

Supporting Information

for

Photophysics and Stability of Cyano-Substituted Boradiazaindacene Dyes

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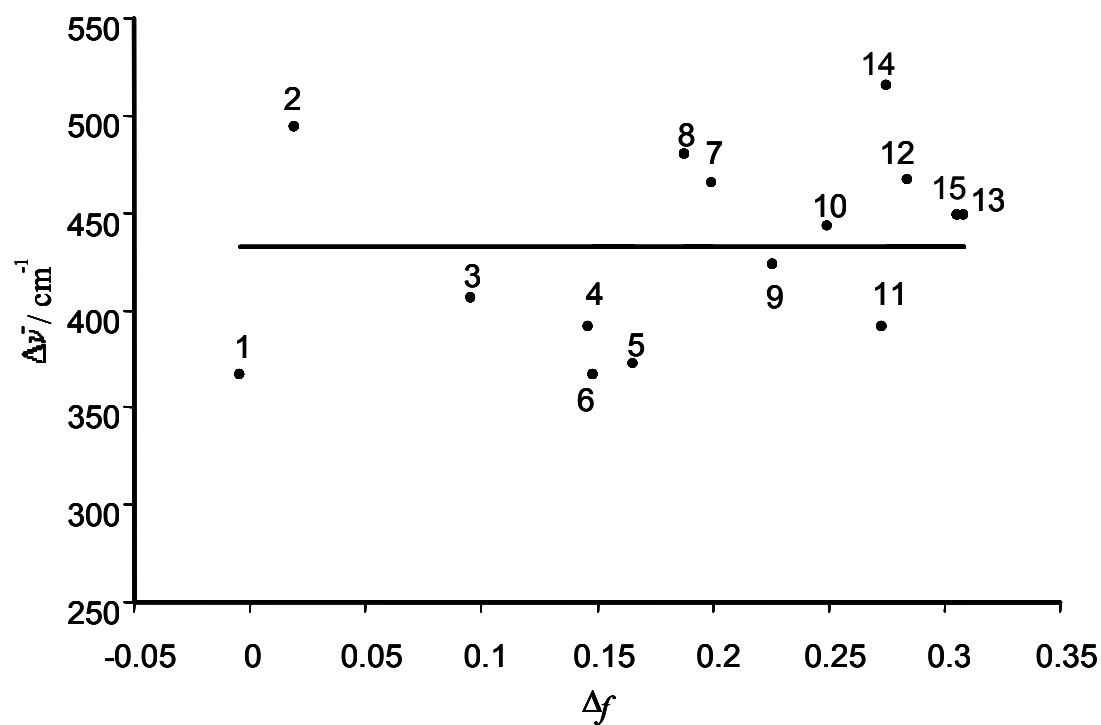


Figure S1. Plot of the Stokes shifts $\Delta\bar{\nu}$ of **4CN** for the solvents of Table 1 versus the Lippert solvent parameter $\Delta f = f(\epsilon) - f(n^2)$. The numbers refer to the solvents of Table 1. The straight line represents the average value of $\Delta\bar{\nu} = (4.3 \pm 0.5) \times 10^2 \text{ cm}^{-1}$.

