Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Oxygen delignification of conventional and high alkali cooked softwood kraft pulps, and study of the residual lignin structure

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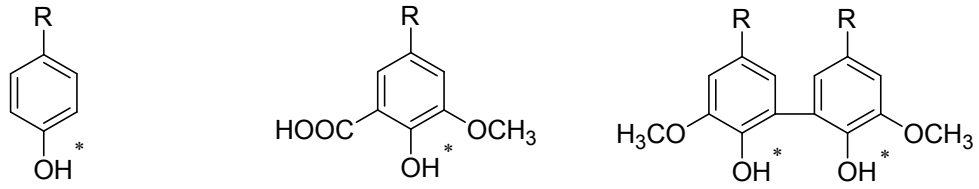

p-Hydroxyphenolic units (137-138.6 ppm) | Guaiacyl phenolic units (138.6-140.2 ppm) | 5-5´ Biphenyl units (140.2-141.4 ppm)

Figure 1. Typical phenolics present in the lignin samples in this study and the corresponding chemical shifts in their ^{31}P NMR spectra.

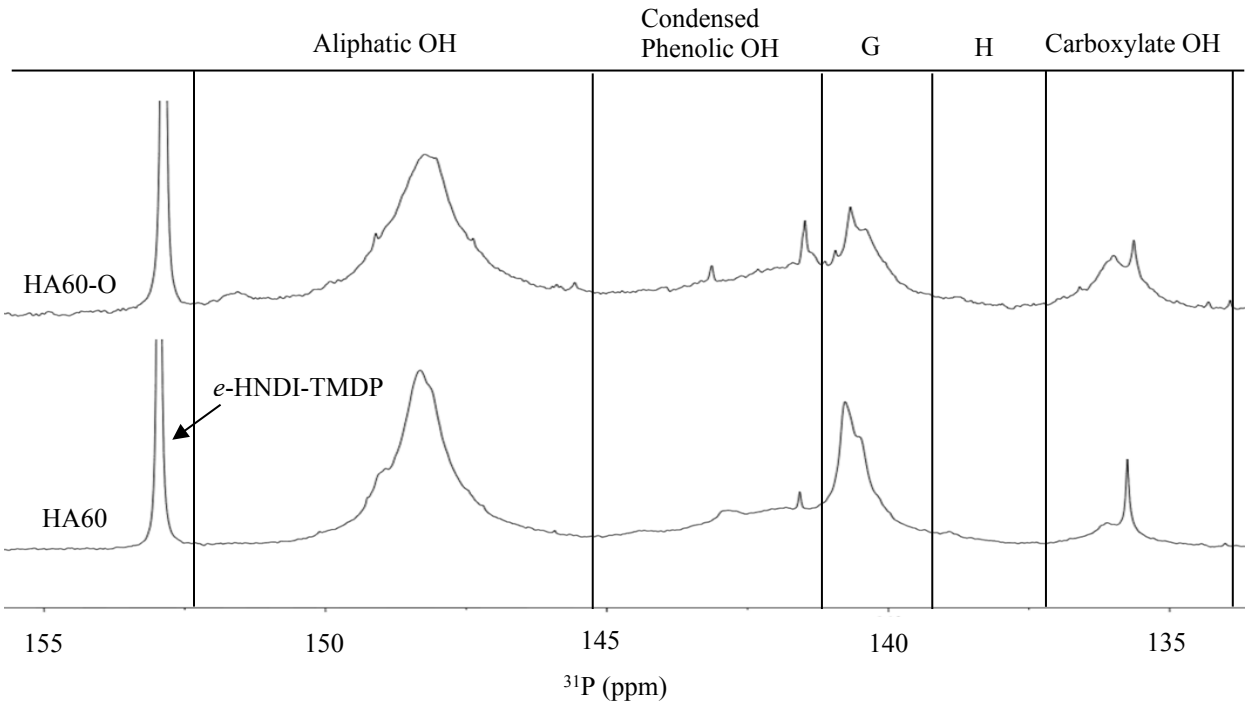

Figure 2. ^{31}P NMR spectra of HA60 and HA60-OD (G: Guaiacyl phenolic OH, H: *p*-Hydroxyphenolic OH).

