Electronic supporting information

Contents

General experimental information

All reagents and solvents were purchased from Sigma-Aldrich, and appropriately purified, if necessary. Unless otherwise noted, all the reactions were carried out under a nitrogen atmosphere and in dry solvents.

^{1}H NMR experiments were performed using Varian VNMR 400 MHz and Bruker 500 MHz NMR spectrometers at the University of Bristol's School of Chemistry NMR service. Samples for MALDI-TOF mass spectra were prepared using of 2,5-dihydroxybenzoic acid (DHB) as a matrix and 2:1 MeCN:water as the solvent. The spectra were run by the University of Bristol School of Chemistry mass spectrometry service. UV-vis-NIR spectra were recorded on a Shimadzu UV2600 spectrophotometer fitted with an ISR- 2600Plus integrating sphere attachment. Spectroscopic grade THF was used as the solvent. ESR spectra were recorded on an Active Spectrum extended-range benchtop Micro-ESR spectrometer.

Synthesis

Dimer (DPPD)

N,*N*'-Diphenyl-1,4-phenylenediamine (**DPPD-LEB**, 97%) was purchased from Alfa Aesar and used without further purification. *N*,*N*'-diphenyl-1,4-phenylenediimine (**DPPD-PB**) was synthesized according to a published procedure.[1]

Tetramer (TANI)

TANI-LEB

N^1,*N*$^{1'}$-(1,4-phenylene)-bis(*N*^{4}-phenylbenzene-1,4-diamine) (**TANI-LEB**) was prepared according to a published procedure.[2, 3]

TANI-EB

4,4'-(cyclohexa-2,5-diene-1,4-diylidenebis(azaneylylidene))bis(*N*-phenylaniline) (**TANI-EB**) was prepared according to a published procedure.[2, 3]

TANI-PB

N^1,*N*$^{1'}$-(1,4-phenylene)-bis(*N*^{4}-phenylbenzene-1,4-diimine) (**TANI-PB**) was prepared in solution without isolation by the same method used to oxidised **DPPD-LEB** to **DPPD-PB**:[1] the precursor **TANI-LEB** (13.3 mg, 30 µmol) was dissolved in THF (30 ml) and stirred at room temperature, to which silver(I) oxide (20.9 mg, 90 µmol, 3 eq.) was added. The solution gradually changed in color from colorless to red and was stirred overnight, then filtered through a cotton wool plug to remove silver residues. *In situ* UV-vis-NIR spectroscopy showed the appearance of a new absorption feature at 504 nm that does not correspond, to either **TANI-LEB** or **TANI-EB**.

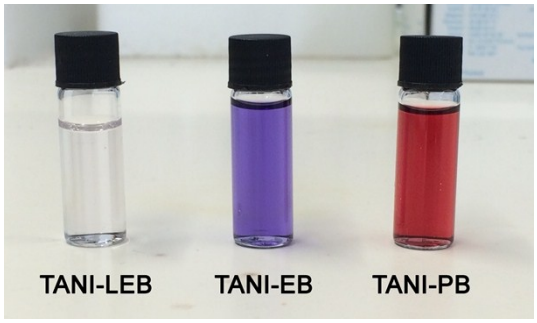


Figure S1. Solutions of **TANI-LEB**, **TANI-EB** and **TANI-PB** dissolved in THF.

Octamer (OANI)

N^1,$N^{1\prime}$-(1,4-phenylene)bis(N_4-(4-((4-(phenylamino)phenyl)amino)phenyl)benzene-1,4-diamine) (OANI-LEB)