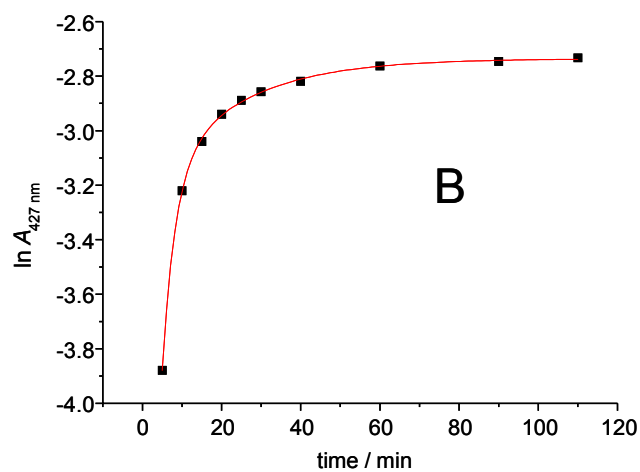
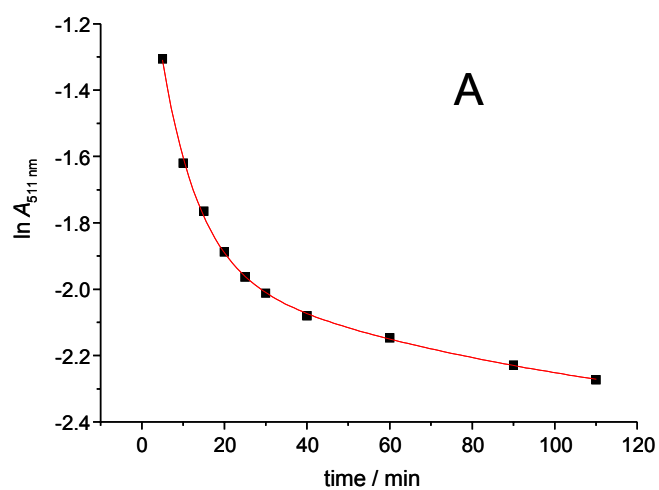


Figure S2. 4CN in acetone. (A) Biexponential fit to $\ln A_{511 \text{ nm}}$ as a function of the ageing time. (B) Biexponential fit to $\ln A_{427 \text{ nm}}$ as a function of the ageing time.

