

Electronic supplementary information

Stereoselective synthesis and properties of 1,3-bis(dicyanomethylidene)indane-5-carboxylic acid acceptor fragment containing nonlinear optical chromophores

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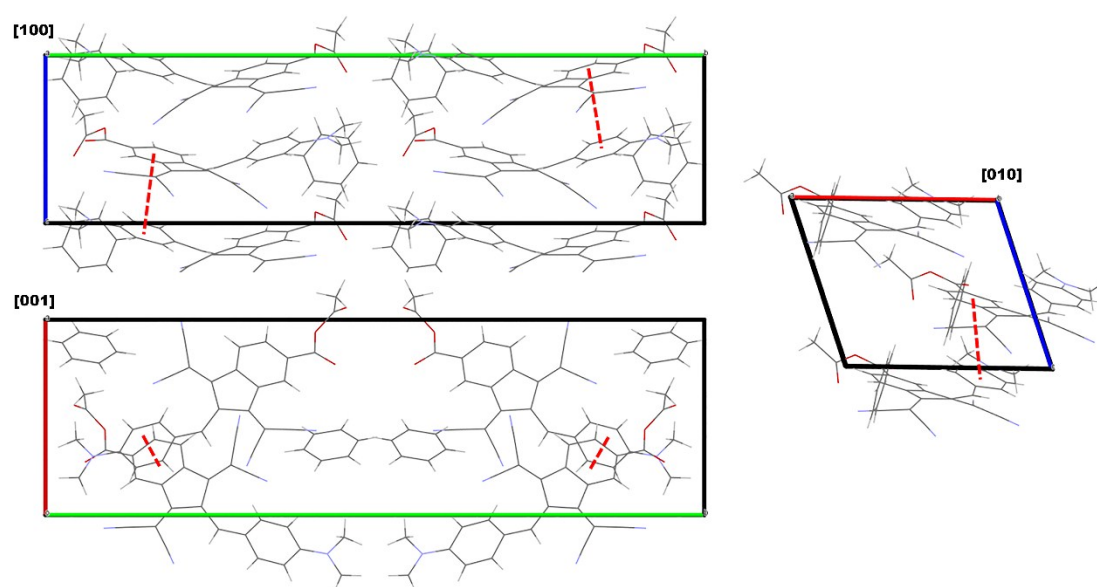


Figure S1. Crystal packing of **7b** viewed along different crystallographic directions. Red dashed lines indicate π - π stacking.