The precursor (**Ph/NH$_2$ TANI**) was synthesised according to a published procedure.[3] A nitrogen-protected Schlenk tube was charged with **Ph/NH$_2$ TANI** (229.6 mg, 0.63 mmol, 2.1 eq.), Pd(dba)$_2$ (10.4 mg, 0.02 mmol, 6 mol%), *rac*-BINAP (16.8 mg, 0.03 mmol, 9 mol%), 1,4-dibromobenzene (70.8 mg, 0.3 mmol, 1 eq.), sodium *tert*-butoxide (86.5 mg, 0.9 mmol, 3 eq.) and anhydrous THF (30 mL). The reaction mixture was heated, with stirring, to 90 °C. After 3 days, TLC analysis indicated complete consumption of the starting dibromide. The reaction mixture was cooled to room temperature and added into deionized water (100 mL). Then, the THF was removed under reduced pressure. The precipitate was collected by centrifugation and dissolved in DMF (30 mL) and a portion of hydrochloric acid (20 mL, 2 M) was added under strong stirring within 2 min. The green suspension was poured into deionized water (100 mL). The precipitate was collected by centrifugation and then treated with a mixture of ammonium hydroxide solution (20 mL, 2 M) and acetone (200 mL) for 1 h. The acetone was removed under reduced pressure and the precipitate was collected by centrifugation. The precipitate was dried under dynamic vacuum and washed with several portions of diethyl ether (20 mL) by centrifugation until full removal of the starting **Ph/NH$_2$ TANI** was achieved, as indicated by TLC analysis on the supernatants. Phenylhydrazine (324.4 mg, 3.0 mmol, 10 eq.) was added to a DMF (40 mL) solution of the product and stirred for overnight. The solution was then poured into isopropanol (150 mL) and left stationary for 1 h. The precipitate was collected by centrifugation to afford the product, in the leucoemeraldine base state **OANI-LEB**, as white powder (157.2 mg, 65%): m.p. 320.6 ˚C; ^{1}H NMR (400 MHz, DMSO-d_6, 25°C): δ=7.73 (s, 2H), 7.54 (s, 2H), 7.46 (s, 2H), 7.44 (s, 2H), 7.13 (m, 4H), 6.91-6.87 (m, 32H), 6.66 (m, 2H); IR (neat, cm^{-1}): 3390, 3022, 1670, 1600, 1512, 1494, 1291, 1214, 813, 745, 693; Anal. calcd. for $C_{54}H_{46}N_8$: C, 80.37; H, 5.75; N, 13.89. Found: C, 79.05; H, 5.95; N, 12.70. HRMS (MALDI) calcd. for $C_{54}H_{46}N_8$: 806.3845. Found: 806.3849.

OANI-EB

A solution of ammonium persulfate (91.3 mg, 0.4 mmol, 2 eq.) in hydrochloric acid (20 mL, 2 M) was added dropwise to a DMF (20 mL) solution of the leucoemeraldine base state **OANI-LEB** (161.4 mg, 0.2 mmol, 1 eq.) under stirring for 30 min. The resulting solution was poured into stirred deionized water (100 mL). The deep green precipitate was collected by centrifugation and treated with a mixture of ammonium hydroxide solution (30 mL, 2 M) and acetone (200 mL) for 6 hours. After removal of acetone under reduced pressure, the residue was filtered to afford the product, in the emeraldine oxidation state **1EB**, as a black powder (158.9 mg, 99%): Anal. calcd. for $C_{54}H_{42}N_8$: C, 80.77; H, 5.27; N, 13.95. Found: C, 80.44; H, 6.08; N, 13.71. MS calcd. for $C_{54}H_{42}N_8$: 802.4. Found: 802.3.

Chemical structures of the oligo(aniline)s' oxidation states

DPPD

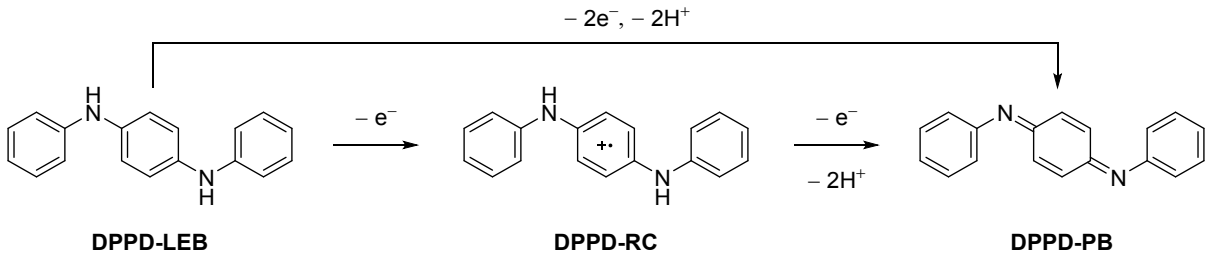


Figure S2. Chemical structures of the known oxidation states and doped forms of **DPPD**.

