

Supporting Information

Fundamental aspects of property tuning in push-pull molecules

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1. Correlations

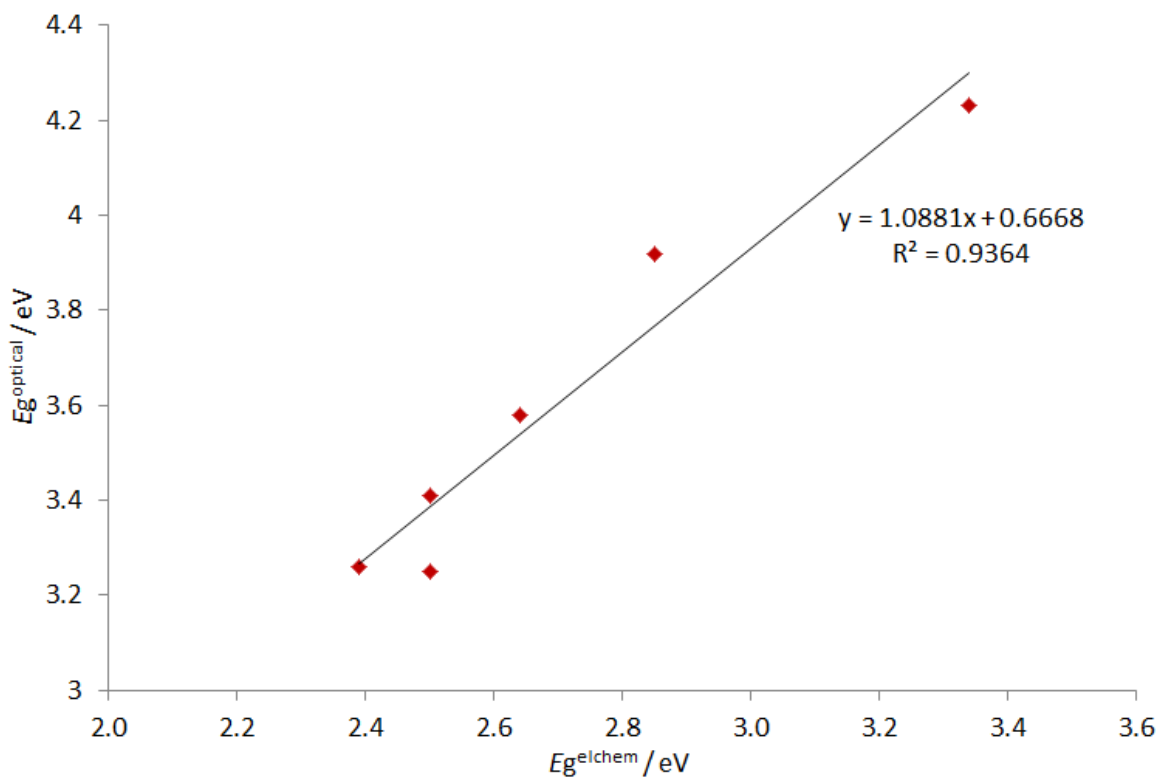


Fig. S1 Correlation of the optical and electrochemical gaps in molecules **1c-6c** (Ref.¹)