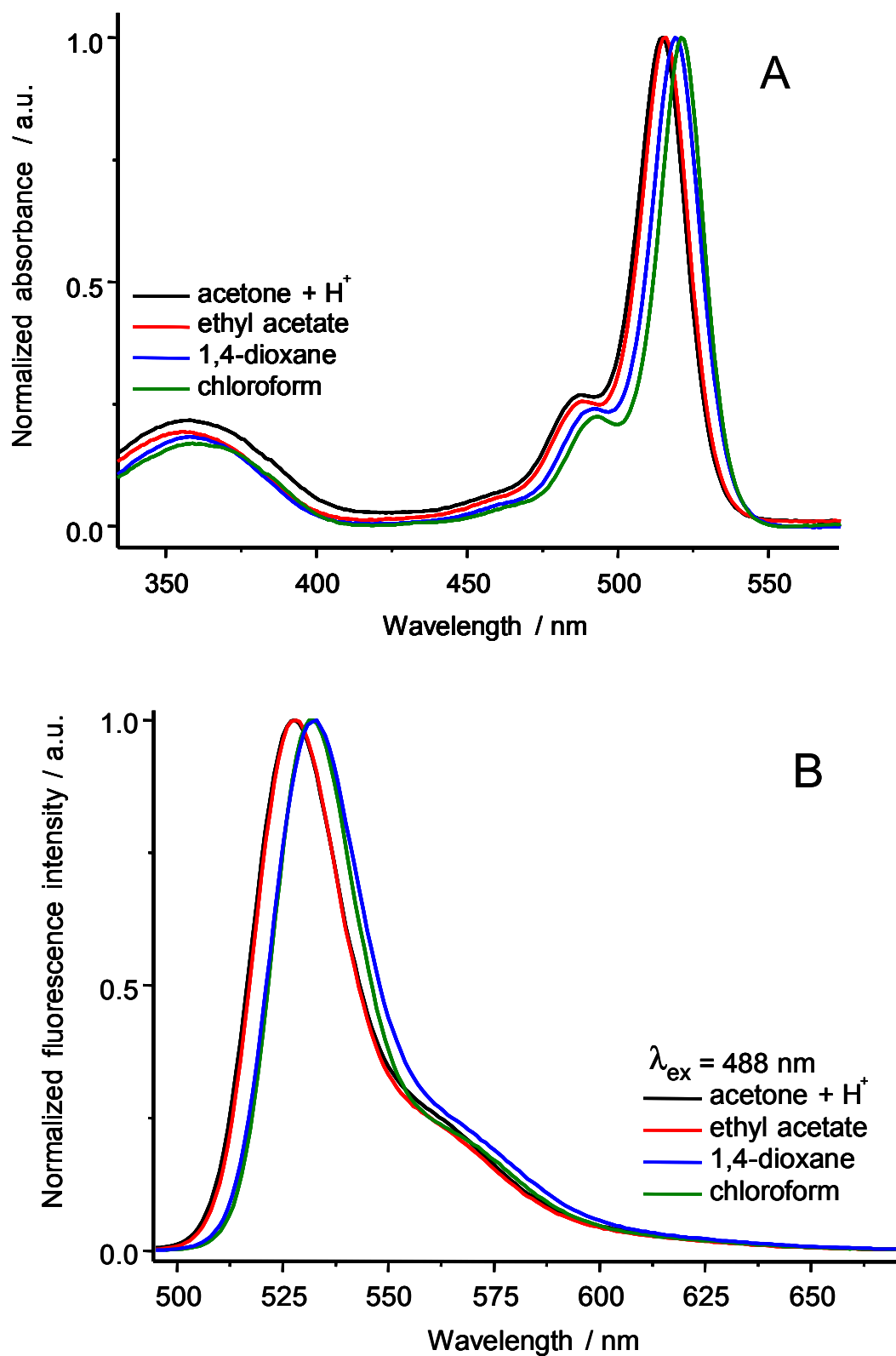


Figure S3. (A) Absorption spectra of 2CN in different solvents normalized to 1.0. (B) Corresponding normalized fluorescence emission spectra ($\lambda_{ex} = 488 \text{ nm}$). Because all the spectra have similar shapes and for better clarity, only a limited number of spectra are shown.