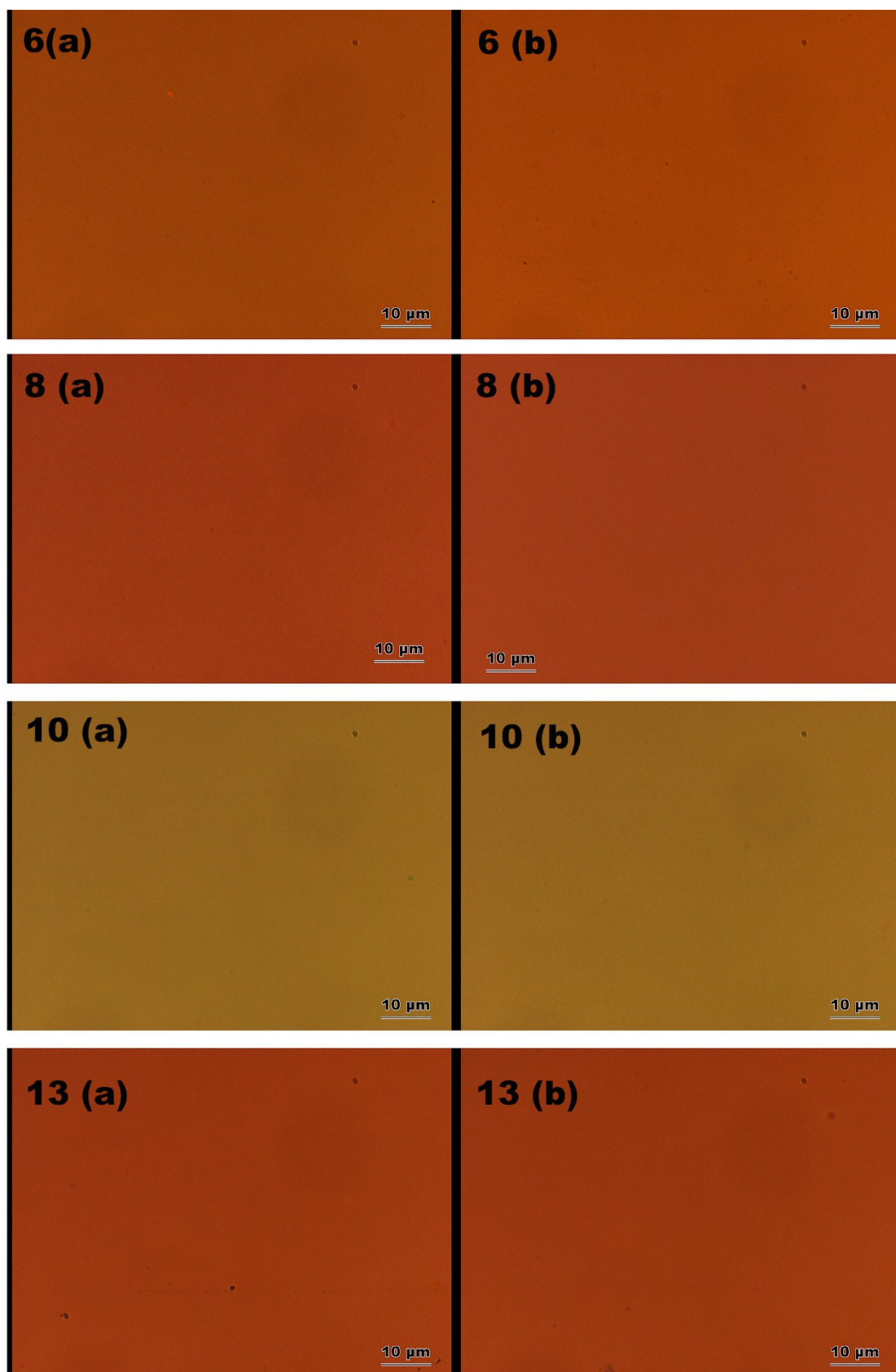


Figure S2. Optical microscope images of freshly cast (a) and 10-12 months stored spin-cast film samples previously used in NLO measurements (b).

Atomic coordinates for geometrically optimized structures used in performed quantum chemical calculations:

Compound 6:

| | | | |
|---|----------|----------|----------|
| C | -3.63367 | 1.91917 | -0.06642 |
| C | -4.15204 | 0.61917 | -0.13308 |
| C | -3.30538 | -0.49007 | -0.15917 |
| C | -5.63643 | 0.47802 | -0.17343 |
| C | -1.94246 | -0.25592 | -0.11755 |
| C | -1.42964 | 1.03538 | -0.05278 |
| C | -2.26334 | 2.14193 | -0.02619 |
| C | 0.06793 | 0.99621 | -0.02072 |
| C | 0.44500 | -0.43272 | -0.06999 |
| C | -0.81245 | -1.22925 | -0.13053 |
| C | 1.63152 | -1.09485 | -0.06984 |
| C | 3.01048 | -0.69169 | -0.02432 |
| C | 3.46937 | 0.63853 | 0.03481 |
| C | 4.81485 | 0.92835 | 0.07366 |
| C | 5.78984 | -0.09529 | 0.05648 |
| C | 5.33388 | -1.43118 | -0.00302 |
| C | 3.98571 | -1.70635 | -0.04163 |
| N | 7.12605 | 0.19700 | 0.09613 |
| C | 7.56879 | 1.57588 | 0.14821 |
| C | 8.10563 | -0.86983 | 0.07357 |
| O | 0.76603 | 1.99444 | 0.03531 |
| O | -0.91149 | -2.43939 | -0.18099 |
| O | -6.40428 | 1.41369 | -0.14381 |
| O | -6.02480 | -0.80273 | -0.25104 |
| C | -7.44401 | -1.04045 | -0.29394 |
| C | -8.04232 | -1.04302 | 1.09771 |
| H | -9.10355 | -1.30096 | 1.04468 |
| H | -4.33816 | 2.74293 | -0.04810 |
| H | -3.69961 | -1.49744 | -0.20985 |
| H | 7.23654 | 2.14375 | -0.72867 |
| H | 8.65721 | 1.60134 | 0.17178 |
| H | 7.19968 | 2.08793 | 1.04438 |
| H | 8.03557 | -1.46889 | -0.84220 |
| H | 7.99216 | -1.54426 | 0.93047 |
| H | 9.10505 | -0.43951 | 0.11673 |
| H | -7.54151 | -2.01478 | -0.77517 |
| H | -7.90756 | -0.27711 | -0.92135 |
| H | -7.95169 | -0.05593 | 1.55422 |
| H | -7.54142 | -1.77701 | 1.73329 |
| H | 1.48636 | -2.17602 | -0.11554 |
| H | -1.84744 | 3.14203 | 0.02459 |
| H | 2.74422 | 1.44327 | 0.04955 |
| H | 5.11824 | 1.96580 | 0.11831 |
| H | 6.03862 | -2.25150 | -0.01947 |
| H | 3.66377 | -2.74285 | -0.08736 |

