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Supplementary information:

Electron Correlation Effects and Dipolar/Octupolar Contribution on the First Hyperpolarizability of Push–Pull Oligomer Systems

Información Suplementaria:

Efectos de Correlación Electrónica y Contribución Dipolar/Octupolar en la Primera Hiperpolarizabilidad de Sistemas Push–Pull Oligómeros

N.S. LABIDI

Department of Matter Sciences, Institute of Sciences and Technology.
University center of Tamanghasset 11000, Algeria
labidi19722004@yahoo.fr

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Table S1: Selected Distances (Å) and torsion Angles (°).Calculated at the B3LYP/6-311G* level for the trans α,ω-nitro,dimethylamino-hexatriene

Parameters	Value
C1-C3	1.366
C3-C5	1.425
C5-C7	1.363
C7-C9	1.426
C9-C11	1.349
C11-N13	1.439
C1-N16	1.358
N13-O14	1.232
N13-O15	1.233
N16-C17	1.454
N16-C21	1.452
θ(C1-C3-C5)	121.6
A(C3-C5-C7)	125.9
θ(C5-C7-C9)	122.6
θ(C7-C9-C11)	125.1
θ(C9-C11-N13)	121.2
θ(C1-N16-C17)	120.1
θ(C1-N16-C21)	120.3
θ(H2-C1-C3)	118.5
θ(H2-C1-N16)	113.8
θ(C3-C1-N16)	127.7
θ(C11-N13-014)	119.5
θ(C11-N13-015)	116.2
θ(C1-C3-H4)	120.6
θ(C3-C5-H6)	116.7
θ(C5-C7-H8)	119.3
θ(C7-C9-H10)	118.3
θ(C9-C11-H12)	126.3
θ(O14-N13-O15)	124.3
θ(C17-N16-C21)	117.2
θ(C1-C3-C5-C7)	180.0
θ(C11-C9-C7-C5)	-179.9

θ(N16-C1-C3-C7)	176.9
θ(N13-C11-C9-C7)	180.0
Energy (a.u.)	-572.0239063
μ (Debye)	11.94

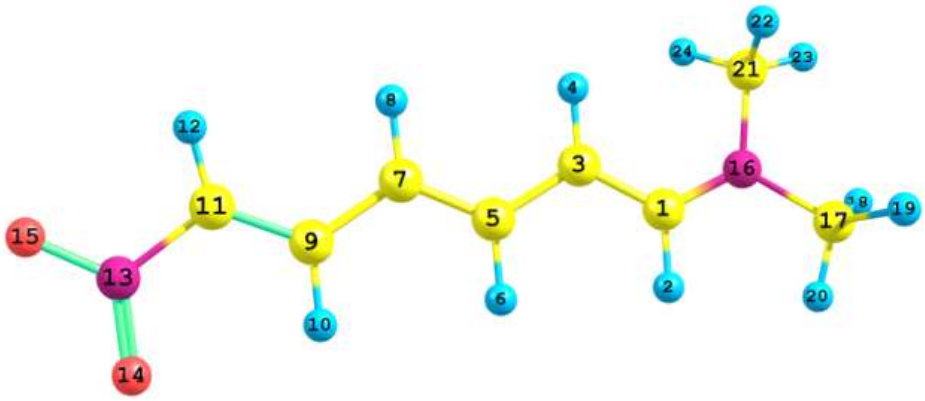


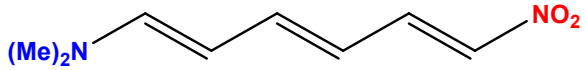
Table S2. Basis set effects on the DFT/ B3LYP static and dynamic first hyperpolarizabilities β_{HRS}, $\beta_{//}$, βvec and depolarization ratios (DR) of trans α,ω-nitro,dimethylamino-hexatriene with taking into account the effects of the solvent using the IEFPCM scheme. The β values are given in atomic units (a.u).