TANI

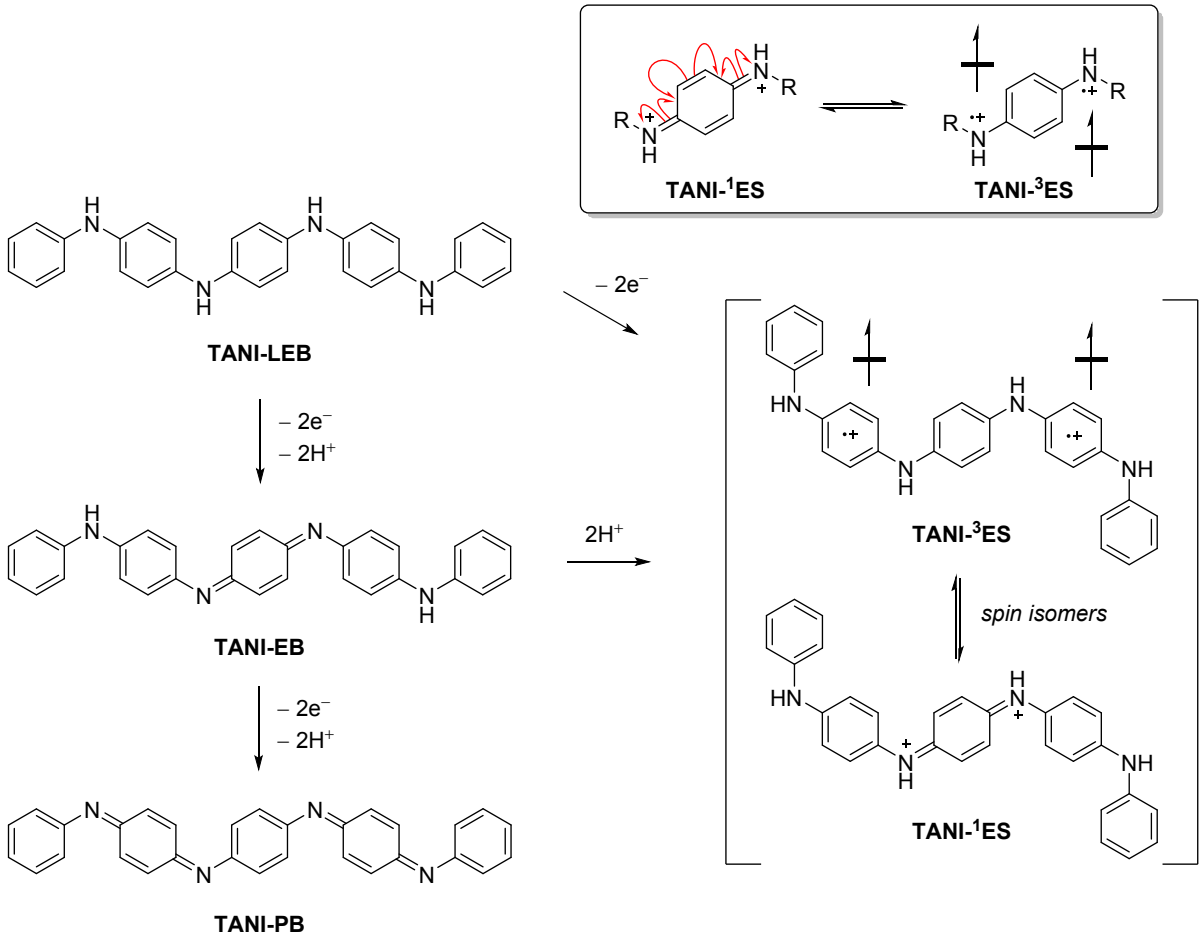


Figure S3. Chemical structures of the known oxidation states and doped forms of **TANI**, with a curly-arrow mechanism for conversion from the ^{1}ES to the ^{3}ES state.

