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UV/Vis Absorption Spectroscopy Theoretical Calculations on Starburst Triphynylamines: A Review.

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Review Article

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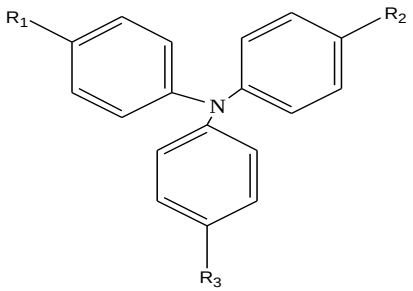
ABSTRACT

A nitrogen atom generally possess a pair of electrons on it in the outermost orbit. These electrons are not movable in inorganic compounds. But where as in the case of dendrimer which is conjugated big molecule is attached to a nitrogen atom then there is possibility of moving of electrons. This review article mainly focused on starburst triphenylamine derivatives and their UV/Vis absorption theoretical calculations were analyzed. The data on triphenylamine derivatives with different methods published over the last years are reviewed here for the first time by searching all chemistry journals. In the present survey of literature on triphenylamine derivatives emphasis mainly laid on title, author, comparison of experimental results with theoretical calculations and concerned references are summarized. This review article may be useful to chemists those who wish to do research on triphenylamine derivatives in general to synthetic chemists and in particular to theoretical chemists. For theoretical calculations the authors have mainly used the methods namely D.F.T, T.D-D.F.T, INDO/SCI, ZINDO/SDCI, AM 1, AFOT and B3LYP to calculate theoretical UV/Vis light absorption of triphenylamine derivatives.

INTRODUCTION

Conjugated polymers because of their unusual optical, electrical and electronic properties conjugated polymers containing electron donor-acceptor pairs have become an important area of study [1,2,3,4,5]. The family of triarylamines attracts us because of their excellent hole transporting properties. However, triphenylamine the smallest number in the family, is electrochemically active toward oxidation [6] and rarely used for device applications. During the past a few decades, polymeric optoelectronic devices based on conjugated or non-conjugated polymers have become extremely important areas of study [7]. The family of triarylamines attracts us because of their excellent electronic properties [8]. Starburst triarylamine derivatives have played an important role in recent electroluminesense applications and have been widely explored [9]. So far no attempt has been made on a review of triphynylamines. In the present survey of literature on triphenylamines emphasis laid mainly on title, author references, results of theoretical UV/Vis absorption are summarized in this review article.

UV/V is /NIR spectral properties of triarylamines and their corresponding radical cations, by Christoph Lambert et al [10].



Structure of Triphynylamine with functional groups

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Table 1: Spectral properties of Triphenylamine with their substituents are OMe, Me and Cl.

S.No	R_1	R_2	R_3	ν_{max} MeCN	ν_{max} CH_2Cl_2	V(theory)
1	OMe	OMe	OMe	33,780	33,330	32,100
2	Me	Me	Me	33,460	33,030	31,630
3	Me	OMe	OMe	33,820	33,280	31,920(32,060)
4	Me	Cl	Cl	33,230	32,890	30,900(32,090)
5	OMe	Me	Me	33,640	33,180	31,800(32,000)
6	OMe	Cl	Cl	33,370	33,090	30,750(32,150)
7	Cl	Me	Me	33,490	33,080	31,130(32,260)
8	Cl	OMe	OMe	33,980	33,340	30,760(32,180)
9	Cl	Cl	Cl	32,900	32,530	31,380
10	Cl	OMe	Me	33,760	33,300	30,950(32,260)

For theoretical calculations in this paper, used AM1-CSID with Gaussian '98 programme.

Theoretical study on Photophysical and charge transport properties of 1,6- Bis(2-hydroxyphenol) pyridylboron bis(4-n-butylphenyl)phenyleneamine compound, by Yue Wang et al [11].

Table 2: (DPPY) BTPA UV light absorption

Compound	Experimental(nm)	Theoretical(nm)
(dppy)BTPA UV Light absorption	304	312
	375	384

These calculations were carried out with Time Dependent Density Functional theory (TD-DFT).

Joint Theoretical and experimental Characterization of the structrural and Electronic properties of Poly(dioctylfluorene-alt-N-butyl diphenylamine), by Bredas et al [12].

Graphical comparison of experimental and calculated absorption spectrum.

They were used INDO/SCI for theoretical calculations.

Charge transfer transitions in Triaryamine Mixed-valence Systems: A Joint Density functional theory and Vibronic coupling study, by Bredas et al [13].

Graphical comparison of experimental and calculated absorption spectrum.