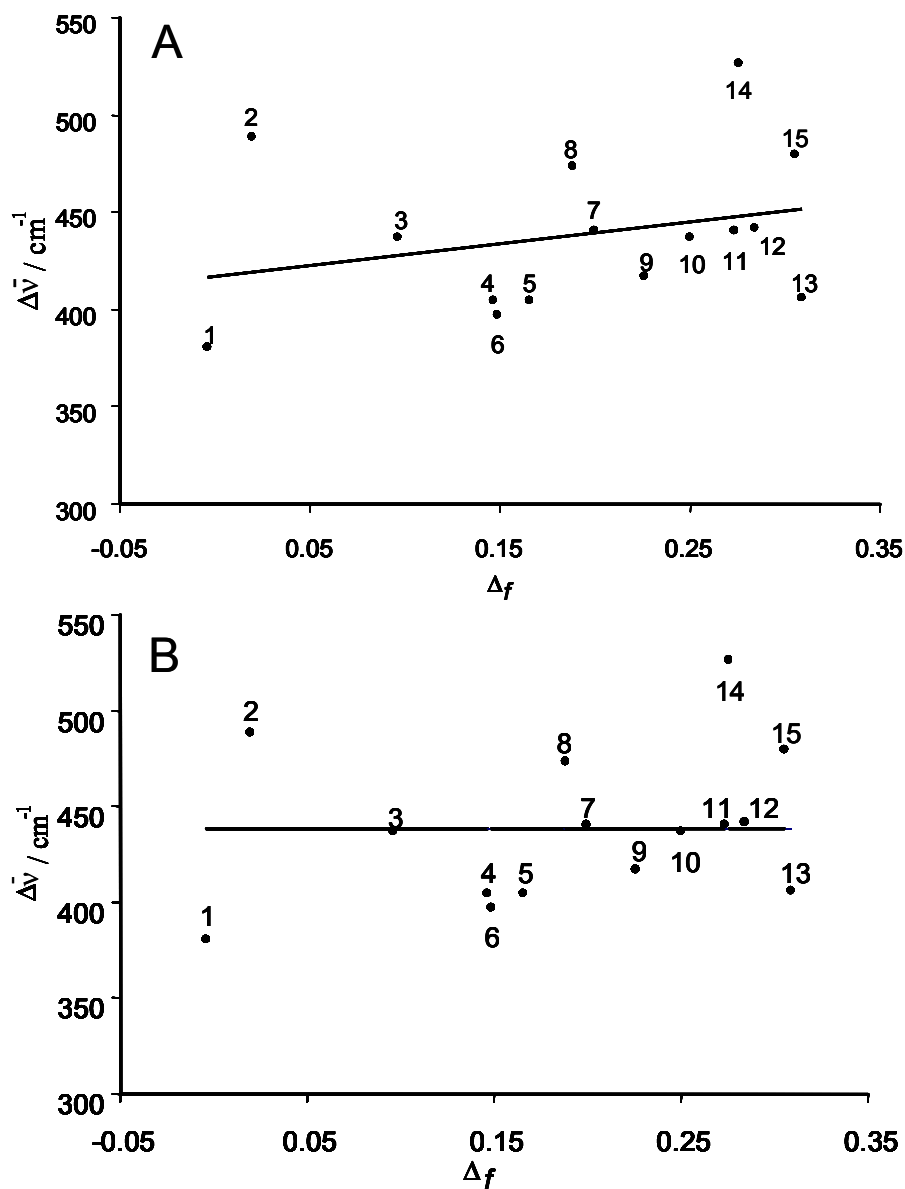


Figure S4. Plots of the Stokes shifts $\Delta\bar{\nu}$ (in cm^{-1}) of **2CN** versus the Lippert solvent parameter $\Delta f = f(\epsilon) - f(n^2)$. The numbers refer to the solvents of Table 3. (A) The straight line represents the best fit to the data: $r = 0.274$, slope = $(1.1 \pm 1.0) \times 10^2 \text{ cm}^{-1}$, intercept = $(4.2 \pm 0.2) \times 10^2 \text{ cm}^{-1}$. (B) The straight line represents the average value of $\Delta\bar{\nu} = (4.4 \pm 0.4) \times 10^2 \text{ cm}^{-1}$.