OANI

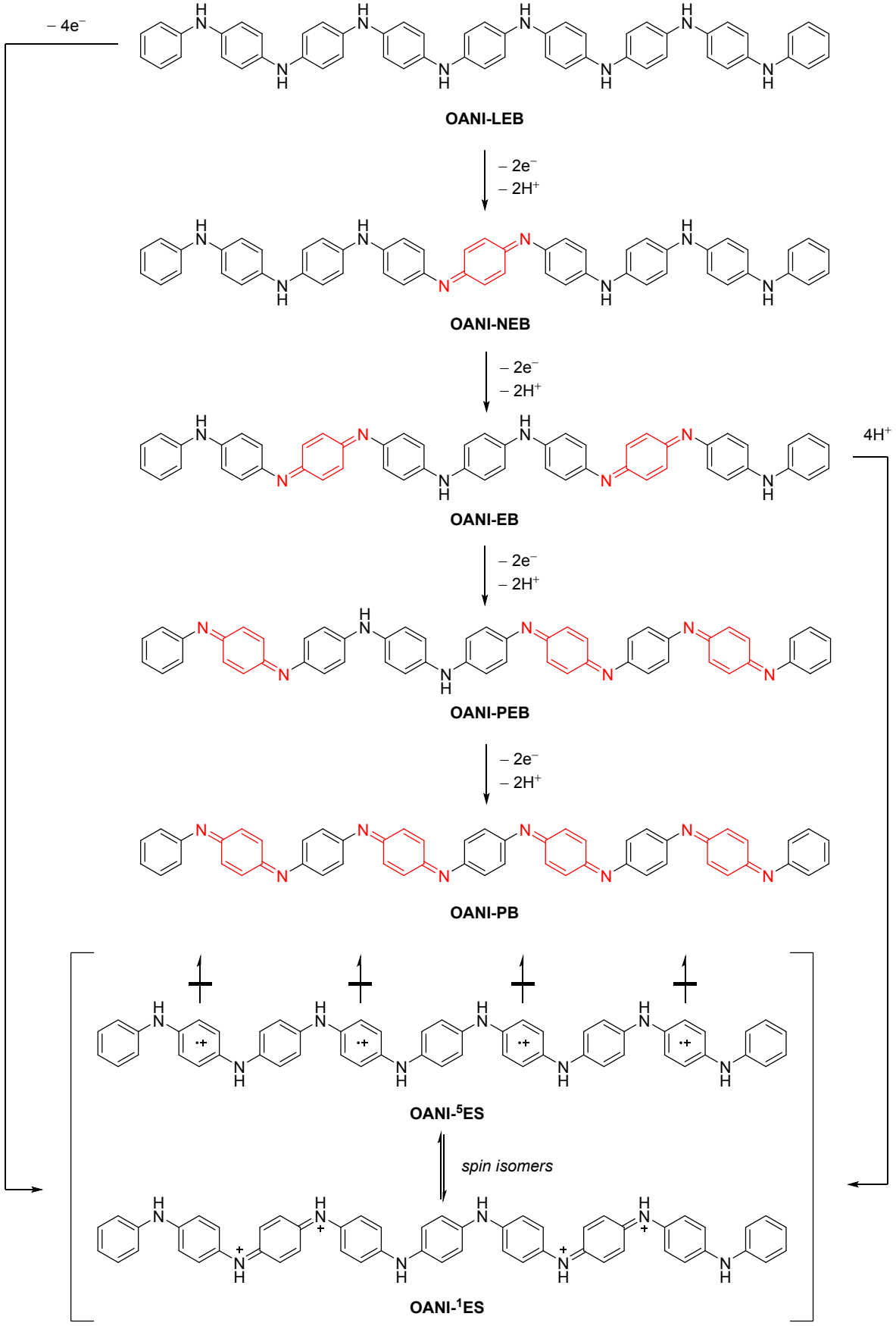


Figure S4. Chemical structures of the known oxidation states and doped forms of **OANI**.