Compound 8:

| | | | |
|---|----------|----------|----------|
| C | -3.22562 | -2.37205 | -0.28218 |
| C | -3.90055 | -1.15739 | -0.39226 |
| C | -3.25088 | 0.04886 | -0.13591 |
| C | -5.33870 | -1.19745 | -0.79519 |
| C | -1.90946 | 0.01715 | 0.22281 |
| C | -1.23122 | -1.21271 | 0.33587 |
| C | -1.88856 | -2.41271 | 0.08899 |
| C | 0.15641 | -0.94102 | 0.74947 |
| C | 0.37330 | 0.50124 | 0.56829 |

| | | | |
|---|----------|----------|----------|
| C | -0.96951 | 1.11356 | 0.52455 |
| C | 1.51589 | 1.19732 | 0.28893 |
| C | 2.83716 | 0.79671 | -0.11349 |
| C | 3.17712 | -0.44645 | -0.67802 |
| C | 4.45527 | -0.72454 | -1.09846 |
| C | 5.49390 | 0.22739 | -0.95702 |
| C | 5.15351 | 1.48830 | -0.41679 |
| C | 3.86170 | 1.75831 | -0.03002 |
| N | 6.77061 | -0.05791 | -1.34343 |
| C | 7.09799 | -1.36693 | -1.87563 |
| C | 7.81930 | 0.93022 | -1.17776 |
| C | 0.98236 | -1.81653 | 1.39439 |
| C | -1.30741 | 2.41832 | 0.75099 |
| O | -5.94573 | -2.22044 | -1.01468 |
| O | -5.87339 | 0.02296 | -0.88315 |
| C | -7.26550 | 0.08256 | -1.24688 |
| C | -7.65107 | 1.54134 | -1.30978 |
| H | -8.70872 | 1.63380 | -1.56861 |
| H | -3.77233 | -3.28324 | -0.49558 |
| H | -3.80188 | 0.97287 | -0.23104 |
| H | 6.87308 | -2.16373 | -1.15776 |
| H | 8.16296 | -1.40570 | -2.09802 |
| H | 6.55296 | -1.57629 | -2.80322 |
| H | 7.94358 | 1.21668 | -0.12722 |
| H | 7.61683 | 1.83694 | -1.75901 |
| H | 8.76226 | 0.51265 | -1.52649 |
| H | -7.84287 | -0.46812 | -0.49956 |
| H | -7.39736 | -0.42570 | -2.20557 |
| H | -7.06355 | 2.06724 | -2.06544 |
| H | -7.48529 | 2.02956 | -0.34714 |
| H | 1.40355 | 2.27573 | 0.29637 |
| H | -1.38001 | -3.36353 | 0.16916 |
| H | 2.41309 | -1.20134 | -0.81953 |
| H | 4.65874 | -1.69024 | -1.54045 |
| H | 5.90425 | 2.25885 | -0.30856 |
| H | 3.62727 | 2.74051 | 0.37005 |
| C | -2.65150 | 2.90173 | 0.67113 |
| C | -0.36202 | 3.42227 | 1.13205 |
| N | 0.38768 | 4.25059 | 1.43601 |
| N | -3.72809 | 3.32314 | 0.61154 |
| C | 2.19662 | -1.41446 | 2.03298 |
| C | 0.65702 | -3.19887 | 1.56994 |
| N | 3.16916 | -1.11966 | 2.58619 |
| N | 0.41966 | -4.32362 | 1.70601 |

