.259981	-0.061381	-0.759281
7	1	0	-0.919005	0.069152	-0.571887
8	1	0	1.189450	0.031828	3.190955
9	1	0	3.395707	-0.058456	2.089197
10	8	0	1.297295	-0.091019	-1.962720
11	8	0	3.641030	-0.151104	-0.522934
12	6	0	-1.226086	0.059601	2.154829
13	1	0	-1.156869	0.674805	3.044823
14	6	0	-2.378933	-0.590552	1.912800
15	6	0	-2.536551	-1.563791	0.768122
16	1	0	-1.560684	-1.974597	0.498260
17	1	0	-3.183334	-2.387056	1.090020
18	8	0	-3.121450	-0.883521	-0.341015
19	1	0	-3.182796	-1.495815	-1.079993
20	6	0	-3.566727	-0.384073	2.767217
21	6	0	-4.812032	-0.511791	2.263229
22	6	0	-3.436966	-0.061010	4.222334
23	6	0	-6.054599	-0.329783	3.028743
24	1	0	-4.925401	-0.743087	1.208170
25	6	0	-4.750417	0.194630	5.026044
26	6	0	-6.026070	0.030615	4.328146

27	1	0	-6.926453	0.236158	4.894871
28	6	0	-7.308977	-0.542340	2.291758
29	1	0	-7.284647	-0.326071	1.225791
30	6	0	-8.428791	-1.014802	2.839365
31	1	0	-8.448936	-1.313684	3.884820
32	6	0	-9.712396	-1.186590	2.094529
33	1	0	-9.553513	-1.012820	1.024042
34	1	0	-10.431508	-0.440392	2.458768
35	8	0	-2.390520	-0.012063	4.811159
36	8	0	-4.662164	0.515450	6.183336
37	8	0	-10.187899	-2.497896	2.344408
38	1	0	-11.090621	-2.570592	2.026761

D1* – GB5G-H2-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.459553
3	6	0	1.293015	0.000000	2.138781
4	6	0	2.442580	0.026454	1.452395
5	6	0	2.476027	0.056428	-0.021798
6	6	0	1.146434	0.025568	-0.708208
7	1	0	-0.964623	-0.021208	-0.491827
8	1	0	1.313382	-0.050990	3.220634
9	1	0	3.409259	0.019336	1.941439
10	8	0	1.258632	0.027616	-2.043345
11	8	0	3.512952	0.103129	-0.644081
12	6	0	-1.173090	-0.003961	2.123626
13	1	0	-2.092440	-0.044528	1.547075
14	6	0	-1.342481	-0.007539	3.618429
15	6	0	-1.190375	-1.432447	4.198372

16	1	0	-1.883036	-1.690352	5.022252
17	8	0	-0.340832	-2.186538	3.832142
18	6	0	-2.645695	0.618236	4.036233
19	6	0	-2.749870	1.782568	4.693144
20	6	0	-3.887733	-0.121607	3.694745
21	6	0	-4.032782	2.395626	5.091078
22	1	0	-1.847894	2.327785	4.959153
23	6	0	-5.248680	0.540022	4.046565
24	6	0	-5.207151	1.820138	4.761462
25	1	0	-6.160276	2.283665	4.987937
26	6	0	-3.948398	3.661880	5.834549
27	1	0	-3.082217	4.286519	5.625368
28	6	0	-4.832340	4.057092	6.750192
29	1	0	-5.685841	3.432436	7.002006
30	6	0	-4.725926	5.336770	7.516721
31	1	0	-3.924589	5.959542	7.102931
32	1	0	-4.477601	5.104765	8.560933
33	8	0	-3.856051	-1.206222	3.172274
34	8	0	-6.268536	-0.012791	3.725045
35	8	0	-5.983360	5.984281	7.436552
36	1	0	-5.998735	6.720506	8.052210
37	6	0	0.061466	-0.016181	-2.791592
38	1	0	-0.505234	-0.925296	-2.567130
39	1	0	-0.559517	0.861544	-2.585681
40	1	0	0.358604	-0.017570	-3.837123
41	1	0	-0.532823	0.562342	4.088167

D4* – SB5G-H2-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000

2	6	0	0.000000	0.000000	1.459291
3	6	0	1.294818	0.000000	2.139071
4	6	0	2.443610	-0.019000	1.450548
5	6	0	2.476726	-0.043199	-0.023878
6	6	0	1.145937	-0.021998	-0.709623
7	1	0	-0.965197	0.009496	-0.490863
8	1	0	1.314642	0.016346	3.220817
9	1	0	3.410807	-0.019288	1.939461
10	8	0	3.512951	-0.082948	-0.647057
11	8	0	1.257314	-0.032916	-2.043507
12	6	0	-1.175165	-0.023063	2.121306
13	1	0	-2.098459	-0.043933	1.544181
14	6	0	-1.374705	-0.056907	3.605158
15	6	0	-2.123409	1.205460	4.026931
16	1	0	-3.226234	1.107651	4.008514
17	8	0	-1.565867	2.218490	4.334018
18	8	0	-2.224366	-1.139469	3.989320
19	6	0	-2.114330	-2.308806	3.290073
20	6	0	-3.261221	-2.817918	2.669193
21	6	0	-0.907322	-3.004523	3.192115
22	6	0	-3.201735	-4.028395	1.982734
23	6	0	-0.844837	-4.205737	2.486272
24	6	0	-1.997173	-4.732470	1.902190
25	1	0	-4.082353	-4.438751	1.507002
26	1	0	0.097649	-4.718046	2.358016
27	8	0	0.154664	-2.421047	3.804151
28	8	0	-4.371055	-2.049745	2.778598
29	6	0	-1.972100	-6.012279	1.168796
30	1	0	-2.615322	-6.058225	0.293664
31	6	0	-1.265448	-7.102805	1.479600
32	6	0	-0.395460	-7.324850	2.685082
33	1	0	0.660150	-7.190623	2.430923

34	1	0	-0.641186	-6.613531	3.480860
35	6	0	1.419429	-3.042997	3.658929
36	1	0	1.413443	-4.048155	4.090200
37	1	0	1.713790	-3.087394	2.606383
38	1	0	2.124607	-2.420314	4.205344
39	6	0	-5.568441	-2.547438	2.215499
40	1	0	-6.332697	-1.805565	2.434578
41	1	0	-5.477069	-2.667775	1.131659
42	1	0	-5.847898	-3.503553	2.667577
43	8	0	-0.499296	-8.661677	3.147219
44	1	0	-1.413745	-8.824008	3.393333
45	6	0	0.059566	-0.011752	-2.792732
46	1	0	-0.551070	-0.893763	-2.575177
47	1	0	-0.516567	0.894122	-2.579615
48	1	0	-1.336004	-7.968618	0.825670
49	1	0	-0.437563	-0.100600	4.156275
50	1	0	0.357347	-0.019977	-3.837975

D5* - SBO4S-H2-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.458385
3	6	0	1.281649	0.000000	2.143167
4	6	0	2.445808	0.000155	1.470433
5	6	0	2.476875	-0.046533	-0.017746
6	6	0	1.149811	-0.008763	-0.700909
7	1	0	-0.962761	0.004440	-0.495109
8	1	0	1.325448	-0.037238	3.224429
9	8	0	1.272817	-0.013902	-2.036592
10	8	0	3.510368	-0.129416	-0.641847

11	6	0	-1.180909	0.010572	2.110610
12	1	0	-2.094802	-0.020132	1.525218
13	6	0	-1.362691	0.000461	3.602089
14	6	0	-1.318699	-1.439625	4.161699
15	1	0	-1.999925	-1.640089	5.011579
16	8	0	-0.559703	-2.265994	3.756313
17	6	0	-2.621512	0.711708	4.020531
18	6	0	-2.646755	1.871344	4.693493
19	6	0	-3.911203	0.066311	3.664314
20	6	0	-3.885102	2.568451	5.093764
21	1	0	-1.709823	2.346791	4.972072
22	6	0	-5.223733	0.819098	4.017309
23	6	0	-5.095627	2.082892	4.750397
24	1	0	-6.014682	2.609856	4.978935
25	6	0	-3.715231	3.814804	5.856141
26	1	0	-2.804803	4.378178	5.661443
27	6	0	-4.574212	4.259358	6.772898
28	1	0	-5.472195	3.694472	7.010760
29	6	0	-4.379998	5.516104	7.559770
30	1	0	-3.532393	6.084741	7.160465
31	1	0	-4.156572	5.250791	8.601639
32	8	0	-3.954577	-1.012204	3.130335
33	8	0	-6.278541	0.345271	3.682275
34	8	0	-5.585859	6.255849	7.482779
35	1	0	-5.554190	6.976815	8.115593
36	6	0	0.078947	-0.030097	-2.791398
37	1	0	-0.511385	-0.923861	-2.566400
38	1	0	-0.521025	0.863758	-2.592488
39	1	0	0.381743	-0.043260	-3.835238
40	1	0	-0.518963	0.504027	4.087134
41	8	0	3.608416	-0.074105	2.154393
42	6	0	4.692437	0.764466	1.744430