Basis set	IEFPCM (acetonitrile)			
	Static (ω=0)			
	β_{VEC}	$\beta_{//}$	β_{HRS}	DR
6-31G*	27163	16262	11442	4.73
6-311G*	28478	17046	12032	4.68
6-311G**	28526	17072	12058	4.68
6-31+G*	31706	18932	13433	4.64
6-311+G*	39039	23371	16433	4.74
6-311+G**	39038	23366	16440	4.73
cc-pVDZ	25425	15218	10747	4.68
cc-pVTZ	30486	18257	12868	4.70
aug-cc-pVTZ	37465	22445	15734	4.77
Basis set	Dynamic (ω= 0.042824 a.u.)			
	β_{VEC}	$\beta_{//}$	β_{HRS}	DR
6-31G*	34549	20709	14446	4.86
6-311G*	36842	22082	15431	4.84
6-311G**	37026	22190	15511	4.84
6-31+G*	58591	35076	24535	4.88
6-311+G*	54550	32697	22789	4.88
6-311+G**	54732	32803	22870	4.88
cc-pVDZ	32294	19356	13531	4.84
cc-pVTZ	40127	24057	16795	4.85
aug-cc-pVTZ	51608	30945	21542	4.89

Table S3. TDDFT calculated norm of the first hyperpolarizability (β_{vec}), the projection on the dipole moment ($\beta_{//}$), HRS first hyperpolarizability (β_{HRS}), depolarization ratio DR and tha anisotropy factor (ρ) for the trans α,ω-nitro,dimethylamino-hexatriene with taking into account the effects of the solvent (acetonitrile) using the IEFPCM scheme at different levels of approximation. All β values are in (a.u.).

Methods	IEFPCM (acetonitrile)				
	Static (ω=0)				
	β_{VEC}	β//	β_{HRS}	DR	ρ
HF	21558	12698	9391	4.28	0.994
LC-BLYP	39558	23673	16653	4.74	0.877
B3LYP	31706	18932	13433	4.64	0.899
B3P86	31161	18613	13179	4.67	0.893
CAM-B3LYP	37610	22478	15879	4.70	0.887
M052X	35735	21357	15099	4.68	0.889
M05	29791	17723	12664	4.60	0.910
M062X	38248	22893	16118	4.72	0.880
BHandHLYP	33327	19871	14149	4.62	0.906
Methods	Dynamic (ω= 0.042824 a.u.)				
	β_{VEC}	β//	β_{HRS}	DR	ρ
HF	25561	15200	10886	4.63	0.903
LC-BLYP	55207	33085	23068	4.88	0.843
B3LYP	58591	35076	24535	4.88	0.844
B3P86	55219	33062	23104	4.88	0.843
CAM-B3LYP	59283	35505	24799	4.87	0.845
M052X	54495	32638	22807	4.87	0.846
M05	53867	32194	22573	4.85	0.850
M062X	59536	35683	24888	4.88	0.842
BHandHLYP	48532	29031	20367	4.83	0.854

Table S4. Contrast between dynamic (λ=1064) and static (λ=∞) calculated first hyperpolarizability ($\beta_{//}$), HRS response (β_{HRS}) and the depolarization ratio DR for all trans α,ω-nitro,dimethylamino-hexatriene at different levels of approximation. All β values are in (a.u.).

Method					
	(6-31+G*) Ratios				
	$\beta_{//\,(1064)}/\beta_{//\,(\infty)}$	$\beta^{HRS}_{(1064)}/\beta^{HRS}_{(\infty)}$	$DR_{(1064)}/DR_{(\infty)}$	β^{HRS}(MP2)/ β^{HRS} (X)	
				λ =1064nm	(λ =∞)
HF	1.78	1.74	1.07	2.39	2.39
MP2	1.78	1.74	1.07	1.00	1.00
SCS-MP2	1.78	1.74	1.07	0.97	0.97
LC-BLYP	0.44	0.44	1.01	1.34	0.34
B3LYP	2.68	2.63	1.07	1.14	1.73
B3P86	2.62	2.58	1.06	1.17	1.74
CAM-B3LYP	2.29	2.26	1.05	1.22	1.58
M052X	2.25	2.22	1.05	1.27	1.62
M05	2.63	2.57	1.07	1.26	1.87
M062X	2.26	2.24	1.04	1.20	1.54
BHandHLYP	2.17	2.14	1.05	1.41	1.74