Density functional theory (DFT) calculations

Computational method

Geometry minimization and electronic structure calculations were performed in *Gaussian 09*, revision D.01.[4] For geometry optimisations, the B3LYP functional as implemented in Gaussian[5, 6] and the standard 6-31G(d) basis set[7] were used. A polarizable continuum model (PCM) was used to account for ethanol solvation, as implemented by default in Gaussian.[8-10] This continuum dielectric model for solvation does not fully capture differences in solvent effects, but it is necessary to obtain reasonable energies; optimisation in vacuum gave unrealistically high energies. The results of the calculations were visualized in *GaussView*, version 5.0.9.[10, 11] The output from geometry optimization was used as the starting point for time-dependent DFT calculations,[12-14] which were carried out using either the B3LYP or CAM-B3LYP functional as stated in the text,[15] again with the 6-31G(d) basis set and PCM solvation, in this case for tetrahydrofuran as this was in better agreement with experiment, where solubility problems had been observed for ethanol. Geometry effects of changing the solvent in PCM were minimal, so optimisations were not repeated. Calculations of triplet and quintet states used the unrestricted DFT approach, which gave better convergence. As the CAM-B3LYP functional generally gave better agreement with available experimental data, maxima were simulated using this functional, unless otherwise specified in the text. For the simulation of UV-vis-NIR spectra, the peak width was set to 0.333 eV in GaussView, as this gave a reasonable match with experimental spectra.

As part of our method evaluation, optimisations with explicit counterions were also explored. These did not reliably improve the agreement between calculation and experiment, but added considerable computational noise to energies and calculated transitions, due to variations in oligomer conformation (see below), counterion positions and potentially also interactions with solvent molecules if these were to be modelled explicitly. In addition, dispersive interactions might arise between oligo-anilines, solvents, and potentially larger counterions, further complicating the analysis. With calculations on relatively simple models achieving satisfying agreement with experimental data already, a full exploration of such effects lay outside of the scope of the present study.

Conformational isomerism (TANI)

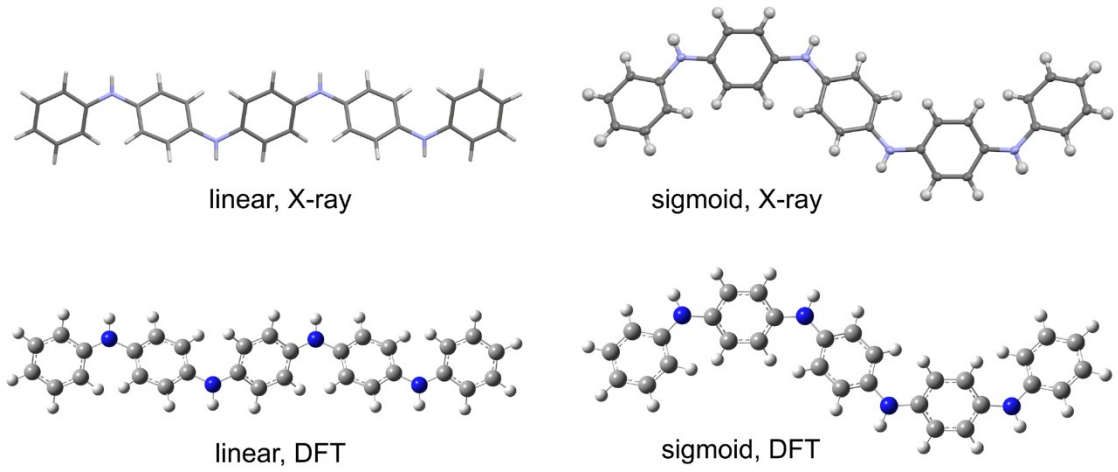


Figure S5. Experimental (X-ray) and calculated (DFT) structures of the linear and sigmoid conformations of **TANI**.