43	1	0	5.300931	0.911641	2.635298
44	1	0	5.274625	0.291978	0.956948
45	1	0	4.321182	1.730846	1.394168

T6- SB5GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.366383	-0.267211	-0.316958
2	6	0	5.121065	0.516163	-0.332286
3	6	0	5.121239	1.869006	-0.342409
4	6	0	6.371622	2.621661	-0.299957
5	6	0	7.697658	1.806759	-0.244221
6	6	0	7.581006	0.312258	-0.268749
7	1	0	6.259207	-1.344682	-0.321257
8	1	0	4.207819	2.444516	-0.426340
9	8	0	6.438139	3.825622	-0.309127
10	8	0	8.766479	-0.299663	-0.232363
11	8	0	8.753712	2.366789	-0.182880
12	6	0	3.893745	-0.286523	-0.380540
13	1	0	3.956397	-1.172847	-1.002846
14	6	0	2.748969	-0.072834	0.289663
15	6	0	2.554268	1.078961	1.247924
16	1	0	3.529842	1.449244	1.571660
17	1	0	2.037797	1.904081	0.735331
18	8	0	1.790893	0.623669	2.351524
19	1	0	1.726566	1.335841	2.991606
20	6	0	1.585128	-0.976520	0.105200
21	6	0	0.292792	-0.437659	0.063774
22	6	0	1.722299	-2.357924	-0.030004
23	6	0	-0.841973	-1.219985	-0.114464
24	1	0	0.171683	0.631683	0.191717

25	6	0	0.584181	-3.158312	-0.226503
26	6	0	-0.680222	-2.605417	-0.281207
27	1	0	-1.538322	-3.228947	-0.485661
28	8	0	2.935684	-2.964120	0.027255
29	1	0	2.783572	-3.916587	-0.021310
30	8	0	0.869817	-4.489736	-0.352433
31	6	0	-2.156503	-0.558919	-0.149003
32	1	0	-2.139080	0.444641	-0.567751
33	6	0	-3.342362	-1.027060	0.275252
34	6	0	-3.525815	-2.390929	0.921428
35	1	0	-3.702864	-3.151039	0.150520
36	1	0	-2.607210	-2.650880	1.450328
37	6	0	-0.219534	-5.384607	-0.474067
38	1	0	-0.890664	-5.297139	0.385407
39	1	0	-0.775851	-5.196949	-1.396698
40	1	0	0.209073	-6.383413	-0.504945
41	6	0	8.763705	-1.715262	-0.248439
42	1	0	9.806623	-2.018345	-0.214853
43	1	0	8.232822	-2.110064	0.622876
44	1	0	8.296623	-2.089949	-1.164105
45	8	0	-4.558067	-2.422196	1.882364
46	1	0	-5.393058	-2.464330	1.407529
47	6	0	-4.532214	-0.144924	0.144497
48	6	0	-5.751033	-0.629251	-0.314597
49	6	0	-4.453127	1.215797	0.470916
50	6	0	-6.855248	0.223794	-0.460125
51	6	0	-5.528388	2.081965	0.308741
52	1	0	-3.534933	1.579030	0.914911
53	6	0	-6.751228	1.567290	-0.152477
54	1	0	-7.599870	2.230287	-0.264298
55	8	0	-5.894459	-1.953398	-0.617806
56	1	0	-6.785793	-2.081200	-0.967736

57	8	0	-7.974942	-0.406042	-0.925116
58	6	0	-5.435878	3.514406	0.641325
59	1	0	-6.337605	3.958593	1.055614
60	6	0	-4.372160	4.306496	0.475241
61	1	0	-4.441901	5.343227	0.795386
62	6	0	-3.056731	3.953583	-0.160139
63	1	0	-2.309960	3.709122	0.601102
64	1	0	-3.163664	3.079736	-0.812906
65	6	0	-9.136100	0.379717	-1.118311
66	1	0	-9.466470	0.821465	-0.174164
67	1	0	-8.951384	1.169980	-1.851251
68	1	0	-9.901600	-0.295274	-1.493069
69	8	0	-2.518100	5.057047	-0.869960
70	1	0	-3.144316	5.309306	-1.553509

T9-D-SB5GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.054861	-0.290901	-0.262742
2	6	0	4.809711	0.489968	-0.322318
3	6	0	4.808024	1.841569	-0.377452
4	6	0	6.056944	2.597688	-0.342100
5	6	0	7.382766	1.787256	-0.240382
6	6	0	7.268154	0.292136	-0.217121
7	1	0	5.949423	-1.368106	-0.232954
8	1	0	3.895337	2.412564	-0.493831
9	8	0	6.121033	3.800678	-0.389834
10	8	0	8.453329	-0.315463	-0.143772
11	8	0	8.436960	2.350662	-0.182157
12	6	0	3.582305	-0.313966	-0.362773
13	1	0	3.652967	-1.219293	-0.956097

14	6	0	2.428257	-0.076148	0.282573
15	6	0	2.222573	1.107830	1.198682
16	1	0	3.194480	1.476079	1.535170
17	1	0	1.730310	1.923345	0.648204
18	8	0	1.424385	0.699030	2.296568
19	1	0	1.401492	1.413167	2.937264
20	6	0	1.263718	-0.981258	0.108330
21	6	0	-0.025519	-0.439870	0.032912
22	6	0	1.396137	-2.366557	0.012942
23	6	0	-1.160730	-1.223605	-0.138838
24	1	0	-0.143389	0.633169	0.128948
25	6	0	0.257483	-3.169002	-0.180210
26	6	0	-1.003882	-2.614378	-0.266160
27	1	0	-1.858699	-3.241927	-0.469916
28	8	0	2.604435	-2.974485	0.103237
29	1	0	2.451713	-3.927831	0.072416
30	8	0	0.541607	-4.501918	-0.269948
31	6	0	-2.466614	-0.553141	-0.203448
32	1	0	-2.425583	0.456824	-0.604626
33	6	0	-3.674041	-1.015847	0.167864
34	6	0	-3.916984	-2.387367	0.773800
35	1	0	-4.044185	-3.133993	-0.017746
36	1	0	-3.040548	-2.661608	1.365114
37	6	0	-0.546143	-5.398831	-0.400815
38	1	0	-1.234390	-5.298121	0.443403
39	1	0	-1.082083	-5.225183	-1.337971
40	1	0	-0.117220	-6.397765	-0.407097
41	6	0	8.454219	-1.731102	-0.112730
42	1	0	9.497276	-2.029721	-0.054292
43	1	0	7.912015	-2.097936	0.763769
44	1	0	8.001244	-2.137114	-1.022059
45	8	0	-5.023126	-2.407908	1.651374

46	1	0	-5.805336	-2.628834	1.138702
47	6	0	-4.840123	-0.118163	0.014126
48	6	0	-6.101345	-0.652245	-0.565399
49	6	0	-4.811639	1.178061	0.379338
50	6	0	-7.291628	0.334426	-0.759868
51	6	0	-5.914063	2.131036	0.171091
52	1	0	-3.934017	1.546434	0.898086
53	6	0	-7.097148	1.722056	-0.333372
54	1	0	-7.931756	2.400240	-0.471103
55	8	0	-6.249840	-1.810187	-0.866762
56	8	0	-8.312403	-0.077197	-1.248424
57	6	0	-5.726759	3.538426	0.564735
58	1	0	-6.618362	4.037821	0.931854
59	6	0	-4.596820	4.246998	0.480644
60	1	0	-4.612493	5.279166	0.821895
61	6	0	-3.269857	3.828464	-0.097665
62	1	0	-2.595372	3.497152	0.697912
63	1	0	-3.389200	2.999206	-0.803322
64	8	0	-2.615441	4.921909	-0.711193
65	1	0	-3.152260	5.230097	-1.446301

