Electronic Supporting Information (Part 1).
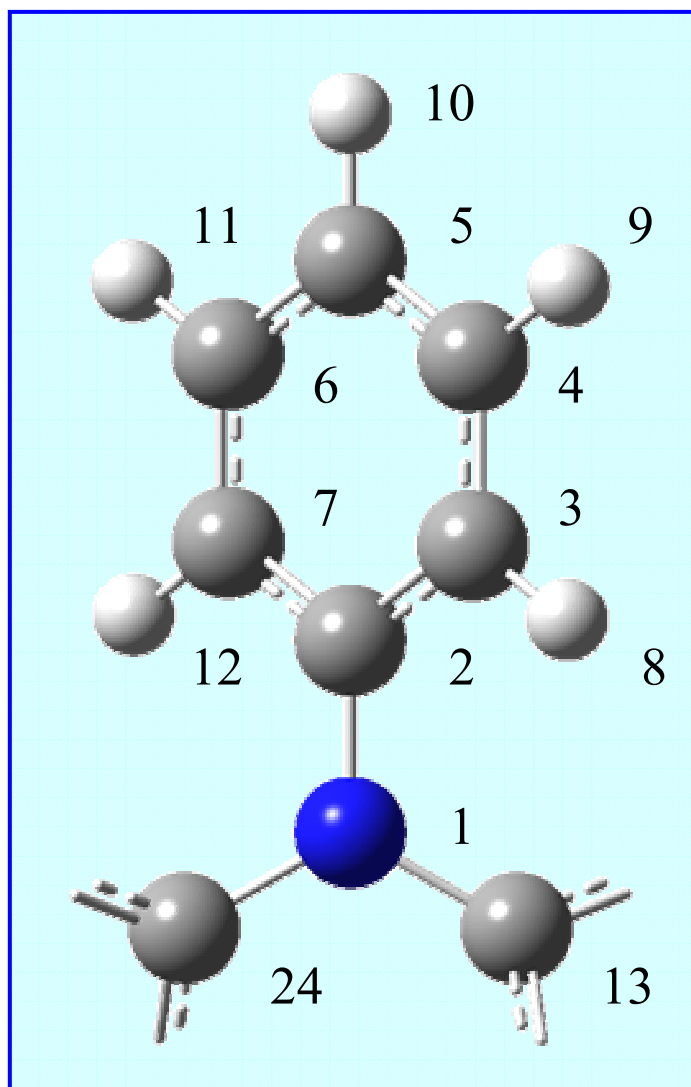

Figure S1.
Atom numbering for one of the phenyl rings in the molecule of triphenylamine, as used in
Table S1. The other two phenyl rings are identical by symmetry.

Table S1.

Optimized geometry parameters for one of the phenyl rings and the central NCCC fragment of the triphenylamine monomer. Other two phenyl rings are identical by symmetry. For atom numbering see Figure S1.

Definition	Value	
	6-31G**	aug-cc-pVDZ

Bond lengths (Angstroms)

R(1,2)	1.4216	1.4211
R(1,13)	1.4216	1.4211
R(1,24)	1.4216	1.4211
R(2,3)	1.4044	1.4058
R(2,7)	1.4044	1.4058
R(3,4)	1.3933	1.3961
R(3,8)	1.0848	1.0889
R(4,5)	1.3962	1.3991
R(4,9)	1.0863	1.0906
R(5,6)	1.3962	1.3991
R(5,10)	1.0856	1.0899
R(6,7)	1.3933	1.3961
R(6,11)	1.0863	1.0906
R(7,12)	1.0848	1.0889

Bond angles (Degrees)

A(2,1,13)	120.0	120.0
A(2,1,24)	120.0	120.0
A(13,1,24)	120.0	120.0
A(1,2,3)	120.5345	120.5261
A(1,2,7)	120.5345	120.5261
A(3,2,7)	118.9309	118.9478
A(2,3,4)	120.3108	120.3394
A(2,3,8)	119.3902	119.5709
A(4,3,8)	120.299	120.0896
A(3,4,5)	120.6234	120.6093
A(3,4,9)	119.2825	119.3463
A(5,4,9)	120.0881	120.0393
A(4,5,6)	119.1916	119.1488
A(4,5,10)	120.4042	120.4256
A(6,5,10)	120.4042	120.4256
A(5,6,7)	120.6234	120.6093
A(5,6,11)	120.0881	120.0393
A(7,6,11)	119.2825	119.3463
A(2,7,6)	120.3108	120.3394
A(2,7,12)	119.3902	119.5709
A(6,7,12)	120.299	120.0896

Table S1 (continued).

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Dihedral angles (Degrees)
D(13,1,2,3)            -41.5041           -41.9752
D(13,1,2,7)            138.4959           138.0248
D(24,1,2,3)            138.4959           138.0248
D(24,1,2,7)            -41.5041           -41.9752
D(1,2,3,4)             179.5529           179.6351
D(1,2,3,8)              -0.3867            -0.2287
D(7,2,3,4)              -0.4471            -0.3649
D(7,2,3,8)             179.6133           179.7713
D(1,2,7,6)             179.5529           179.6351
D(1,2,7,12)             -0.3867            -0.2287
D(3,2,7,6)              -0.4471            -0.3649
D(3,2,7,12)            179.6133           179.7713
D(2,3,4,5)               0.9017             0.7358
D(2,3,4,9)            -179.9943           179.9149
D(8,3,4,5)            -179.1592          -179.4011
D(8,3,4,9)              -0.0553            -0.222
D(3,4,5,6)              -0.4505            -0.3673
D(3,4,5,10)            179.5495           179.6327
D(9,4,5,6)            -179.5473          -179.5407
D(9,4,5,10)              0.4527             0.4593
D(4,5,6,7)              -0.4505            -0.3673
D(4,5,6,11)           -179.5473          -179.5407
D(10,5,6,7)            179.5495           179.6327
D(10,5,6,11)             0.4527             0.4593
D(5,6,7,2)               0.9017             0.7358
D(5,6,7,12)           -179.1592          -179.4011
D(11,6,7,2)           -179.9943           179.9149
D(11,6,7,12)            -0.0553            -0.222
```

Dipole moment = 0 Debye (Full point group D_3)

Standard basis 6-31G**. Rotational constants (GHZ):
0.4002826   0.4002826   0.2203502

Standard basis Aug-CC-pVDZ. Rotational constants (GHZ):
0.3991689   0.3991689   0.2201991

Table S2.

Calculated frequencies (cm^{-1}) of the non-infrared-active modes (symmetry A$_1$, theoretical intensities are equal to zero) in the TPA monomer.

DFT(B3LYP)		Description and
6-31G**	aug-cc-pVDZ	(Whiffen symbol)
79.3	79.7	change of blade pitch
279.7	279.6	N-Phenyl stretching
417.4	417.9	R tors (w)
712.8	714.1	R bend (t)
833.1	828.3	CH oop (g)
949.9	962.7	CH oop (h)
991.8	992.5	R bend (p)
1031.0	1029.5	CH bend (b)
1174.0	1170.2	CH bend (a), CN str
1189.1	1187.6	CH bend (a), CN str
1504.5	1492.6	R str (m), CH bend(b)
1626.9	1624.5	R str (k)
3110.3	3127.6	CH str
3133.3	3150.0	CH str
3143.9	3159.8	CH str

Theoretical frequencies calculated with the 6-31G** basis set were scaled with a factor of 0.978, and those calculated with the aug-cc-pVDZ basis set were scaled by 0.986.
Str – stretching, bend – bending, oop – out-of-plane, tors – torsion.