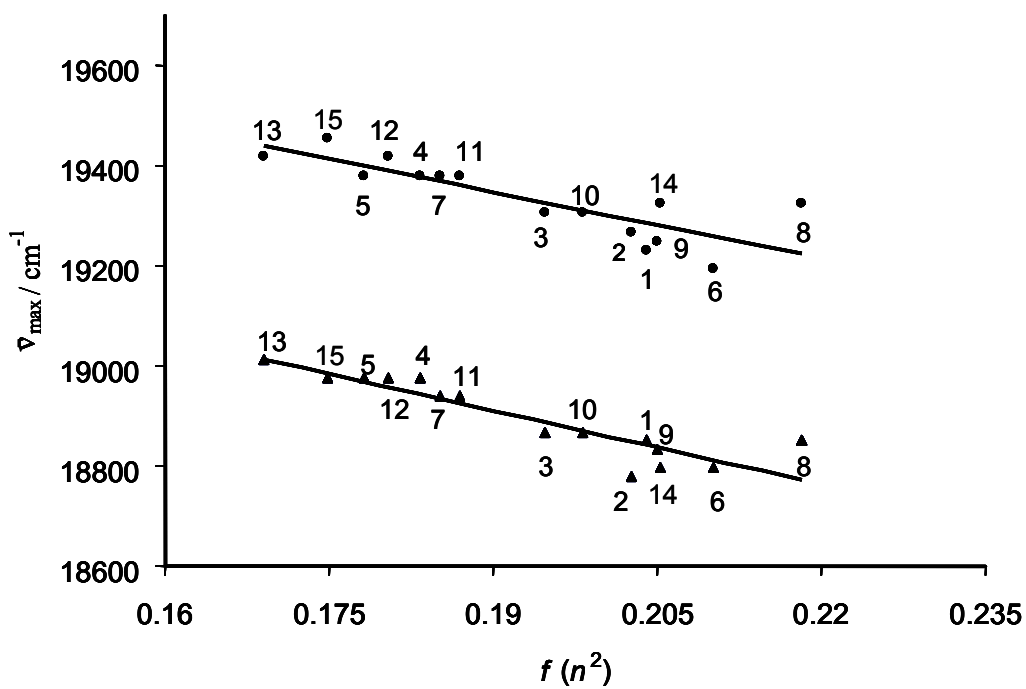


Figure S5. Plots of the experimental $\bar{\nu}_{\text{abs}}$ and $\bar{\nu}_{\text{em}}$ (both in cm^{-1}) of **2CN** as a function of $f(n^2)$. The numbers refer to the solvents of Table 3. The straight lines represent the best fits to $\bar{\nu}_{\text{abs}}$ [$r = 0.830$, slope = $(-4.4 \pm 0.8) \times 10^3 \text{ cm}^{-1}$, intercept = $(20.2 \pm 0.2) \times 10^3 \text{ cm}^{-1}$] and $\bar{\nu}_{\text{em}}$ [$r = 0.910$, slope = $(-4.9 \pm 0.6) \times 10^3 \text{ cm}^{-1}$, intercept = $(19.8 \pm 0.1) \times 10^3 \text{ cm}^{-1}$].

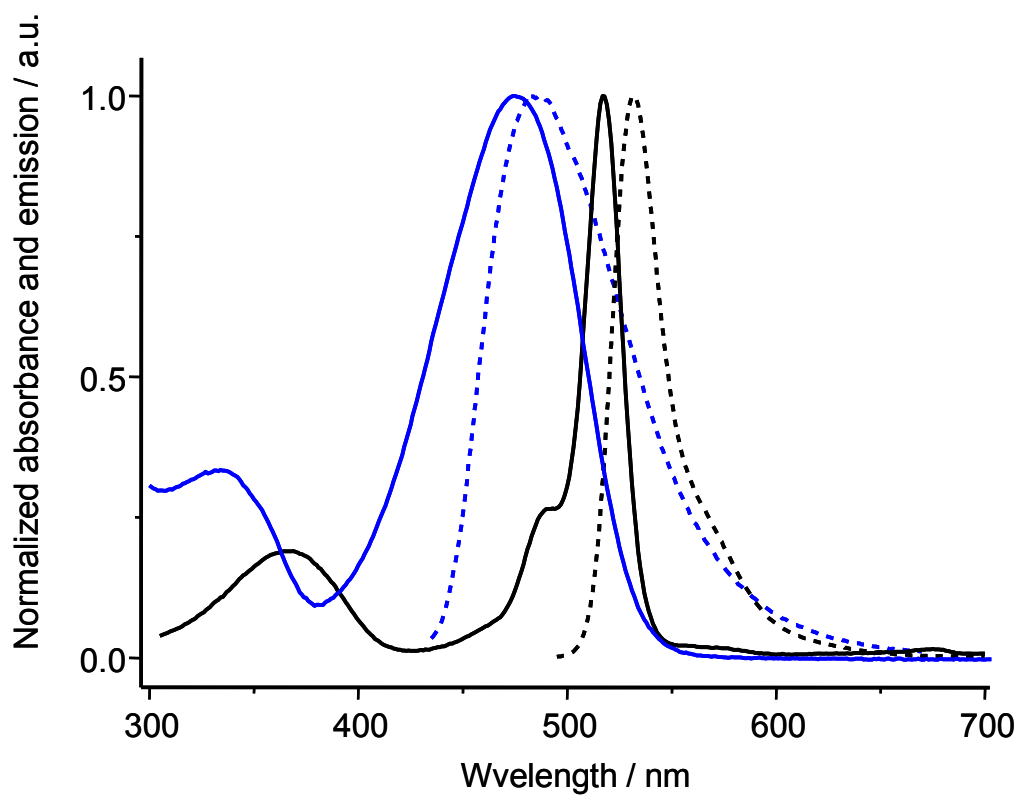


Figure S6. Normalized absorption spectra of **2CN** in DMF (blue solid line) and in DMF + H⁺ (black solid line). Corresponding normalized fluorescence emission spectra of **2CN** in DMF ($\lambda_{\text{ex}} = 430$ nm, blue dotted line) and in DMF + H⁺ ($\lambda_{\text{ex}} = 488$ nm, black dotted line).