T10-T-SB5GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.088930	-1.894907	-0.483436
2	6	0	4.139069	-0.544232	-0.454815
3	6	0	5.413759	0.182881	-0.431334
4	6	0	6.612846	-0.427334	-0.407772
5	6	0	6.671353	-1.919732	-0.474256
6	6	0	5.314757	-2.687381	-0.423940
7	1	0	3.148758	-2.433990	-0.501274

8	1	0	5.398267	1.264466	-0.482726
9	8	0	7.736244	0.304642	-0.482205
10	8	0	7.697156	-2.529596	-0.609304
11	8	0	5.343472	-3.888518	-0.336479
12	6	0	8.906803	-0.135007	0.218387
13	1	0	9.479099	-0.834800	-0.386019
14	1	0	9.483930	0.767536	0.408358
15	1	0	8.637171	-0.603395	1.166871
16	6	0	2.876080	0.213445	-0.483267
17	1	0	2.107449	-0.221123	-1.115984
18	6	0	2.575266	1.324629	0.208682
19	6	0	3.520640	2.007041	1.186526
20	1	0	4.207123	1.262816	1.592258
21	1	0	4.108976	2.769154	0.665722
22	8	0	2.835956	2.571514	2.284102
23	1	0	2.639877	3.487778	2.070438
24	6	0	1.209712	1.887670	0.075763
25	6	0	1.034891	3.358984	-0.036098
26	6	0	0.116240	1.101798	0.029766
27	6	0	-0.391623	3.890792	-0.357818
28	6	0	-1.256130	1.603198	-0.164249
29	1	0	0.246007	0.029279	0.106849
30	6	0	-1.485463	2.915809	-0.389150
31	1	0	-2.479214	3.307091	-0.577801
32	8	0	1.932460	4.152077	0.099421
33	8	0	-0.548094	5.069320	-0.546174
34	6	0	-2.407025	0.688155	-0.166560
35	1	0	-3.255796	1.063883	-0.733630
36	6	0	-2.556781	-0.498777	0.449060
37	6	0	-1.491875	-1.187308	1.294941
38	1	0	-0.954984	-0.438972	1.879951
39	1	0	-1.979276	-1.862741	2.004758

40	8	0	-0.525591	-1.878137	0.530751
41	1	0	-0.982806	-2.603197	0.086577
42	6	0	-3.865524	-1.182970	0.338309
43	6	0	-3.886133	-2.646031	0.068866
44	6	0	-5.044191	-0.548533	0.493069
45	6	0	-5.266957	-3.362661	0.046291
46	6	0	-6.363780	-1.194535	0.374018
47	1	0	-5.036514	0.500446	0.769348
48	6	0	-6.462936	-2.529263	0.205640
49	1	0	-7.420979	-3.034840	0.159767
50	8	0	-2.887883	-3.292211	-0.129124
51	8	0	-5.299866	-4.554642	-0.111148
52	6	0	-7.577593	-0.369655	0.504086
53	1	0	-8.418977	-0.857490	0.986758
54	6	0	-7.740146	0.879042	0.057265
55	1	0	-8.695781	1.366725	0.232532
56	6	0	-6.778858	1.716796	-0.745176
57	1	0	-6.255677	2.423099	-0.093045
58	1	0	-6.026279	1.092972	-1.240490
59	8	0	-7.467186	2.515866	-1.685364
60	1	0	-7.915698	1.941317	-2.311813

T2*-GBO4SB5G-H2-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.471042	3.057539	-1.870855
2	6	0	6.938128	2.192685	-0.791819
3	6	0	7.109079	2.792795	0.521924
4	6	0	6.852054	4.095190	0.750721
5	6	0	6.328464	4.973831	-0.338480
6	6	0	6.200718	4.354198	-1.668022

7	1	0	6.352842	2.610662	-2.852539
8	1	0	7.443323	2.191423	1.359393
9	1	0	5.846352	5.005593	-2.457831
10	8	0	6.961628	4.576484	2.006104
11	8	0	6.000091	6.126210	-0.130097
12	6	0	7.207276	0.897962	-1.062833
13	1	0	7.068947	0.516479	-2.071792
14	6	0	7.760230	-0.116180	-0.102486
15	6	0	9.278821	0.052279	-0.057983
16	1	0	9.594185	1.058499	0.286483
17	6	0	7.542020	5.871358	2.195498
18	1	0	6.789356	6.650980	2.107505
19	1	0	7.965509	5.856125	3.198351
20	1	0	8.336885	6.047853	1.467350
21	8	0	10.064459	-0.789073	-0.368482
22	8	0	7.465082	-1.430128	-0.510592
23	6	0	6.126910	-1.727980	-0.520212
24	6	0	5.472417	-1.916325	-1.742153
25	6	0	5.427977	-1.920707	0.675662
26	6	0	4.131583	-2.297023	-1.764778
27	6	0	4.088090	-2.300686	0.654324
28	6	0	3.433600	-2.472221	-0.567660
29	1	0	3.612467	-2.441712	-2.702519
30	1	0	3.551876	-2.498772	1.572711
31	8	0	6.143340	-1.722055	1.810803
32	8	0	6.223040	-1.693933	-2.850852
33	6	0	2.018339	-2.877066	-0.608996
34	1	0	1.720229	-3.599214	-1.363196
35	6	0	1.069618	-2.455415	0.228181
36	6	0	1.201122	-1.408166	1.296649
37	1	0	2.067578	-0.784004	1.089285
38	1	0	0.313464	-0.764162	1.290092

39	6	0	5.487444	-1.963524	3.044944
40	1	0	6.219999	-1.745946	3.818497
41	1	0	4.616154	-1.313462	3.164732
42	1	0	5.173230	-3.007849	3.120595
43	6	0	5.648636	-2.007966	-4.103391
44	1	0	4.786946	-1.367868	-4.317401
45	1	0	6.426363	-1.828879	-4.842303
46	1	0	5.342939	-3.057445	-4.142725
47	8	0	1.389962	-1.978616	2.583605
48	1	0	0.620622	-2.535899	2.756705
49	8	0	-0.146746	-3.129447	0.191936
50	6	0	-1.303621	-2.409375	0.309654
51	6	0	-1.985080	-2.380468	1.529151
52	6	0	-1.831230	-1.744451	-0.800519
53	6	0	-3.204632	-1.716800	1.632416
54	6	0	-3.054920	-1.081969	-0.698786
55	6	0	-3.751787	-1.086947	0.511226
56	1	0	-3.745227	-1.683257	2.568654
57	1	0	-3.453821	-0.531933	-1.539457
58	8	0	-1.364751	-3.009679	2.562531
59	8	0	-1.075557	-1.799135	-1.918977
60	6	0	-5.040259	-0.387945	0.675275
61	1	0	-5.134877	0.165101	1.602213
62	6	0	-6.083207	-0.384418	-0.175558
63	6	0	-6.104509	-1.206568	-1.451477
64	1	0	-5.951999	-0.571522	-2.330092
65	1	0	-5.291152	-1.934119	-1.427559
66	6	0	-2.039827	-3.046357	3.811031
67	1	0	-1.397426	-3.613259	4.480683
68	1	0	-2.184712	-2.037989	4.207503
69	1	0	-3.004054	-3.551308	3.714426
70	6	0	-1.564408	-1.146867	-3.074426

71	1	0	-1.667419	-0.070877	-2.905954
72	1	0	-0.824886	-1.322515	-3.851757
73	1	0	-2.526655	-1.565538	-3.385110
74	8	0	-7.345150	-1.855421	-1.667828
75	1	0	-7.521031	-2.435042	-0.921286
76	6	0	-7.271502	0.453375	0.096267
77	6	0	-8.089696	0.872216	-0.892212
78	6	0	-7.660506	0.822245	1.492775
79	6	0	-9.260938	1.744938	-0.711196
80	1	0	-7.901102	0.547585	-1.909204
81	6	0	-8.765897	1.904747	1.673196
82	6	0	-9.563681	2.260295	0.500722
83	1	0	-10.349219	2.990763	0.648234
84	8	0	-7.212181	0.301461	2.479799
85	8	0	-8.926867	2.391511	2.763911
86	6	0	-10.030018	2.044374	-1.924041
87	1	0	-9.465610	2.042460	-2.851948
88	6	0	-11.348644	2.254407	-1.995203
89	1	0	-11.792651	2.443274	-2.968532
90	6	0	-12.346156	2.218496	-0.880538
91	1	0	-12.029966	1.511790	-0.103432
92	1	0	-12.420747	3.213407	-0.418636
93	8	0	-13.586228	1.844553	-1.453558
94	1	0	-14.259834	1.844700	-0.770107
95	1	0	7.393830	0.058983	0.917604