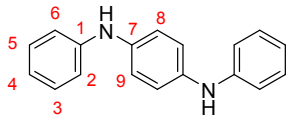
Table S1. Energies of linear and sigmoid conformers of **TANI** in six different oxidation states, calculated with DFT (B3LYP/6-31G*). The most stable conformer in each state is indicated with an asterisk (*).

Oxidation state	**Conformation**	**Energy / Ha**	$E_{linear} - E_{sigmoid}$ / kJ mol^{-1}
LEB	Linear *	-1377.87208424	−0.01
	Sigmoid	-1377.87208023	
EB	Linear	-1376.63403783	+1.17
	Sigmoid *	-1376.63469040	
PB	Linear	-1375.38575966	+1.54
	Sigmoid *	-1375.38634719	
RC	Linear	-1377.71964612	+1.25
	Sigmoid *	-1377.72012032	
^{1}ES	Linear	-1377.54000901	+2.09
	Sigmoid *	-1377.54080402	
^{3}ES	Linear	-1377.54075224	+1.54
	Sigmoid *	-1377.54133901	

These results suggest that the energy difference between these conformers is small and unlikely to have a considerable impact on energies or predicted transitions; indeed, in the absence of other interactions one might expect both conformers to be present in solution.

Comparison with crystal structures

DPPD



DPPD-LEB

Figure S6. Structure of **DPPD**-LEB with atom numbering.

Table S2. Selected geometric parameters of **DPPD**-LEB in its two crystalline polymorphs and in the DFT model.

Geometric parameter	**Orthorhombic[16]**	**Triclinic[17] (1)**	**Triclinic[17] (2)**	**DFT**
C8-C8′ bond length / Å	1.385	1.384	1.386	1.392
C7-C8 bond length / Å	1.384	1.395	1.390	1.405
C7-N bond length / Å	1.410	1.413	1.413	1.404
C1-N bond length / Å	1.402	1.415	1.395	1.396
C7–N–C1 angle / °	129.7	126.1	127.3	129.4
Sum of bond angles at N / °	357.7	354.9	359.8	359.7
C9-C7-C1-C2 torsion angle / °	29.1	42.1	45.4	41.7

Table S3. Selected geometric parameters of **DPPD**-PB in the crystalline state and in the DFT model.

Geometric parameter	**Crystal**	**DFT[16]**
C8–C8′ bond length / Å	1.337	1.350
C7–C8 bond length / Å	1.462	1.464
C7=N bond length / Å	1.297	1.302
C1–N bond length / Å	1.413	1.400
C7–N–C1 angle / °	121.7	123.4
C9-C7-C1-C2 torsion angle / °	49.2	48.0

TANI

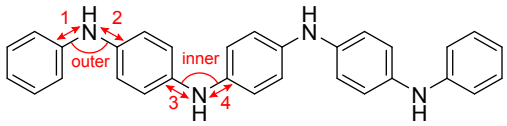


Figure S7. Structure of **TANI**-LEB with selected bond lengths and angles labelled.

Table S4. Selected geometric parameters of **TANI**-LEB in the crystalline state[18] and in the DFT model.

Geometric parameter	**Crystal (1)**	**Crystal (2)**	**DFT**
Length of C-N bond #1 / Å	1.397	1.392	1.395
Length of C-N bond #2 / Å	1.411	1.403	1.407
Length of C-N bond #3 / Å	1.407	1.397	1.400
Length of C-N bond #4 / Å	1.405	1.402	1.402
Outer C–N–C angle / °	125.7	127.6	128.9
Inner C–N–C angle / °	126.0	127.2	129.0
Sum of bond angles at outer N / °	354.5	358.4	359.9
Sum of bond angles at inner N / °	355.8	359.3	359.5
Dihedral angle between outer rings / °	50.3	46.1	42.1
Dihedral angle between inner rings / °	49.9	47.8	42.7

Table S5. Selected geometric parameters of **TANI**-ES in the crystalline state (see Table 22) and in DFT models of **TANI**-^{1}ES and ^{3}ES.