Dications of Bis-triarylamino-[2.2] paracyclophanes: Evaluation of Excitated state couplings by GMH Analysis, by Christoph Lambert et al [14].

Table 3: Dications of Bis-triarylamino-[2.2] paracyclophanes light absorption

Dication	v/cm^{-1}(Theo)	v/cm^{-1}(Exp)
1^{2+}	14100	13090
2^{+}	15740	13400
3^{+}	14460	13260
4^{2+}	14540	13300
5^{2+}	14490	13260
6^{2+}	14520	13160
7^{+}	14970	13440
8^{+}	15500	13050
9^{2+}	14390	13000

The theoretical values are higher than experimental values in the case of pi and pi* transitions are occurred. When CT bridge transitions are occurred the theoretical values are very higher than experimental values.

Theoretical investigation of electro-luminescent properties in red emission DCM, DCJ, RED and DAD Derivatives, by Bo-Cheng Wang et al [15]

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Table 4: Theoretical electro-luminescent of RED3

Compound calculated (max)	Zindo/AM1	DFT/TD-DFT	Experimental
RED3	401	502	505

The experimental values and DFT/TD-DFT theoretical values are in good agreement than AM1.

Theoretical study of two-photon absorption properties for triphenylamine (boron, aluminum)-cored dendritic compounds, by Ji-Kang Feng et al [16]

One electron absorption properties

Table 5: Theoretical one electron absorption of Triphenylamines

Compound	(Exp)nm	Theoretical
1.	392	399
2.	400	399
2-B	----	357
2-Al	----	383
3.	420	413

Two photon absorption for studied molecules

Table 6: Theoretical two electron absorption of Triphenylamines

Compound	(Exp)nm	Theoretical
1.	----	527
2.	----	511
2-B	----	485
2-Al	----	496
3.	----	523

For calculation of theoretical absorption, the authors have used Zindo/SDCI methods.

Theoretical investigation on dendritic molecules with large two-photon absorption cross section, by Xin Zhou et al [17].

One electron absorption properties

Table 7: Theoretical one-electron absorption on dendritic molecules

Compound	(Exp)nm	Theoretical
m1	392	402
M2	----	407
M3	----	401
M4	----	392
M5	----	393
m13	----	357

Two photon absorption for studied molecules

Table 8: Theoretical one-electron absorption on dendritic molecules

Compound	(Exp)nm	Theoretical
m1	690	616
M2	----	580
M3	----	583
M4	----	563
M5	----	576
m13	----	568

The authors used AM1 and Zindo method to investigate OPA and TPA spectra.

Theoretical study on triphenylamine-based sensors of dicarboxylic acids, by Theodorakopoulos et al [18]

Results of the TDDFT calculations: wavelength of absorption lines of the different complexes.

Table 9: Triphenylamine-based sensors of dicarboxylic acids, TDDFT calculations

Compound	Lamda (nm) theoretical
1.(triphenylamine-based chemosensor)	363.6
1+ 2-Dimethyl malonic	384.4
1 + Malonic	384.0
1 + Succinic	377.0
1 +Glutaric	376.6
1 +Adipic	368.8
1 + Suberic	368.1

Ab initio fragment orbital theory (AFOT): application to some two-photon-absorbing (TPA) molecules, By G.P. Das et al [19].

Charge-transfer transitions in triarylamine mixed-valence systems: the effect of temperature, by Bridas et al [21].

- bis-{4-[N,N-di(4-methoxyphenyl)amino]-phenyl}butadiyne,
- (4,4O-bis[N,N-di(4-methoxyphenyl)amino]biphenyl,
- N,N,N',N'-tetraphenyl-1,4-phenylenediamine.

For the above three compounds absorption bands theoretically calculated and compared with experimental values through graphical representation.

Subchromophore interactions in tricyanovinyl-substituted triarylamines—a combined experimental and computational study, by Christoph Lambert et al [22].

Table 12: Tricyanovinyl-triarylamines experimental and computational study

Name	Exp(v_{max}/cm^{-1})	Theoretical (AM1)
A) mono (tricyanovinyl)-substituted Triphenylamines	19660	20440
B) bis (tricyanovinyl)-substituted Triphenylamines	18430	---------
C)2+OMe	20920	19220
D) tris (tricyanovinyl)-substituted Triphenylamines	19950	20600

Intra molecular Charge Transfer in a Star-Shaped Oligoarylamine, by Akihiro Ito et al [23].

Table 13: Theoretical(TD-DFT) calculations of Oligoarylamine

Compound	Exp.hv(cm^{-1})	Theoretical (TD-DFT)
Triamine 2^+	8117	8700
	14350	14210

Dications of Bis-triarylamino-[2.2]paracyclophanes: Evaluation of Excited State Couplings by GMH Analysis, by Christoph Lambert et al [24].