T3*-GB5GBO4S-CH2-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.639313	0.837934	1.326525
2	6	0	7.836896	0.399401	0.186667

3	6	0	8.361253	-0.675856	-0.643361
4	6	0	9.571880	-1.216775	-0.406024
5	6	0	10.436853	-0.754271	0.719475
6	6	0	9.853278	0.314817	1.582021
7	1	0	8.224513	1.622005	1.947462
8	1	0	7.732143	-1.082440	-1.419256
9	8	0	10.137692	-2.214719	-1.100291
10	8	0	10.676202	0.655344	2.586553
11	8	0	11.528198	-1.222329	0.925835
12	6	0	6.659860	1.025104	-0.036471
13	1	0	6.364742	1.785133	0.681899
14	6	0	5.660945	0.841669	-1.155511
15	6	0	6.252862	0.357249	-2.470410
16	1	0	7.182989	0.885131	-2.762168
17	6	0	9.404197	-2.729204	-2.194174
18	1	0	10.020623	-3.511841	-2.628851
19	1	0	8.448981	-3.148897	-1.862820
20	1	0	9.213948	-1.949276	-2.938428
21	6	0	10.229503	1.661663	3.469772
22	1	0	11.020226	1.792089	4.204263
23	1	0	10.062388	2.603269	2.936842
24	1	0	9.305270	1.358496	3.972303
25	8	0	5.760411	-0.471948	-3.181619
26	6	0	4.418061	0.090238	-0.728862
27	6	0	4.482657	-1.262305	-0.422916
28	6	0	3.195663	0.754327	-0.622143
29	6	0	3.330825	-1.942410	0.004568
30	6	0	2.038785	0.086937	-0.219417
31	1	0	3.159239	1.819293	-0.816913
32	6	0	2.125996	-1.275983	0.116775
33	1	0	1.237957	-1.798638	0.450468
34	8	0	5.656207	-1.925742	-0.513999

35	1	0	5.506933	-2.841808	-0.247387
36	8	0	3.546147	-3.260965	0.284064
37	6	0	0.725925	0.732184	-0.095009
38	1	0	0.076160	0.277002	0.650841
39	6	0	0.226747	1.778448	-0.779060
40	6	0	0.984903	2.522425	-1.864004
41	1	0	1.572717	1.800991	-2.435370
42	6	0	2.443501	-4.025441	0.731933
43	1	0	1.654039	-4.046877	-0.024752
44	1	0	2.818239	-5.032632	0.896789
45	1	0	2.046901	-3.623666	1.668698
46	6	0	-1.157633	2.214963	-0.495942
47	6	0	-1.433082	3.670468	-0.350034
48	6	0	-2.193743	1.361209	-0.380786
49	6	0	-2.908281	4.117872	-0.136052
50	6	0	-3.579196	1.760807	-0.069606
51	1	0	-2.019065	0.309161	-0.578264
52	6	0	-3.915215	3.068330	0.001525
53	1	0	-4.933995	3.388932	0.186296
54	8	0	-0.568165	4.509926	-0.395945
55	8	0	-3.153782	5.296640	-0.079981
56	6	0	-4.612673	0.729180	0.057744
57	1	0	-5.595435	0.992725	-0.319639
58	6	0	-4.459361	-0.472356	0.626275
59	6	0	-3.281681	-1.030242	1.382499
60	1	0	-2.910199	-1.919523	0.854700
61	1	0	-2.481312	-0.297058	1.452986
62	8	0	-3.658851	-1.350708	2.703528
63	1	0	-4.569341	-1.670467	2.686513
64	1	0	0.270745	2.988239	-2.551615
65	8	0	1.899509	3.486969	-1.377777
66	1	0	1.379141	4.146556	-0.902996

67	8	0	-5.461043	-1.408044	0.687725
68	6	0	-6.769823	-1.012028	0.557755
69	6	0	-7.476128	-0.705180	1.722230
70	6	0	-7.387244	-0.958028	-0.689546
71	6	0	-8.817488	-0.343466	1.641282
72	6	0	-8.735030	-0.600004	-0.768083
73	6	0	-9.451080	-0.308873	0.394792
74	1	0	-9.384110	-0.104733	2.531353
75	1	0	-9.221281	-0.503246	-1.728173
76	8	0	-6.755168	-0.795188	2.863843
77	8	0	-6.598001	-1.243774	-1.746911
78	6	0	-10.878104	0.064603	0.337746
79	1	0	-11.186745	0.830522	1.044289
80	6	0	-11.807687	-0.454056	-0.469213
81	1	0	-12.820430	-0.062985	-0.409206
82	6	0	-11.653070	-1.585299	-1.447410
83	1	0	-11.538216	-1.201708	-2.465548
84	1	0	-10.766947	-2.185605	-1.214494
85	6	0	-7.379490	-0.396790	4.072572
86	1	0	-6.621279	-0.494874	4.845434
87	1	0	-7.710393	0.643437	4.013294
88	1	0	-8.228863	-1.044824	4.305340
89	6	0	-7.189753	-1.221781	-3.033625
90	1	0	-7.552067	-0.220349	-3.282844
91	1	0	-6.403260	-1.506351	-3.727833
92	1	0	-8.012874	-1.939402	-3.098295
93	8	0	-12.819360	-2.389648	-1.482994
94	1	0	-12.958422	-2.759663	-0.607238
95	1	0	5.331544	1.860484	-1.410915

T7*-GBO4SBO4G-H2-CH4

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-6.561095	-0.296241	2.297345
2	6	0	-6.968266	0.623008	1.241792
3	6	0	-7.850639	0.113777	0.203711
4	6	0	-8.270432	-1.163837	0.194926
5	6	0	-7.892969	-2.109588	1.284582
6	6	0	-6.984205	-1.569803	2.334093
7	1	0	-5.887366	0.057394	3.069916
8	1	0	-8.173016	0.756773	-0.604367
9	8	0	-9.113125	-1.575487	-0.777455
10	8	0	-6.536155	-2.419932	3.287844
11	8	0	-8.299957	-3.253136	1.310924
12	6	0	-6.488396	1.884900	1.254733
13	1	0	-5.799559	2.175530	2.045152
14	6	0	-6.807461	2.981433	0.280269
15	6	0	-8.863160	-2.838665	-1.405244
16	1	0	-9.330336	-3.648331	-0.850216
17	1	0	-9.292848	-2.759303	-2.402471
18	1	0	-7.788949	-3.023930	-1.483868
19	6	0	-7.529903	-2.943101	4.172815
20	1	0	-6.990472	-3.540231	4.904573
21	1	0	-8.044644	-2.121522	4.679878
22	1	0	-8.243896	-3.565919	3.636167
23	6	0	-7.662860	4.005891	1.023123
24	1	0	-8.678830	3.631595	1.262129
25	8	0	-7.294256	5.093420	1.348985
26	8	0	-5.645440	3.636497	-0.187631
27	6	0	-4.541007	2.875351	-0.465834
28	6	0	-3.319674	3.320569	0.014906
29	6	0	-4.592753	1.720477	-1.264647
30	6	0	-2.151625	2.622209	-0.259837

31	1	0	-3.313642	4.227460	0.607309
32	6	0	-3.424170	1.008353	-1.509852
33	6	0	-2.192848	1.438584	-0.998059
34	1	0	-1.204139	2.986285	0.120356
35	1	0	-3.452850	0.140777	-2.152534
36	8	0	-5.810177	1.378865	-1.766012
37	6	0	-0.939661	0.708821	-1.247498
38	1	0	-0.065434	1.344293	-1.367700
39	6	0	-0.758821	-0.620558	-1.334093
40	6	0	-1.868180	-1.644354	-1.158655
41	1	0	-2.607286	-1.239081	-0.464153
42	1	0	-2.365292	-1.830023	-2.116550
43	8	0	-1.403516	-2.856865	-0.602923
44	1	0	-1.155628	-3.439235	-1.325963
45	6	0	-5.914476	0.141971	-2.449364
46	1	0	-5.330013	0.153097	-3.373473
47	1	0	-5.586815	-0.683003	-1.808310
48	1	0	-6.968636	0.015433	-2.688852
49	6	0	0.610263	-1.131264	-1.573588
50	6	0	0.816729	-2.223788	-2.561438
51	6	0	1.688223	-0.655957	-0.921811
52	6	0	2.271803	-2.722242	-2.805788
53	6	0	3.076471	-1.090595	-1.165939
54	1	0	1.533945	0.062386	-0.124048
55	6	0	3.339083	-2.094868	-2.031128
56	1	0	4.347826	-2.449023	-2.209598
57	8	0	-0.089872	-2.754262	-3.154209
58	8	0	2.454279	-3.594852	-3.617403
59	6	0	4.162653	-0.484374	-0.389458
60	1	0	4.963834	-1.152276	-0.090003
61	6	0	4.263207	0.809165	-0.063701
62	6	0	3.411506	1.972068	-0.501187