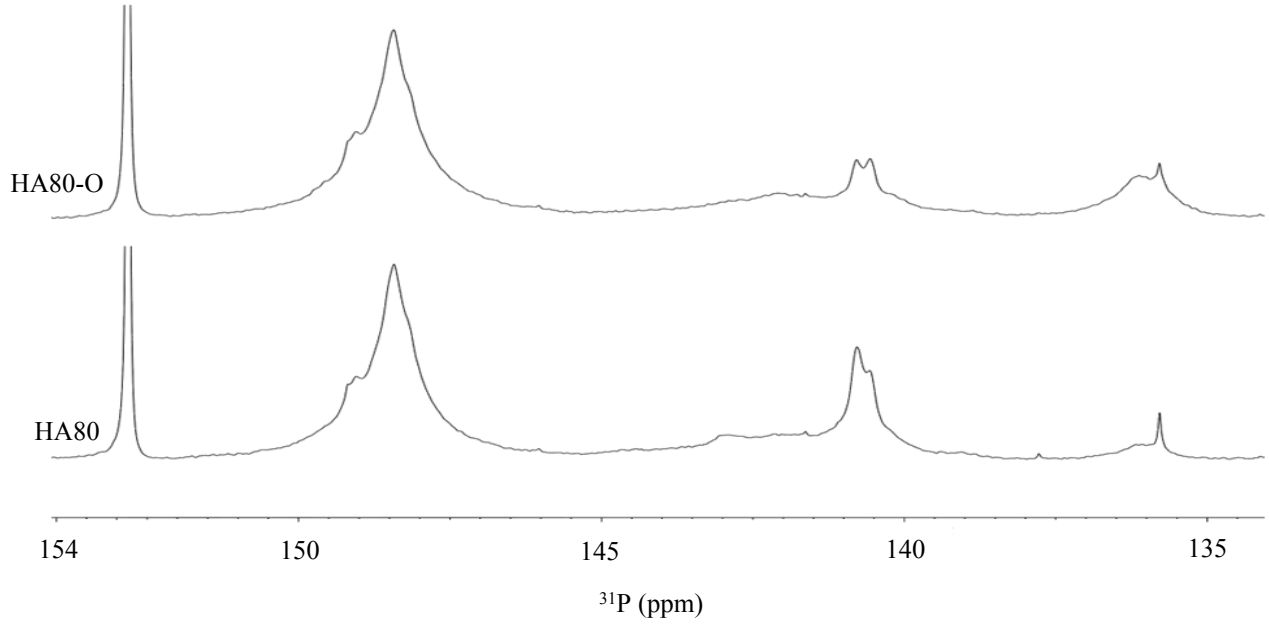

Figure 3. ^{31}P NMR spectra of HA80 and HA80-OD (G: Guaiacyl phenolic OH, H: *p*-Hydroxyphenolic OH).

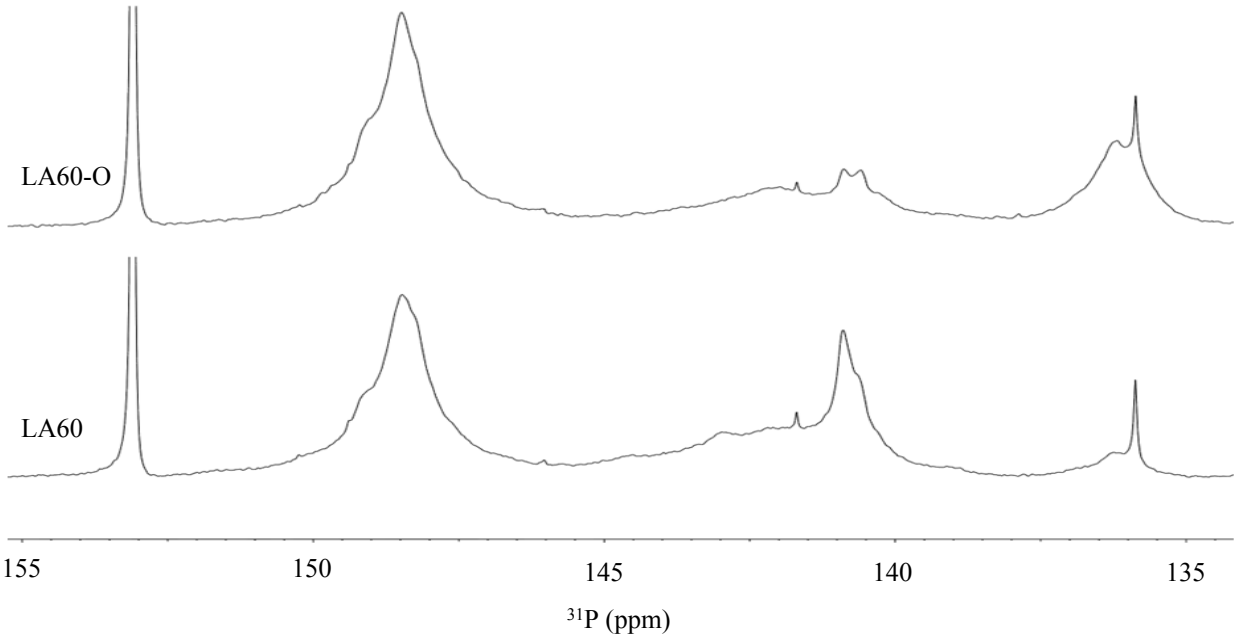

Figure 4. ^{31}P NMR spectra of LA60 and LA60-OD (G: Guaiacyl phenolic OH, H: *p*-Hydroxyphenolic OH).