Geometric parameter	**Crystal**	**DFT ^{1}ES**	**DFT ^{3}ES**
C-N bond lengths / Å	1.415	1.410	1.408
	1.355	1.363	1.363
	1.370	1.381	1.366
	1.365	1.361	1.407
C–N–C angles / °	129.4	129.7	129.9
	128.8	131.8	129.6
Central ring C(H)-C(H) bond length / Å	1.366	1.369	1.388
Central ring C(N)-C(H) bond lengths / Å	1.411	1.426	1.405
	1.417	1.424	1.405
Dihedral angles between rings / °	37.0	41.0	40.3
	32.2	32.7	41.1

Charge distribution in ES state spin isomers

TANI-ES

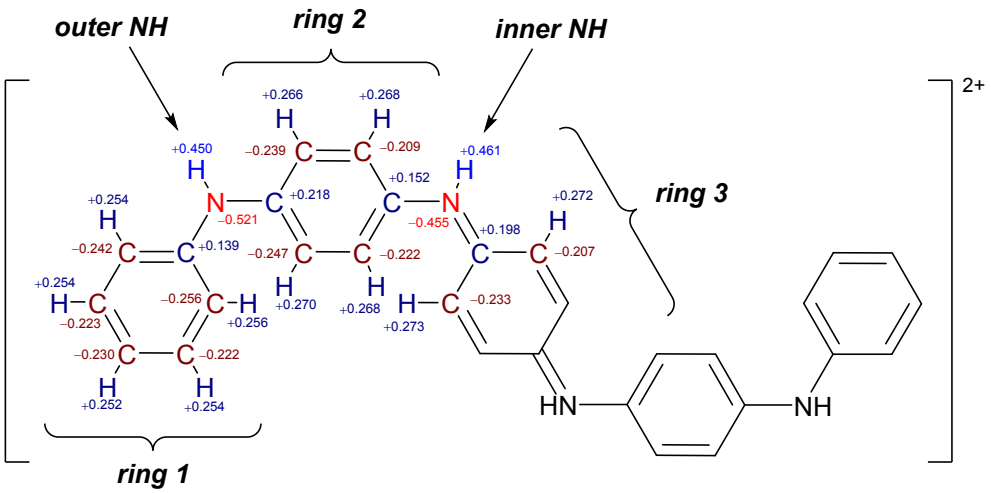


Figure S8. Charge distribution in the ^{1}ES state of **TANI** calculated with natural bond orbital (NBO) population analysis.

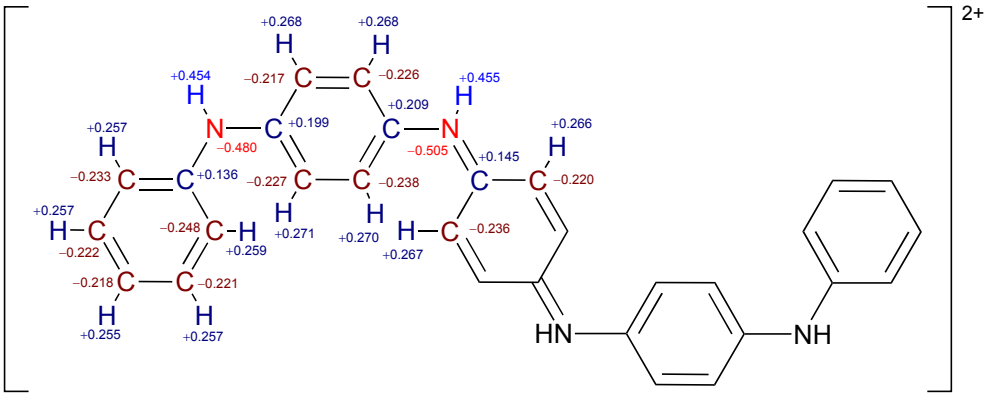


Figure S9. Charge distribution in the ^{3}ES state of **TANI** calculated with natural bond orbital (NBO) population analysis.