63	1	0	2.624416	1.646230	-1.177633
64	1	0	2.956303	2.434552	0.385186
65	8	0	4.197103	2.905601	-1.209893
66	1	0	5.067848	2.938486	-0.795446
67	8	0	5.289340	1.320303	0.689538
68	6	0	6.454289	0.606358	0.824995
69	6	0	6.613250	-0.324811	1.851452
70	6	0	7.489108	0.869914	-0.070926
71	6	0	7.830957	-0.991963	1.981691
72	6	0	8.706049	0.202660	0.061933
73	6	0	8.880111	-0.716178	1.099818
74	1	0	7.982171	-1.716941	2.770146
75	1	0	9.501853	0.358540	-0.652308
76	8	0	5.534286	-0.510404	2.640750
77	8	0	7.198043	1.780982	-1.027620
78	6	0	10.157830	-1.433857	1.277820
79	1	0	10.068700	-2.468695	1.597706
80	6	0	11.385405	-0.935900	1.106340
81	1	0	12.236296	-1.595372	1.258948
82	6	0	11.769286	0.479134	0.773775
83	1	0	12.007477	0.574250	-0.289736
84	1	0	10.949031	1.170102	0.995886
85	6	0	8.180746	2.036577	-2.016619
86	1	0	9.089028	2.448752	-1.567639
87	1	0	8.420563	1.125346	-2.570995
88	1	0	7.741355	2.767565	-2.690644
89	6	0	5.640093	-1.458429	3.687140
90	1	0	4.675735	-1.456964	4.188632
91	1	0	5.845348	-2.457537	3.292085
92	1	0	6.422364	-1.173505	4.396309
93	8	0	12.953330	0.857581	1.455020
94	1	0	12.788333	0.803195	2.400001

95	1	0	-7.400610	2.611278	-0.558744

OG12-GB5GBO4SBO4S-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.174649	6.120778	-0.732760
2	6	0	0.072193	4.863741	-0.174548
3	6	0	-0.972044	4.231168	0.513027
4	6	0	-2.227940	4.809776	0.605702
5	6	0	-2.470746	6.049802	0.001051
6	6	0	-1.433483	6.701162	-0.657544
7	1	0	0.625909	6.642329	-1.244929
8	1	0	-0.819175	3.279890	1.011998
9	1	0	-1.616503	7.668698	-1.114801
10	8	0	-3.232125	4.147444	1.261631
11	8	0	-3.728044	6.561995	0.100015
12	1	0	-3.772032	7.401788	-0.365473
13	6	0	1.425431	4.288270	-0.268496
14	1	0	2.233941	4.999447	-0.145275
15	6	0	1.740431	2.996736	-0.479678
16	6	0	0.686090	1.942464	-0.765524
17	1	0	0.474502	1.340163	0.120877
18	1	0	-0.246646	2.432198	-1.051946
19	6	0	-3.614242	4.748528	2.495710
20	1	0	-4.422876	4.140137	2.899770
21	1	0	-2.770407	4.749234	3.192416
22	1	0	-3.972069	5.767616	2.340108
23	8	0	1.078010	1.024114	-1.781760
24	1	0	1.305893	1.527454	-2.569074
25	6	0	3.140740	2.529031	-0.392290
26	6	0	3.425713	1.252194	-0.067629

27	6	0	4.302132	3.419937	-0.690543
28	6	0	4.776339	0.676958	0.057806
29	1	0	2.610668	0.557117	0.104159
30	6	0	5.734779	2.870273	-0.388617
31	6	0	5.875064	1.450372	-0.065778
32	1	0	6.877663	1.079384	0.108127
33	8	0	4.206839	4.515349	-1.178053
34	8	0	6.663457	3.637052	-0.442832
35	6	0	4.748813	-0.759657	0.336864
36	1	0	3.941158	-1.071287	0.992678
37	6	0	5.441409	-1.727482	-0.275850
38	6	0	6.530181	-1.607676	-1.298986
39	1	0	6.797153	-0.563304	-1.448338
40	1	0	7.410224	-2.144628	-0.921678
41	8	0	6.126069	-2.131841	-2.547451
42	1	0	5.450860	-2.802463	-2.389818
43	8	0	5.131918	-3.059838	-0.086930
44	6	0	3.818205	-3.314130	0.243366
45	6	0	3.455247	-3.666882	1.542593
46	6	0	2.844872	-3.102002	-0.732378
47	6	0	2.099469	-3.751797	1.870775
48	6	0	1.496054	-3.171623	-0.400811
49	6	0	1.125219	-3.453609	0.915178
50	1	0	1.790407	-3.973085	2.883253
51	1	0	0.732165	-2.992315	-1.145523
52	8	0	3.321523	-2.780230	-1.958255
53	8	0	4.473969	-3.831025	2.414225
54	6	0	-0.295823	-3.399176	1.318098
55	1	0	-0.719697	-4.246269	1.848873
56	6	0	-1.085672	-2.345169	1.121361
57	6	0	-0.717003	-1.012438	0.526591
58	1	0	0.310747	-1.034081	0.169696

59	1	0	-1.364249	-0.788121	-0.332226
60	6	0	2.456039	-2.073095	-2.838573
61	1	0	2.006755	-1.215396	-2.328856
62	1	0	3.086749	-1.731496	-3.656792
63	1	0	1.675779	-2.731545	-3.229599
64	6	0	4.146264	-4.133585	3.756814
65	1	0	5.094566	-4.229112	4.279854
66	1	0	3.557760	-3.329968	4.209249
67	1	0	3.595127	-5.076012	3.824199
68	8	0	-2.366311	-2.387964	1.665541
69	6	0	-3.401937	-1.967527	0.867574
70	6	0	-4.063175	-0.772632	1.165882
71	6	0	-3.827167	-2.744632	-0.213867
72	6	0	-5.146277	-0.359686	0.394861
73	6	0	-4.912426	-2.330750	-0.986070
74	6	0	-5.583918	-1.147534	-0.672000
75	1	0	-5.658948	0.567233	0.613311
76	1	0	-5.215961	-2.899084	-1.853526
77	8	0	-3.564733	-0.074569	2.220856
78	8	0	-3.112938	-3.871199	-0.433944
79	6	0	-6.740152	-0.687480	-1.465044
80	1	0	-6.806418	0.388012	-1.607491
81	6	0	-7.701063	-1.448681	-1.996181
82	1	0	-8.483053	-0.964484	-2.576089
83	6	0	-4.143143	1.191519	2.511455
84	1	0	-3.583528	1.580205	3.360004
85	1	0	-4.039619	1.874929	1.664740
86	1	0	-5.194285	1.078072	2.790061
87	6	0	-3.513916	-4.706761	-1.502461
88	1	0	-3.428311	-4.188512	-2.462110
89	1	0	-2.835666	-5.556442	-1.487122
90	1	0	-4.541609	-5.056350	-1.363994

91	6	0	-7.886800	-2.933344	-1.850303
92	1	0	-7.517371	-3.458737	-2.736021
93	1	0	-7.336210	-3.312797	-0.982835
94	8	0	-9.262230	-3.268317	-1.767119
95	1	0	-9.631256	-2.834477	-0.993305
96	8	0	-0.799019	0.018718	1.496678
97	1	0	-1.667865	-0.023629	1.919956

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-10.373568	2.334655	0.110478
2	6	0	-8.907345	2.187694	-0.020338
3	6	0	-8.178223	3.138013	-0.644727
4	6	0	-8.810255	4.312318	-1.258204
5	6	0	-10.359036	4.420850	-1.162552
6	6	0	-11.059178	3.354280	-0.418076
7	1	0	-10.893647	1.551527	0.652765
8	1	0	-7.095915	3.095814	-0.684780
9	1	0	-12.135373	3.443646	-0.328907
10	8	0	-8.187341	5.184114	-1.810327
11	8	0	-10.931551	5.345310	-1.676252
12	6	0	-8.322728	1.000971	0.602508
13	1	0	-8.730678	0.694193	1.561759
14	6	0	-7.357173	0.229820	0.093551
15	6	0	-6.713458	0.305532	-1.264579
16	1	0	-7.151149	1.121722	-1.834742
17	1	0	-5.638328	0.503418	-1.151214
18	8	0	-6.935255	-0.877352	-2.002333
19	1	0	-6.809971	-1.650293	-1.436869
20	8	0	-7.001849	-0.881625	0.832895