Experimental and AM1-CISD Computed Absorption Energies.

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Table 14: Dications of Bis-triarylamino-[2.2]paracyclophanes values of Experimental and AM1-CISD Computed Absorption Energies

Compound	$\tilde{V}$Exp/cm-1	$\tilde{V}$/cm-1(Theory)
1^{2+}	11300	20160
2^{+}	11500	14390
3^{+}	15500	14590
4^{2+}	10900	16100
5^{2+}	11260	15370
6^{2+}	10870	16140
7^{+}	10680	12960
7^{+}	11500	11780
9^{2+}	13000	14392

[2.2]Paracyclophane-Bridged Mixed-Valence Compounds: Application of a Generalized Mulliken-Hush Three-Level Model, by Christoph Lambert et al [25].

Transition Energies (computed (AM1+CSID) and experimental) and Diabatic Electronic Couplings (GMH).

Table 15: Transition Energies (computed (AM1 + CSID) and experimental) of [2.2]Paracyclophane

Compound	V/cm^{-1}(EXP)	V/cm^{-1}(Theory)
1^{+}	10730	16120
4^{+}	10030	13060
5^{+}	10370	16390
6^{+}	5620	11380
9^{+}	10790	145701

Electronic Coupling in Tetraanisylarylenediamine Mixed-Valence Systems: The Interplay between Bridge Energy and Geometric Factors, by Bridas et al [26].

Experimental Data and TD-DFT Vertical Excitation Energies Systems 1^{+}-3^{+} Obtained at the UB3LYP/6-31G**.

Table 16: Tetraanisylarylenediamine, experimental data and TD-DFT Vertical Excitation Energies from UB3LYP/6-31G

Compound	Vexp(abs/cm^{-1})	V theoretical (abs/cm^{-1})
1^{+}	9480	9290
4^{+}	8000	7710
3^{+}	5140	9390

Crystal, Molecular and Electronic Structure of N,N'-Diphenyl-N,N'-bis(2,4-dimethylphenyl)-(1,1'-biphenyl)-4,4'-diamine and the Corresponding Radical Cation, by Paul J. Low et al [27].
Calculated (TD-DFT) and observed electronic transitions.

Table 17: Observed and calculated (TD-DFT) and electronic transitions of N,N'-Diphenyl-N,N'-bis(2,4-dimethylphenyl)-(1,1'-biphenyl)-4,4'-diamine radical cation

Compound	Observed Lamda(max)[nm]	Calculated Lamda(max)[nm]
1a	310	305
1a+	484	426
$1b^{+}$	305	304
1b+	476	422
1c	----	304
1c+	----	424

Optically and Thermally Induced Electron Transfer Pathways in Hexakis[4-(N,N-diarylamino)phenyl]benzene Derivatives, by Christoph Lambert et al [28]

Optical properties of the IV-CT band of 5^{3+} and 6^{3+}.

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Table 18: Optical properties of the IV-CT band of 5^{3+} and 6^{3+}

Compound	Vmax [cm^{-1}]	Lamda [cm^{-1}]
5^{3+}	7450	7050
6^{3+}	7040	6960

Charge-Transfer Transitions in Triarylamine Mixed-Valence Systems: A Joint Density Functional Theory and Vibronic Coupling Study, by Bredas et al [29].

Experimental absorption and TD-DFT Calculated absorption energy.

Table 19: Experimental absorption and TD-DFT calculated absorption energy of Triarylamine Mixed-Valence Systems

Compound	Lamda(exp)cm^{-1}	Calculated cm^{-1}
1^{+}	10950	9250
2^{+}	7000	6920
3^{+}	7200	6550
4^{+}	8150	6040

Electronic and vibronic contributions to two-photon absorption of molecules with multi-branched structures, by Yi Luo et al [30]

Calculated one-photon absorption of the lowest excited states of PRL-101 compound E and their dimers and trimers. The corresponding experimental results are also included.

Table 20: Calculated and experimental values of PRL-101 compound E and their dimers and trimmers

Compound	HF/6-31G Lamda OP (nm)	Exp. Lamda OP (nm)
PRL-101	323	399
PRL-501	331	417
PRL-701	314	426
E	309	----
E dimer	321	----
	299	----
E trimer	319	----
	317	----
	288	----

Mulliken–Hush analysis of a bis(triarylamine) mixed-valence system with a N... N distance of 28.7 A°, by Christoph Lambert et al [31].

Absorption maxima of the bands in the UV/Vis/NIR spectra of neutral compounds 1a and 1b, the monocation $1b^{+}$ and dications $1a^{2+}$ and $1b^{2+}$.