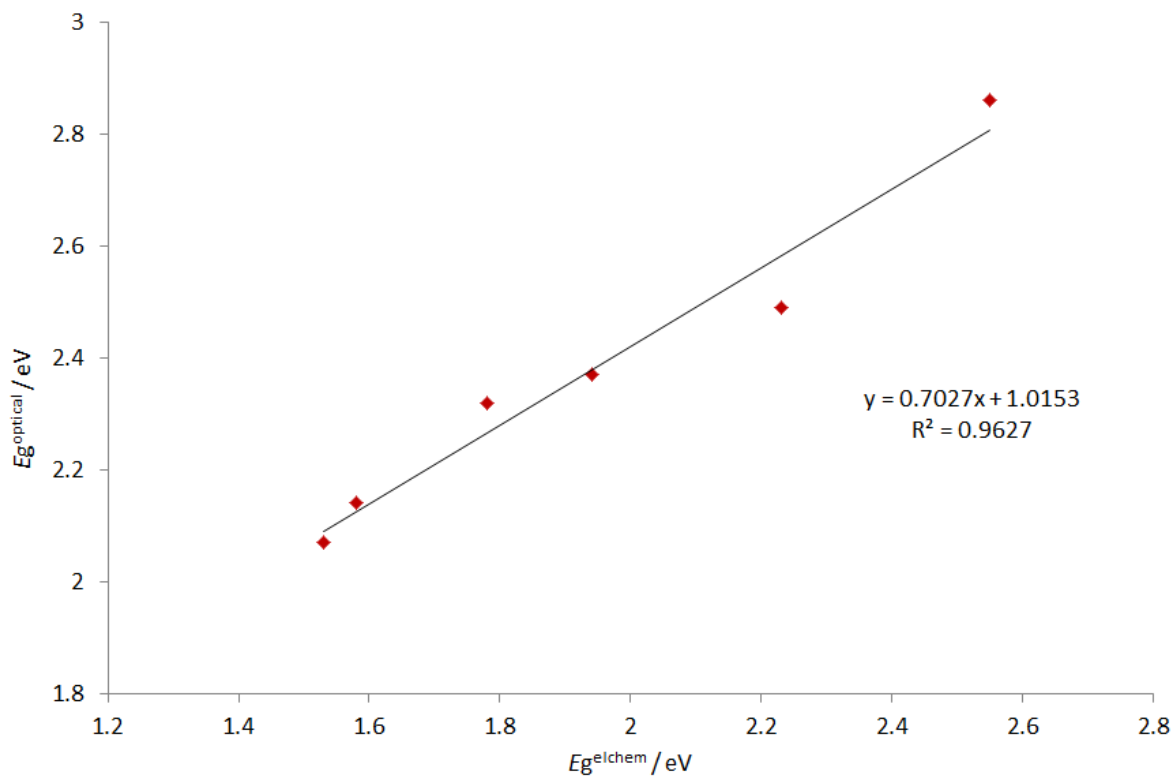


Fig. S2 Correlation of the optical and electrochemical gaps in molecules **19a-19f** (Ref.²)

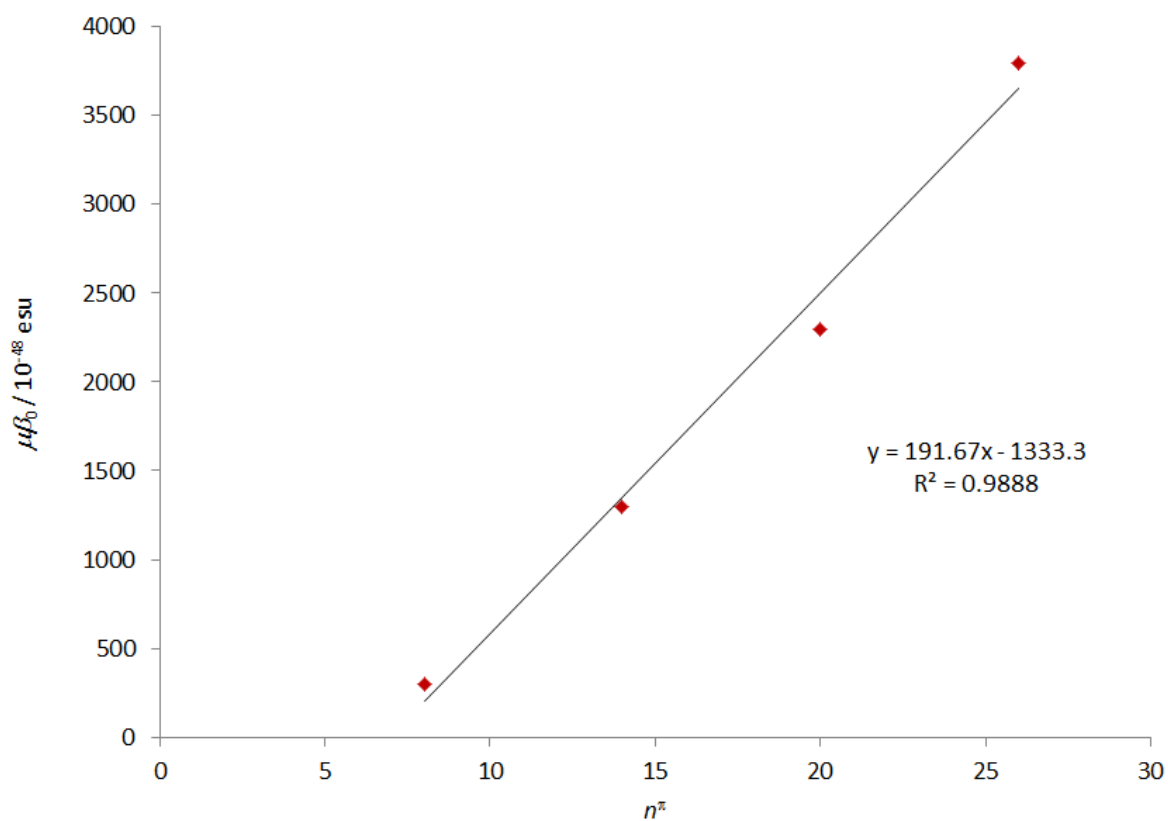


Fig. S3 Correlation of the NLO response ($\mu\beta$ product) vs. number of π -electrons in **22b-c** (Ref.³)

2. References

- 1 J. Kulhánek, F. Bureš, O. Pytela, T. Mikysek, J. Ludvík and A. Růžička, *Dyes Pigm.*, 2010, **85**, 57.
- 2 F. Bureš, W. B. Schweizer, J. C. May, C. Boudon, J.-P. Gisselbrecht, M. Gross, I. Biaggio and F. Diederich, *Chem. Eur. J.*, 2007, **13**, 5378.
- 3 A. K.-Y. Jen, V. P. Rao, K. Y. Wong and K. J. Drost, *J. Chem. Soc., Chem. Commun.*, 1993, 90.