21	6	0	-5.665505	-1.205268	0.903071
22	6	0	-4.764593	-0.371749	1.574309
23	6	0	-5.227829	-2.417569	0.372754
24	6	0	-3.434100	-0.755960	1.710144
25	6	0	-3.897390	-2.808094	0.520169
26	6	0	-2.993547	-1.971013	1.175278
27	1	0	-2.723649	-0.119524	2.220085
28	1	0	-3.567459	-3.770892	0.158603
29	8	0	-6.172349	-3.140807	-0.284392
30	8	0	-5.290464	0.783742	2.040362
31	6	0	-1.578534	-2.339006	1.355850
32	1	0	-1.121728	-2.085063	2.305684
33	6	0	-0.790123	-2.923933	0.455086
34	6	0	-5.773957	-4.367539	-0.875728
35	1	0	-6.659787	-4.760729	-1.368049
36	1	0	-4.983101	-4.205869	-1.613727
37	1	0	-5.435096	-5.072979	-0.112911
38	6	0	-4.427090	1.673177	2.722476
39	1	0	-3.613290	2.005997	2.071606
40	1	0	-5.039666	2.526000	3.004447
41	1	0	-4.013808	1.205956	3.621009
42	6	0	-1.170337	-3.374274	-0.936122
43	1	0	-1.492799	-4.425075	-0.888201
44	1	0	-2.013583	-2.779567	-1.288055
45	8	0	-0.133246	-3.222092	-1.872091
46	1	0	0.567794	-3.846046	-1.647235
47	8	0	0.488007	-3.316940	0.855463
48	6	0	1.597992	-2.602413	0.480362
49	6	0	2.547221	-3.214148	-0.346815
50	6	0	1.868598	-1.334018	1.004607
51	6	0	3.736713	-2.568048	-0.661256
52	6	0	3.059116	-0.681671	0.682202

53	6	0	4.004408	-1.303178	-0.133198
54	1	0	4.467321	-3.031369	-1.310361
55	1	0	3.245351	0.320740	1.040177
56	8	0	2.201390	-4.441311	-0.826012
57	8	0	0.928423	-0.819272	1.832098
58	6	0	5.270880	-0.650787	-0.512166
59	1	0	5.550791	-0.787013	-1.550105
60	6	0	6.097743	0.058228	0.278803
61	6	0	5.863921	0.229014	1.768761
62	1	0	5.485339	1.231186	1.994922
63	1	0	5.111576	-0.489027	2.100846
64	6	0	3.164868	-5.148146	-1.592283
65	1	0	2.714888	-6.111526	-1.819163
66	1	0	3.391823	-4.620329	-2.522326
67	1	0	4.081335	-5.297117	-1.016262
68	6	0	1.156537	0.465710	2.373588
69	1	0	1.223417	1.220598	1.584828
70	1	0	0.298528	0.679357	3.007672
71	1	0	2.067094	0.483924	2.980523
72	8	0	7.049374	0.094704	2.532839
73	1	0	7.422989	-0.775272	2.366016
74	6	0	7.286271	0.729354	-0.290459
75	6	0	7.840809	1.813597	0.291215
76	6	0	7.973235	0.191942	-1.505816
77	6	0	8.992756	2.562427	-0.236347
78	1	0	7.433959	2.178346	1.227624
79	6	0	9.056645	1.086133	-2.178846
80	6	0	9.549830	2.236780	-1.423664
81	1	0	10.324213	2.831858	-1.891327
82	8	0	7.779572	-0.903471	-1.962836
83	8	0	9.451242	0.789434	-3.278320
84	6	0	9.451992	3.691364	0.580391

85	1	0	8.688773	4.182198	1.177203
86	6	0	10.712119	4.122148	0.699908
87	1	0	10.914383	4.959535	1.361761
88	6	0	11.940290	3.558283	0.057548
89	1	0	12.093657	4.028908	-0.924148
90	1	0	11.830081	2.478728	-0.102499
91	8	0	13.024189	3.850619	0.921240
92	1	0	13.836740	3.530755	0.523408

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.467636	2.960451	-0.330426
2	6	0	-6.373212	1.963377	-0.208226
3	6	0	-7.808898	2.237408	-0.082060
4	6	0	-8.324064	3.480409	-0.040467
5	6	0	-7.410106	4.654214	-0.195185
6	6	0	-5.880659	4.359079	-0.261669
7	1	0	-4.406855	2.764971	-0.434618
8	1	0	-8.501545	1.405662	-0.071894
9	8	0	-9.654904	3.648198	-0.019200
10	8	0	-7.805312	5.781573	-0.315529
11	8	0	-5.117945	5.291676	-0.248593
12	6	0	-5.899754	0.569278	-0.241287
13	1	0	-5.061595	0.398787	-0.911961
14	6	0	-6.357399	-0.474371	0.471319
15	6	0	-7.489643	-0.399583	1.485764
16	1	0	-7.509333	0.600197	1.921897
17	1	0	-8.446592	-0.575218	0.984604
18	6	0	-10.215261	4.762552	0.687849
19	1	0	-10.245184	5.646166	0.054779

20	1	0	-11.221892	4.452138	0.959613
21	1	0	-9.641065	4.976250	1.591160
22	8	0	-7.310990	-1.306923	2.550765
23	1	0	-7.776746	-2.119251	2.334327
24	6	0	-5.681396	-1.781909	0.305410
25	6	0	-6.501576	-3.016590	0.190589
26	6	0	-4.341330	-1.904552	0.267092
27	6	0	-5.756340	-4.365638	-0.032982
28	6	0	-3.619398	-3.171764	0.049222
29	1	0	-3.732726	-1.024378	0.447428
30	6	0	-4.290131	-4.337123	-0.054267
31	1	0	-3.780024	-5.284979	-0.184883
32	8	0	-7.703161	-3.020810	0.284535
33	8	0	-6.405872	-5.367996	-0.178697
34	6	0	-2.143577	-3.163772	0.030627
35	1	0	-1.677770	-3.956159	0.601997
36	6	0	-1.361621	-2.292566	-0.634267
37	6	0	-1.946599	-1.243683	-1.568335
38	1	0	-3.011336	-1.437252	-1.719981
39	1	0	-1.850303	-0.241422	-1.138455
40	8	0	-1.284174	-1.186591	-2.815734
41	1	0	-1.308189	-2.058536	-3.220859
42	6	0	0.111471	-2.313475	-0.497912
43	6	0	0.863014	-1.242446	-0.832328
44	6	0	0.842153	-3.524247	-0.017880
45	6	0	2.327259	-1.130842	-0.686900
46	1	0	0.374642	-0.372288	-1.255102
47	6	0	2.359682	-3.367953	0.290038
48	6	0	3.036707	-2.152020	-0.149964
49	1	0	4.103158	-2.103162	0.007479
50	8	0	0.343294	-4.611559	0.111562
51	8	0	2.916043	-4.263658	0.876743

52	6	0	2.875893	0.152311	-1.117915
53	1	0	2.156851	0.892877	-1.447378
54	6	0	4.159016	0.539314	-1.161698
55	6	0	4.605255	1.913109	-1.580104
56	1	0	3.728107	2.531911	-1.763536
57	1	0	5.180046	2.371243	-0.763377
58	8	0	5.357568	1.883747	-2.773084
59	1	0	6.058890	1.224440	-2.688420
60	8	0	5.164181	-0.360021	-0.921196
61	6	0	6.242462	0.048411	-0.164263
62	6	0	6.091515	0.193145	1.218506
63	6	0	7.490849	0.217229	-0.758062
64	6	0	7.194407	0.515107	2.003551
65	6	0	8.596117	0.535834	0.030158
66	6	0	8.445948	0.699672	1.408140
67	1	0	7.094859	0.634822	3.074071
68	1	0	9.577479	0.619488	-0.413095
69	8	0	7.527264	0.061168	-2.107391
70	8	0	4.836078	0.000193	1.675268
71	6	0	9.590775	1.050986	2.269526
72	1	0	9.578096	0.608233	3.261640
73	6	0	10.598472	1.871120	1.963555
74	1	0	11.367663	2.027253	2.717214
75	6	0	8.782026	0.200429	-2.757558
76	1	0	9.191093	1.203004	-2.604208
77	1	0	9.487779	-0.552090	-2.397714
78	1	0	8.587006	0.042016	-3.815137
79	6	0	4.624859	0.052413	3.075169
80	1	0	5.231992	-0.698327	3.588209
81	1	0	4.851898	1.047195	3.468526
82	1	0	3.570799	-0.167756	3.224234
83	6	0	10.789593	2.668411	0.701435