Table 21: Triarylamine mixed-valence system, bands of absorption maxima

Compound	v˜max/cm^{-1} B and A (neutral triarylamine)	p–p*-transition Bridge band	
1b	22300		
1a	24600		
$1b^{+}$ [a] —		12800	14100
$1b^{2+}$ [a] —		12800	14300
$1a^{2+}$ [b] —		13200	11500

[a] Data obtained from a fit of the spectra of the monocation $1b^{+}$ with four gaussian functions. [b] Data of the bands for the dications $1a^{2+}$ and $1b^{2+}$ were obtained from a fit of the observed bands assigned to a p–p*-transition and a hole transfer from one redox centre to the bridge unit by the three Gaussian functions.

Theoretical studies on two-photon absorption properties of newly synthesized triaryl boron-based A-p-A and triaryl nitrogen-based D-p-D quadrupolar compounds, by Chuan-Kui Wang et al [32].

The maximum TPA cross section sigma tp (cm^4 s photon^{-1}), the excitation energy E(eV) and the corresponding two-photon wavelength lamda tp (nm) of all compounds. Two kinds of hybrid functional B3PW91 and B3LYP are used.

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Table 22: Theoretical studies on triaryl boron-based A-p-A and triaryl nitrogen based D-p-D quadrupolar compounds.

Compound	B3LYP lamdatp	B3PW91 lamdatp	Experiment lamdatp
1.	723	725	720
2.	715	715	720
3.	756	749	730
4.	820	820	745

Organic Mixed-Valence Systems: Intervalence Transition in Partly Oxidized Aromatic Polyamines. Electrochemical and Optical Studies, by Jacques Bonvoisin' and Jean-Pierre Launay [33].

Table 23: Aromatic Polyamines and their Optical studies

Compound	Lamda exp(cm^{-l})	Marcus theory(cm^{-l})
Monocation I	6880	7180
Dication II	7210	715

Effects of Conjugation in Length and Dimension on Spectroscopic Properties of Fluorene-Based Chromophores from Experiment and Theory, by Nguyen et al [34].

Experimental Results compared with other calculations TD-PBE0/6-31G(d), Excitation Energies (in eV).

Table 24: Spectroscopic properties of Fluorene-based Chromophores from Experiment and Theory

Compound	Experimental	Theoretical
AF-240	3.17	3.05
AF-287	2.97	2.86
AF-380	2.90	2.83
AF-389	2.84	2.59
AF-270	3.29	3.05
AF-295	3.21	2.94
AF-350	3.15	2.95
AF-457	2.99	2.90
AF-450	2.98	2.91
AF-459-2	3.20	3.23
AF-240	4.07	3.96
AF-287	3.97	3.88
AF-380	3.87	3.76
AF-350	3.56	3.58
AF-459-2	3.88	3.84

Multidimensional Electron Transfer Pathways in a Tetrahedral Tetrakis□4-[N,N-di(4-methoxyphenyl) amino] phenyl□Phosphonium Salt: One-Step vs Two-Step Mechanism, by Christoph Lambert et al [35].

Table 25: Amino Phenyl Phosphonium salt Opticalstudies theoretial and experimental

Compound	Theoretical(cm^{-1})	Experimental (nm)
Tetrakis-□4-[N,N-di(4-methoxyphenyl)amino] phenyl□phosphonium tetrafluoroborate1$^{+}BF_4$	11800(IVCT)	800

Excited Mixed-Valence States of Symmetrical Donor-Acceptor-Donor ð Systems, by Christoph Lambert et al[36].
Calculated Transient IVCT Absorption Energies S_2-S_1 trans in cm^{-1}.

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Table 26: Donor-Acceptor-Donor ð systems, calculated IVCT Absorption energies

Compound	S_2-S_1trans
C_6H_{12}	3080
MeCN	5660
C_6H_{12}	2570
MeCN	4840
C_6H_{12}	3400
CH_2Cl_2	3920
C_6H_{12}	3600
MeCN	3600

Efficient UV-sensitive organic photovoltaic devices using a starburst amine as electron donor, by Chun-Sing Lee et al [37].

Triphenylamine derivative, 4,49,40-tris (N-3-methylphenyl- N-(9-ethylcarbazyl-3)amino) triphenylamine (PCATA), absorption spectra experimental and theoretical represented through graphically.

From Valence Trapped to Valence Delocalized by Bridge State Modification in Bis(triarylamine) Radical Cations: Evaluation of Coupling Matrix Elements in a Three-Level System, by Christoph Lambert et al [38].

