*Table S2* CAM-B3LYP/6-311+G(d) results for the total electric dipole (in D), static linear polarizability , first static hyperpolarizability and second static hyperpolarizability for DFC in several medium solvent.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Solvent Medium |  |  |  |  |
| Gas phase | 4.39 | 36.41 | -8.97 | 108.74 |
| Argon | 4.71 | 38.77 | -11.88 | 138.95 |
| Heptane | 4.95 | 40.55 | -14.24 | 164.57 |
| Toluene | 5.10 | 41.78 | -15.92 | 183.62 |
| Chloroform | 5.50 | 44.95 | -20.42 | 237.63 |
| ChloroBenzene | 5.58 | 45.63 | -21.40 | 250.08 |
| TetraHydroFuran | 5.68 | 46.45 | -22.58 | 265.40 |
| Dichloromethane | 5.73 | 46.93 | -23.27 | 274.63 |
| DiChloroEthane | 5.77 | 47.22 | -23.69 | 280.28 |
| 2-Methyl-2-Propanol | 5.82 | 47.65 | -24.31 | 288.58 |
| 1-Butanol | 5.88 | 48.19 | -25.08 | 299.26 |
| Acetone | 5.91 | 48.41 | -25.40 | 303.68 |
| Ethanol | 5.93 | 48.63 | -25.71 | 308.05 |
| Methanol | 5.96 | 48.88 | -26.06 | 313.07 |
| Acetonitrile | 5.97 | 48.95 | -26.16 | 314.48 |
| dmso | 5.99 | 49.13 | -26.41 | 318.09 |
| FormicAcid | 6.00 | 49.18 | -26.48 | 319.07 |
| Water | 6.02 | 49.36 | -26.74 | 322.87 |
| Formamide | 6.03 | 49.46 | -26.88 | 324.90 |
| n-MethylFormamide-mixture | 6.04 | 49.57 | -27.02 | 327.00 |

*Table S3*: CAM-B3LYP/6-311+G(d) results for the total electric dipole (in D), static linear polarizability , first static hyperpolarizability and second static hyperpolarizability for DFC in several medium solvent for

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |
| Gas phase | 42.57 | -32.13 | 107.18 | 346.13 | 63.21 |
| Argon | 46.07 | -44.95 | 126.46 | 484.24 | -191.13 |
| Heptane | 48.84 | -56.57 | 143.69 | 615.54 | -490.48 |
| Toluene | 50.23 | -63.94 | 152.51 | 702.75 | -668.36 |
| Chloroform | 50.29 | -73.04 | 148.31 | 822.90 | -604.11 |
| ChloroBenzene | 51.24 | -78.14 | 155.11 | 886.98 | -740.53 |
| TetraHydroFuran | 50.10 | -76.26 | 144.52 | 869.23 | -531.36 |
| Dichloromethane | 50.40 | -78.58 | 146.36 | 899.81 | -565.91 |
| DiChloroEthane | 50.68 | -80.37 | 148.30 | 923.01 | -602.96 |
| 2-Methyl-2-Propanol | 50.09 | -79.22 | 142.90 | 911.79 | -497.83 |
| 1-Butanol | 50.31 | -81.38 | 144.06 | 941.16 | -517.85 |
| Acetone | 49.85 | -80.14 | 140.03 | 927.50 | -441.31 |
| Ethanol | 49.92 | -80.89 | 140.28 | 937.89 | -444.93 |
| Methanol | 49.54 | -79.99 | 136.89 | 928.58 | -381.68 |
| Acetonitrile | 49.75 | -80.97 | 138.51 | 940.85 | -410.79 |
| Dmso | 50.67 | -85.00 | 145.82 | 991.30 | -546.94 |
| FormicAcid | 50.13 | -82.96 | 141.31 | 966.64 | -461.52 |
| Water | 49.67 | -81.58 | 137.40 | 950.90 | -388.63 |
| Formamide | 51.08 | -87.39 | 148.76 | 1022.95 | -601.50 |
| n-MethylFormamide-mixture | 50.92 | -86.99 | 147.32 | 1018.71 | -573.07 |