84	1	0	11.393853	2.103796	-0.023209
85	1	0	9.827688	2.880742	0.231991
86	8	0	11.385053	3.926065	0.962336
87	1	0	12.279017	3.788780	1.285201

OG8*-SBO4GBO4SB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.370322	1.834789	-2.099442
2	6	0	6.460705	1.142571	-1.421203
3	6	0	7.075134	1.793110	-0.274643
4	6	0	6.627850	2.969153	0.198264
5	6	0	5.467712	3.662029	-0.427231
6	6	0	4.903015	3.015750	-1.650717
7	1	0	4.942654	1.350948	-2.968326
8	1	0	7.894195	1.317580	0.247918
9	8	0	7.161720	3.471231	1.333449
10	8	0	4.990769	4.673533	0.033855
11	8	0	3.902032	3.733086	-2.179408
12	6	0	6.837412	-0.075632	-1.864377
13	1	0	6.318182	-0.505928	-2.718211
14	6	0	7.903969	-0.962285	-1.287443
15	6	0	9.023768	-1.047123	-2.319327
16	1	0	9.589555	-0.098830	-2.424476
17	6	0	7.460657	4.870963	1.384061
18	1	0	6.585931	5.444592	1.680627
19	1	0	8.255482	4.973100	2.120777
20	1	0	7.818139	5.221983	0.413074
21	6	0	3.266531	3.203419	-3.325044
22	1	0	2.810084	2.233653	-3.102943
23	1	0	2.495365	3.918361	-3.599843

24	1	0	3.978292	3.092357	-4.149112
25	8	0	9.272448	-2.007726	-2.984110
26	8	0	7.428860	-2.270801	-1.039990
27	6	0	6.155008	-2.404474	-0.545376
28	6	0	5.318313	-3.320865	-1.161606
29	6	0	5.702324	-1.697428	0.581668
30	6	0	4.023463	-3.526295	-0.698594
31	1	0	5.709273	-3.862437	-2.014653
32	6	0	4.402319	-1.894586	1.031904
33	6	0	3.541962	-2.791782	0.383813
34	1	0	3.378320	-4.242225	-1.194348
35	1	0	4.047255	-1.379311	1.915277
36	8	0	6.588523	-0.855167	1.175672
37	6	0	2.164384	-2.985749	0.866112
38	1	0	1.764714	-3.995397	0.873969
39	6	0	1.368690	-2.020053	1.325776
40	6	0	1.645127	-0.543949	1.348064
41	1	0	2.432240	-0.306209	0.635114
42	1	0	0.742393	0.001340	1.046348
43	6	0	6.100435	-0.033017	2.226731
44	1	0	5.242866	0.559169	1.893613
45	1	0	5.814546	-0.635801	3.092547
46	1	0	6.916999	0.633933	2.495570
47	8	0	2.084506	-0.103589	2.624175
48	1	0	1.359690	-0.280908	3.236047
49	8	0	0.194517	-2.411726	1.967587
50	6	0	-0.970998	-1.793311	1.609963
51	6	0	-1.491474	-0.766719	2.401926
52	6	0	-1.673785	-2.225963	0.481418
53	6	0	-2.715429	-0.187631	2.078242
54	6	0	-2.901728	-1.649201	0.159396
55	6	0	-3.436785	-0.642640	0.969123

56	1	0	-3.130983	0.607588	2.682159
57	1	0	-3.423281	-1.972954	-0.728374
58	8	0	-0.718718	-0.387709	3.453047
59	8	0	-1.079982	-3.206963	-0.231183
60	6	0	-4.726674	0.018497	0.704570
61	1	0	-4.761309	1.051995	1.026911
62	6	0	-5.848034	-0.506797	0.170252
63	6	0	-1.205263	0.652808	4.287349
64	1	0	-0.451687	0.794209	5.058574
65	1	0	-1.329132	1.580627	3.722784
66	1	0	-2.153064	0.367593	4.750417
67	6	0	-1.757849	-3.692173	-1.374747
68	1	0	-1.874010	-2.905823	-2.126692
69	1	0	-1.133718	-4.486816	-1.775918
70	1	0	-2.740617	-4.094892	-1.111881
71	6	0	-5.939382	-1.950975	-0.259562
72	1	0	-5.232218	-2.555331	0.311321
73	1	0	-6.941655	-2.335815	-0.063130
74	8	0	-5.718513	-2.122834	-1.662725
75	1	0	-5.119657	-1.432464	-1.960409
76	6	0	-7.049510	0.322870	-0.062805
77	6	0	-7.968621	-0.018512	-0.992598
78	6	0	-7.337492	1.537925	0.764293
79	6	0	-9.199275	0.732905	-1.284973
80	1	0	-7.801903	-0.906981	-1.594639
81	6	0	-8.550318	2.426358	0.348855
82	6	0	-9.463664	1.904585	-0.668149
83	1	0	-10.309680	2.527847	-0.930222
84	8	0	-6.717728	1.852308	1.744832
85	8	0	-8.689512	3.497605	0.881756
86	6	0	-10.077709	0.148651	-2.306329
87	1	0	-9.576678	-0.412733	-3.090116

88	6	0	-11.413869	0.197617	-2.320100
89	1	0	-11.926672	-0.303896	-3.137993
90	6	0	-12.326201	0.817474	-1.298813
91	1	0	-11.855152	0.820282	-0.313875
92	1	0	-12.535693	1.863546	-1.560297
93	8	0	-13.528724	0.084182	-1.166503
94	1	0	-14.080907	0.239591	-1.936382
95	1	0	8.330016	-0.534854	-0.377036

OG9*-SBO4SB5GB5G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.275063	-0.058006	1.455236
2	6	0	-6.851084	-0.934851	0.369856
3	6	0	-7.526714	-0.819063	-0.913812
4	6	0	-8.507894	0.076413	-1.113162
5	6	0	-8.931874	1.018253	-0.040104
6	6	0	-8.251497	0.853100	1.279791
7	1	0	-6.769929	-0.169552	2.406366
8	1	0	-7.259573	-1.478201	-1.730375
9	8	0	-9.074741	0.209670	-2.335739
10	8	0	-9.761781	1.879230	-0.223772
11	8	0	-8.719256	1.711252	2.199270
12	6	0	-5.867131	-1.830942	0.592415
13	1	0	-5.412641	-1.901154	1.577663
14	6	0	-5.328100	-2.816554	-0.404782
15	6	0	-10.482988	-0.026863	-2.395230
16	1	0	-11.029411	0.712502	-1.811383
17	1	0	-10.753718	0.054270	-3.445669
18	1	0	-10.703929	-1.037272	-2.038932
19	6	0	-8.134803	1.658326	3.483055

20	1	0	-7.064160	1.881610	3.433391
21	1	0	-8.640098	2.415765	4.076895
22	1	0	-8.281453	0.673621	3.938547
23	6	0	-6.206311	-4.066009	-0.436806
24	1	0	-5.792875	-4.928432	0.119455
25	8	0	-7.256246	-4.105558	-1.009666
26	8	0	-4.038804	-3.278606	-0.020436
27	6	0	-3.070037	-2.313431	0.046825
28	6	0	-2.546929	-1.951845	1.291668
29	6	0	-2.549950	-1.739315	-1.118332
30	6	0	-1.507732	-1.024346	1.368858
31	6	0	-1.520186	-0.804034	-1.039332
32	6	0	-1.007352	-0.438084	0.206173
33	1	0	-1.092089	-0.735119	2.324629
34	1	0	-1.093252	-0.368501	-1.932578
35	8	0	-3.110464	-2.165750	-2.275806
36	8	0	-3.119510	-2.550273	2.365994
37	6	0	0.115409	0.522492	0.305444
38	1	0	0.956447	0.177292	0.903216
39	6	0	0.186515	1.748111	-0.239934
40	6	0	-2.627583	-1.607014	-3.485531
41	1	0	-3.212498	-2.064913	-4.279394
42	1	0	-2.769960	-0.522865	-3.502236
43	1	0	-1.569423	-1.841757	-3.629184
44	6	0	-2.560864	-2.285013	3.637686
45	1	0	-2.655711	-1.226779	3.899685
46	1	0	-3.127798	-2.886444	4.344508
47	1	0	-1.507445	-2.577276	3.673041
48	6	0	-1.004820	2.415897	-0.899679
49	1	0	-1.776535	1.678987	-1.104239
50	1	0	-1.424245	3.142299	-0.197901
51	8	0	-0.687414	3.038301	-2.129108