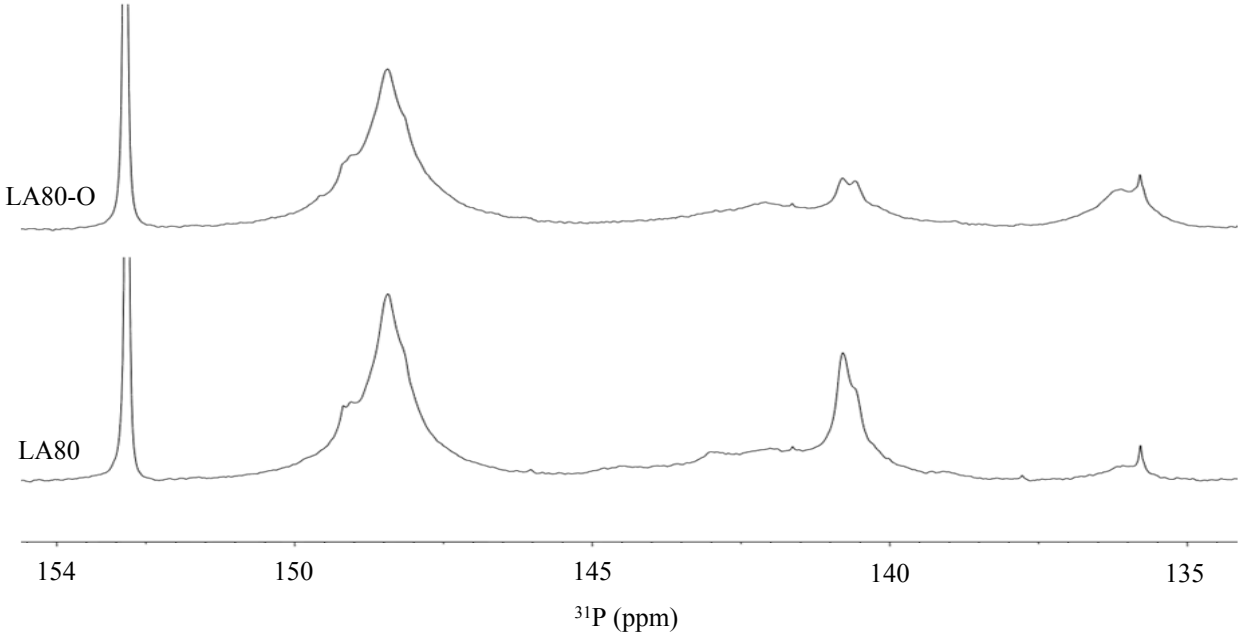

Figure 5. ^{31}P NMR spectra of HA80 and HA80-OD (G: Guaiacyl phenolic OH, H: *p*-Hydroxyphenolic OH).

Table 1. ^{31}P NMR chemical shifts of typical hydroxyl groups within residual Kraft lignin[1]

Reactive groups	^{31}P (ppm)
Carboxyl OH	133-137
p-Hydroxy-phenolic OH	137-138.6
Guaiacyl OH	138-140.2
Total condensed phenolic OH	140.2-145.2
5-5´ Condensed OH	140.2-141.4
Aliphatic OH	145.2-151.4

Table 2. Integral values of typical hydroxyl groups within residual Kraft lignin in ^{31}P NMR spectra

Lignin sample	*Carboxyl OH*	*p-Hydroxy-phenolic OH*	*Guaiacyl OH*	*Total condensed phenolic OH*	*5-5´ Condensed OH*	*Aliphatic OH*
HA60	37.24	18.11	57.03	58.13	29.49	75.09
HA60-O	46.95	20.49	45.2	58.54	38.36	74.02
LA60	32.12	14.53	54.51	59.96	28.07	74.77
LA60-O	55.05	18.5	38.15	50.68	29.82	75.37
HA80	30.75	14.27	51.6	51.2	24.7	75.99
HA80-O	45.4	16.27	39.75	49.22	28.37	76.1
LA80	27.56	14.32	53.27	55.66	32.46	75.2
LA80-O	45.93	12.42	40.1	47.75	31.15	74.96

Integral values are measured against the phosphitylated internal standard.

References:

1. Jiang, Z., D.S. Argyropoulos, and A. Granata, *Correlation analysis of 31P NMR chemical shifts with substituent effects of phenols.* Magnetic Resonance in Chemistry, 1995. **33**(5): p. 375-382.