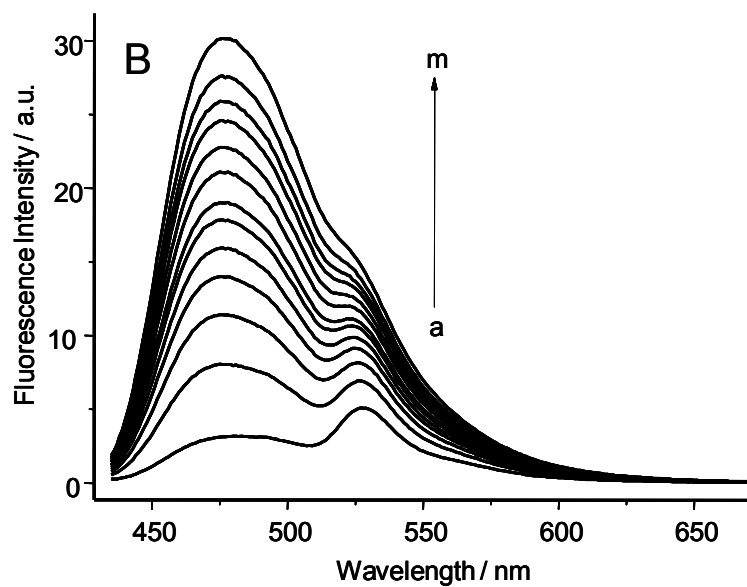
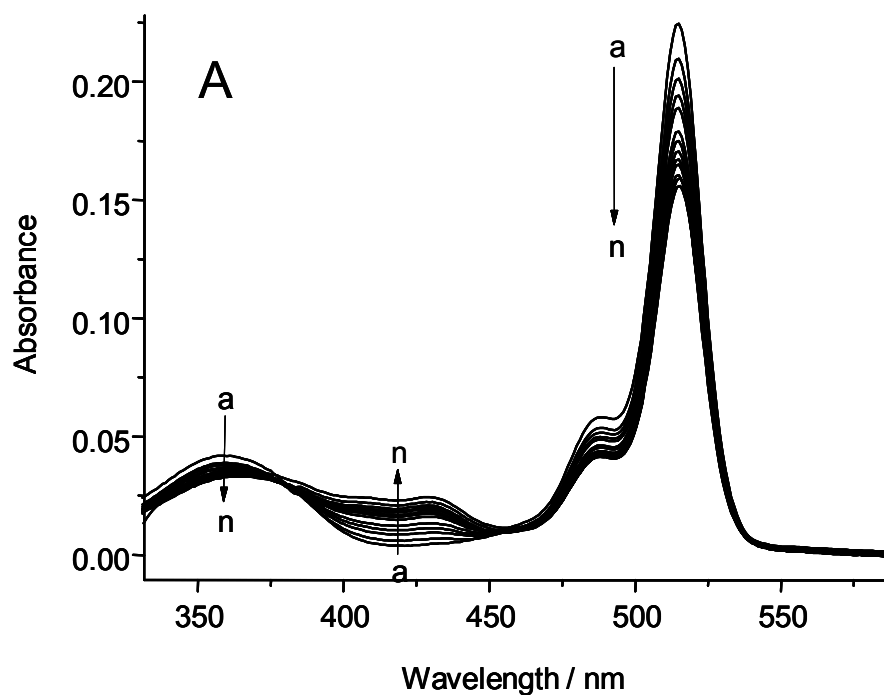


Figure S7. (A) Absorption spectra of **2CN** in acetone for different ageing times: 5' (a), 10' (b), 15' (c), 20' (d), 30' (e), 40' (f), 50' (g), 60' (h), 70' (i), 85' (j), 100' (k), 115' (l), 135' (m), 195' (n).

(B) Fluorescence emission spectra ($\lambda_{\text{ex}} = 430 \text{ nm}$) of **2CN** in acetone for different ageing times: 5' (a), 10' (b), 15' (c), 20' (d), 25' (e), 30' (f), 35' (g), 45' (h), 55' (i), 70' (j), 85' (k), 115' (l), 175' (m).