Compound 10:

| | | | |
|---|----------|----------|----------|
| C | -3.39350 | 2.29736 | -0.42661 |
| C | -3.99815 | 1.04049 | -0.41076 |
| C | -3.26225 | -0.10366 | -0.11119 |
| C | -5.45621 | 0.97021 | -0.73168 |
| C | -1.90819 | 0.03083 | 0.17033 |
| C | -1.30105 | 1.30652 | 0.16690 |
| C | -2.04526 | 2.44328 | -0.13300 |
| C | 0.11548 | 1.16618 | 0.53822 |
| C | 0.41862 | -0.28823 | 0.45545 |
| C | -0.89341 | -0.98379 | 0.47189 |
| N | 1.48033 | -0.98876 | 0.31462 |
| C | 2.76895 | -0.68305 | -0.03227 |
| C | 3.19144 | 0.45936 | -0.73858 |
| C | 4.50104 | 0.61047 | -1.12689 |
| C | 5.47943 | -0.35673 | -0.79015 |

| | | | |
|---|----------|----------|----------|
| C | 5.04875 | -1.51457 | -0.10092 |
| C | 3.72636 | -1.67956 | 0.23465 |
| N | 6.78817 | -0.18494 | -1.13716 |
| C | 7.20898 | 1.01591 | -1.83241 |
| C | 7.77117 | -1.19400 | -0.79220 |
| C | 0.90169 | 2.12944 | 1.09642 |
| C | -1.06081 | -2.31303 | 0.69874 |
| O | -6.12910 | 1.93796 | -1.00307 |
| O | -5.92536 | -0.27835 | -0.68271 |
| C | -7.32821 | -0.44176 | -0.96709 |
| C | -7.64150 | -1.91460 | -0.85292 |
| H | -8.70200 | -2.08361 | -1.05509 |
| H | -4.00570 | 3.15696 | -0.67355 |
| H | -3.75533 | -1.06534 | -0.11000 |
| H | 6.73169 | 1.10619 | -2.81528 |
| H | 8.28627 | 0.98126 | -1.98561 |
| H | 6.97898 | 1.91819 | -1.25484 |
| H | 7.54753 | -2.15688 | -1.26546 |
| H | 7.82730 | -1.34948 | 0.29110 |
| H | 8.75173 | -0.87024 | -1.13696 |
| H | -7.52808 | -0.04923 | -1.96750 |
| H | -7.89846 | 0.16153 | -0.25597 |
| H | -7.41673 | -2.28387 | 0.14986 |
| H | -7.05639 | -2.49432 | -1.57000 |
| H | -1.59410 | 3.42586 | -0.14928 |
| H | 2.47008 | 1.21528 | -1.02732 |
| H | 4.77744 | 1.48962 | -1.69264 |
| H | 5.75386 | -2.29446 | 0.15159 |
| H | 3.38863 | -2.58269 | 0.73142 |
| C | -2.35242 | -2.93053 | 0.69076 |
| C | 0.01333 | -3.21796 | 0.99510 |
| N | 0.79328 | -4.03257 | 1.25312 |
| N | -3.39262 | -3.43811 | 0.68395 |
| C | 2.15808 | 1.85013 | 1.71904 |
| C | 0.48463 | 3.49461 | 1.20956 |
| N | 3.15866 | 1.65846 | 2.26724 |
| N | 0.17174 | 4.60568 | 1.29243 |