52	1	0	-0.301054	3.895370	-1.927162
53	6	0	1.468904	2.497286	-0.153536
54	6	0	1.534553	3.880575	-0.004869
55	6	0	2.685775	1.801477	-0.241910
56	6	0	2.775201	4.537691	0.077078
57	6	0	3.919172	2.431620	-0.134382
58	1	0	2.650012	0.742042	-0.462210
59	6	0	3.957464	3.828978	0.010764
60	1	0	4.914720	4.331486	0.068521
61	8	0	0.402752	4.636172	0.051151
62	1	0	0.668283	5.555138	0.189741
63	8	0	2.663776	5.889647	0.224456
64	6	0	5.196677	1.709002	-0.241019
65	1	0	5.962716	2.226603	-0.806439
66	6	0	5.504522	0.509012	0.287506
67	6	0	4.554611	-0.260083	1.186764
68	1	0	3.752640	0.404188	1.515686
69	1	0	4.090293	-1.095031	0.652570
70	6	0	3.861098	6.642185	0.311903
71	1	0	4.456361	6.528600	-0.597945
72	1	0	3.559195	7.680361	0.424681
73	1	0	4.449327	6.332682	1.179928
74	8	0	5.204581	-0.841599	2.304813
75	1	0	5.655082	-0.144219	2.789560
76	6	0	6.804472	-0.129984	-0.009330
77	6	0	6.969562	-1.468837	0.042426
78	6	0	8.019489	0.684931	-0.318953
79	6	0	8.214729	-2.180268	-0.284188
80	1	0	6.138608	-2.092169	0.353706
81	6	0	9.280866	-0.064337	-0.846938
82	6	0	9.303991	-1.524438	-0.738635
83	1	0	10.194804	-2.045085	-1.072596

84	8	0	8.101620	1.871305	-0.136660
85	8	0	10.185901	0.585837	-1.305393
86	6	0	8.175627	-3.645678	-0.151337
87	1	0	7.227998	-4.112767	-0.408093
88	6	0	9.169017	-4.426629	0.281999
89	1	0	9.000052	-5.498451	0.306697
90	6	0	10.512750	-3.952929	0.756110
91	1	0	10.874660	-4.631177	1.535463
92	1	0	10.429166	-2.946941	1.180949
93	8	0	11.403238	-3.956448	-0.355681
94	1	0	12.295241	-3.792596	-0.038267
95	1	0	-5.295986	-2.402308	-1.416218

OG10*-SBO4SB5GBO4G-CH4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.027265	0.764082	-0.307551
2	6	0	8.820895	-0.033749	-0.501976
3	6	0	8.631288	-1.229786	0.305728
4	6	0	9.561453	-1.613582	1.201338
5	6	0	10.809039	-0.823780	1.429438
6	6	0	10.963048	0.406606	0.591590
7	1	0	10.139209	1.651535	-0.917679
8	1	0	7.723940	-1.798930	0.166321
9	8	0	11.641679	-1.153025	2.234952
10	8	0	9.502998	-2.700043	1.979377
11	8	0	12.106958	1.052982	0.856406
12	6	0	7.916246	0.357830	-1.425768
13	1	0	8.117259	1.251295	-2.007441
14	6	0	6.624816	-0.369220	-1.724501

15	6	0	8.365571	-3.531529	1.827991
16	1	0	8.287021	-3.899660	0.800596
17	1	0	8.509651	-4.362606	2.513455
18	1	0	7.452037	-2.987730	2.086065
19	6	0	12.364721	2.231132	0.122113
20	1	0	13.322810	2.603861	0.475198
21	1	0	12.423923	2.017088	-0.949819
22	1	0	11.587443	2.980629	0.302218
23	6	0	6.953577	-1.683901	-2.429086
24	1	0	7.347313	-1.551778	-3.456834
25	8	0	6.854190	-2.766709	-1.930497
26	8	0	5.877934	-0.619391	-0.542444
27	6	0	4.616676	-0.109016	-0.492663
28	6	0	4.289079	0.778943	0.540603
29	6	0	3.639522	-0.493541	-1.414607
30	6	0	2.986952	1.264318	0.646899
31	6	0	2.337632	-0.006809	-1.306560
32	6	0	2.005989	0.857680	-0.262017
33	1	0	2.714613	1.952280	1.436133
34	1	0	1.588878	-0.269996	-2.040830
35	8	0	4.065820	-1.340283	-2.387499
36	8	0	5.299463	1.098394	1.376045
37	6	0	0.648931	1.416110	-0.110820
38	1	0	0.621641	2.473783	0.123097
39	6	0	-0.521058	0.758441	-0.212928
40	6	0	-0.599262	-0.742335	-0.422161
41	1	0	-0.914970	-0.983571	-1.442108
42	1	0	0.388068	-1.182170	-0.270533
43	6	0	3.092367	-1.905944	-3.244145
44	1	0	2.320303	-2.423228	-2.667145
45	1	0	2.630152	-1.143004	-3.877523
46	1	0	3.622644	-2.623601	-3.865961

47	6	0	5.012266	1.974088	2.449027
48	1	0	5.944393	2.087734	2.996997
49	1	0	4.680698	2.950774	2.084174
50	1	0	4.249056	1.551324	3.108920
51	8	0	-1.553013	-1.363631	0.424159
52	1	0	-1.325713	-1.157729	1.335354
53	6	0	-1.806445	1.486203	-0.132709
54	6	0	-2.938270	0.995320	-0.679608
55	6	0	-1.929601	2.774163	0.618381
56	6	0	-4.244187	1.675945	-0.680732
57	1	0	-2.920676	0.018933	-1.150533
58	6	0	-3.241203	3.595926	0.437989
59	6	0	-4.380778	2.926689	-0.183402
60	1	0	-5.303885	3.489213	-0.271940
61	8	0	-1.102997	3.186651	1.389182
62	8	0	-3.259760	4.738190	0.824072
63	6	0	-5.336508	0.943414	-1.320135
64	1	0	-5.090084	0.352693	-2.197602
65	6	0	-6.615313	0.923137	-0.922491
66	6	0	-7.175796	1.528448	0.335614
67	1	0	-6.356407	1.841516	0.976755
68	1	0	-7.752529	0.775243	0.880122
69	8	0	-7.962340	2.675214	0.066045
70	1	0	-8.814969	2.390825	-0.277961
71	8	0	-7.506975	0.326666	-1.781450
72	6	0	-8.717156	-0.125974	-1.312264
73	6	0	-9.883635	0.399242	-1.839195
74	6	0	-8.769412	-1.179828	-0.386846
75	6	0	-11.119206	-0.097447	-1.435607
76	1	0	-9.802103	1.188750	-2.577572
77	6	0	-10.006843	-1.665784	0.018615
78	6	0	-11.194903	-1.118124	-0.488371

79	1	0	-12.029625	0.317838	-1.851048
80	1	0	-10.059051	-2.505467	0.697512
81	8	0	-7.571717	-1.633797	0.047326
82	6	0	-12.517234	-1.608708	-0.060212
83	1	0	-13.291716	-1.571129	-0.821206
84	6	0	-12.857784	-2.047586	1.153922
85	1	0	-13.885933	-2.371285	1.302550
86	6	0	-12.000413	-2.106760	2.389614
87	1	0	-11.500821	-3.083330	2.467334
88	1	0	-11.222859	-1.341696	2.353724
89	6	0	-7.567783	-2.683656	0.997918
90	1	0	-6.522282	-2.877896	1.223241
91	1	0	-8.092477	-2.386653	1.911426
92	1	0	-8.027298	-3.586152	0.585151
93	8	0	-12.750259	-1.845930	3.561561
94	1	0	-13.397269	-2.545459	3.681392
95	1	0	6.036512	0.231493	-2.424