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CARBON ISOTOPES IN WOOD COMBUSTION/PYROLYSIS PRODUCTS: EXPERIMENTAL AND MOLECULAR SIMULATION APPROACHES

SUPPLEMENTARY MATERIALS

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Table S1. *Thermal corrections to energy (kcal/mol) for all the studied molecules at different temperatures.*

molecule	temperature (°C)	total	translational	rotational	vibrational
^{12}C-pyrene	27	136.297	0.894	0.894	134.508
	427	165.845	2.087	2.087	161.672
^{13}C-pyrene	27	134.178	0.894	0.894	132.389
	427	164.317	2.087	2.087	160.143
$^{12}CO_2$	27	8.966	0.894	0.596	7.476
	427	12.388	2.087	1.391	8.911
$^{13}CO_2$	27	8.825	0.894	0.596	7.335
	427	12.273	2.087	1.391	8.795
^{12}C-formaldehyde	27	18.57	0.894	0.894	16.781
	427	21.908	2.087	2.087	17.735
^{13}C-formaldehyde	27	18.458	0.894	0.894	16.669
	427	21.813	2.087	2.087	17.64
^{12}C-glycoldehyde	27	41.065	0.894	0.894	39.277
	427	49.432	2.087	2.087	45.259
^{13}C-glycoldehyde	27	40.814	0.894	0.894	39.025
	427	49.239	2.087	2.087	45.066
^{12}C-acetone	27	54.844	0.894	0.894	53.055
	427	63.138	2.087	2.087	58.965
^{13}C-acetone	27	54.492	0.894	0.894	52.703
	427	62.869	2.087	2.087	58.696

Table S2. *Different contribution to entropy for all the studied molecules at different temperatures.*

molecule	temperature (°C)	total	translational	rotational	vibrational
^{12}C-pyrene	27	97.838	41.846	31.777	24.216
	427	159.052	46.055	34.302	78.694
^{13}C-pyrene	27	99.467	42.074	31.989	25.405
	427	161.938	46.283	34.515	81.14
$^{12}CO_2$	27	51.169	37.301	13.125	0.743
	427	59.929	41.51	14.808	3.611
$^{13}CO_2$	27	51.29	37.368	13.125	0.797
	427	60.106	41.578	14.808	3.72
^{12}C-formaldehyde	27	53.693	36.161	17.44	0.092
	427	62.212	40.37	19.966	1.876
^{13}C-formaldehyde	27	53.845	36.259	17.49	0.096
	427	62.399	40.468	20.016	1.914
^{12}C-glycoldehyde	27	70.313	38.227	23.71	8.376
	427	89.054	42.437	26.236	20.382
^{13}C-glycoldehyde	27	70.554	38.325	23.758	8.471
	427	89.419	42.535	26.283	20.602
^{12}C-acetone	27	65.333	38.127	24.198	3.008
	427	83.714	42.337	26.723	14.654
^{13}C-acetone	27	65.716	38.278	24.312	3.126
	427	84.272	42.487	26.838	14.947