The AM1 computed energies of the IVCT transition and the bridge transition are in very good agreement with experiment for 1^+ and 2^+ but differ strongly for the transition observed in 3^+.

Experimental and Adiabatic and Diabatic Energy (cm^{-1}) 1^+, 2^+, and 3^+ Computed at the AM1-CISD Level.

Table 27: Bis(triarylamine) radical cations, experimental and computed energies

Compound	Experimental(IVCT)cm^{-1}	Theoretical(Vb)
1^+	7000-8000:11000	6940; 8060:10260
2^+	7000-8000:11000	5880:6520:10560
3^+	7000-8000:11000	9550:4640:13060

Electron-Rich Tetrathiafulvalene–Triarylamine Conjugates: Synthesis and Redox Properties, by Christoph Lambertetal [39]
Photophysical data from chemical oxidant titrations of triarylamine T AA, 9^+.

Table 28: Photophysical data of Triarylamine 9^+

Compound	Exp (ox1 [cm^{-1}])	Theoretical(Graph)
9^+ TAA	8100, 10500 and 15700	7900, 11000 and 15800

Cationic Pi-electron systems with high quadratic hyperpolarisability, by Christoph Lambert et al[40],
AM1 computed linear and nonlinear optical properties of 1–5 and 11 in MeCN. Values in italics refer to the gas phase.

Table 29: AM1 computed optical properties of Cationic Pi-electron systems

Compound	Experimental (nm)	Theoretical(nm)
1	329	357
2	360	356
3	395	338
4	454	397
5	354	309
6	454	----
7	354	----
8	237	----
9	322	----
10	270	----
11	----	353
12	----	297
13	----	285
14	----	261

Delocalization in Platinum-Alkynyl Systems: A Metal-Bridged Organic Mixed-Valence Compound, by Seth R. Marder et al [41].

Calculations of the excited state of 1 performed at the time-dependent density functional theory (TD-DFT) level reveal that both S1 and T1 states originate from orbitals with mixed triarylamine and alkyne character and are, thus, delocalized over the entire system.

The energy of 3.4 eV (364 nm) derived for S1 compares well with the experimental absorption data.

Intervalence Transitions in the Mixed-Valence Monocations ofBis(triarylamines) Linked with Vinylene and Phenylene-Vinylene Bridges, by Seth R. Marder et al [42].

Excitation Energies, E, for Compounds 1^+-4^+ According to ZINDO/CIS Calculations at the Neutral AM1 Geometries, along with the Geometric N-N Distance (AM1, neutral), Diabatic Electron-Transfer Distances, R, and Estimated Adiabatic Electron-Transfer Distance, R12.

Table 30: Excitation energies, (ZINDO/CIS calculations) of Bis(triarylamines) linked Vinylene and Phenylene-Vinylene bridges

Compound	E/eV
1^+	0.389
2^+	0.287
3^+	0.249
4^+	0.043
$L1^+$	0.436

The role of vibronic interactions on intramolecular and intermolecular electron transfer in p-conjugated oligomers, by J.L. Bredas et al [43]

Table 31: Calculated absorption profiles of 9^+ compared with experimental Absorption spectrum.

Compound	Experimental	Calculated
9^+	9680	9680

The same trend is observed for system 8^+.

Intervalence transition in triarylamine mixed-valence systems: A time-dependent density functional theory study, by J. L. Bre´das et al [44].

The first excited state of 1+ (N,N,N8,N8-tetrakis~4-methoxyphenyl!-1,4-benzenediamine molecule ~1) is calculated to be at 9330 cm^{-1} above the ground state, in very good agreement with the lowest optical peak at 9530 cm^{-1} assigned experimentally as the CT transition ~in CH_2Cl_2.

Joint Experimental and Theoretical Characterization of the Electronic Structure of 4,4□-Bis(N-m-tolyl-N-phenylamino)biphenyl (TPD) and Substituted Derivatives, by J. L. Bre´das et al [45]. Energy (in eV) of the HOMO (H) and HOMO-1 (H-1) Levels in NTD, TPD, and Substituted Derivatives, as Inferred from Gas-Phase UPS Spectra and Calculated at the AM1 and INDO Levels.

Table 32: Calculated at the AM1 and INDO energy levels of TPD and derivatives

Compound	E/eV
TPD	3.66
TPDMf-	3.67
TPD-mmF2	3.69
TPD-mmpF3	3.65
TPD-pF	3.65
TPD-mMeO-	3.67
TPD-pMeO-	3.63
NTD	3.60

The column provides the lowest transition energy (in eV) and related oscillator strength (OS, in arbitrary units) obtained at the INDO/SCI level.

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