Table S6. Summary of NBO charges for benzene rings and NH groups in the ^{1}ES and ^{3}ES states of **TANI**.

State	Ring 1 (terminal)	Outer NH	Ring 2	Inner NH	Ring 3 (central)	Total charge
^{1}ES	+0.236	−0.071	+0.525	+0.006	+0.606	+1.998
^{3}ES	+0.279	−0.026	+0.577	−0.050	+0.444	+2.004

OANI-ES

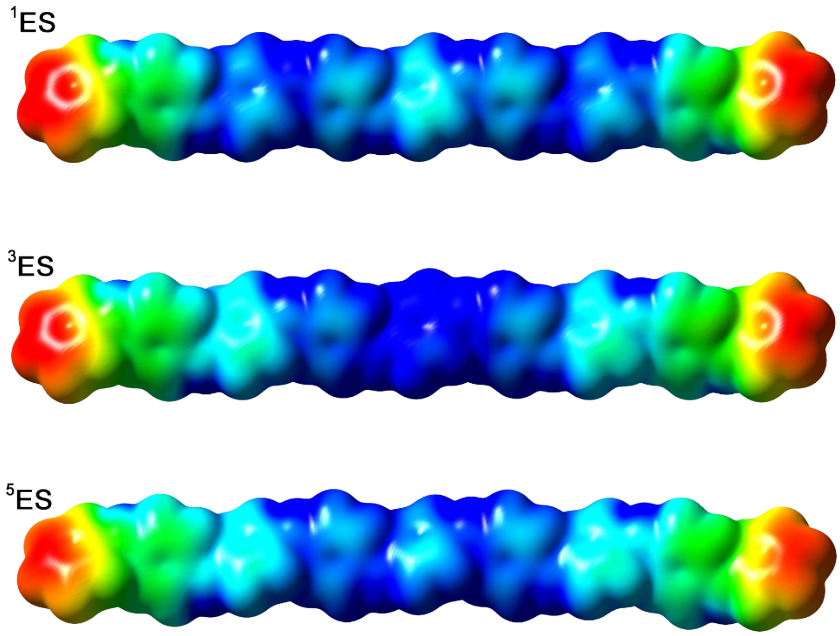


Figure S10. Electrostatic potential (ESP) surfaces for the OANI-^{1}ES, ^{3}ES and ^{5}ES.

Spin density in ES state spin isomers

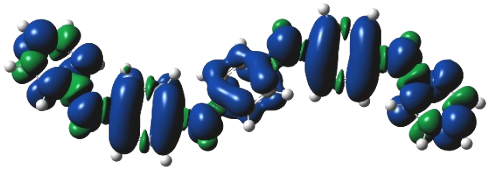


Figure S11. Spin density surface for TANI-^{3}ES.

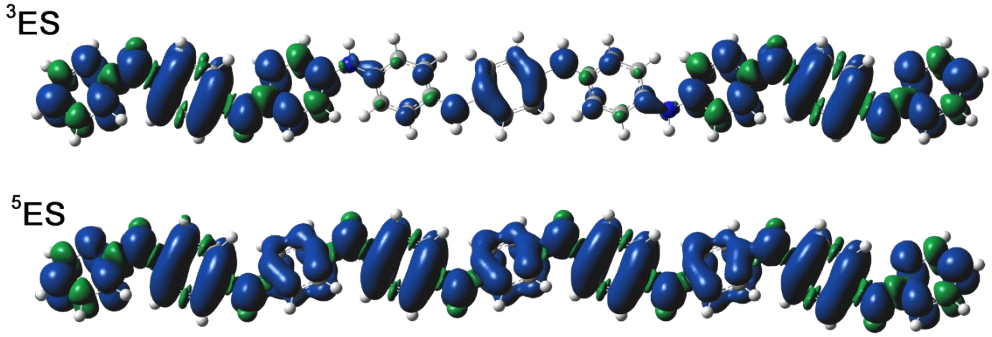
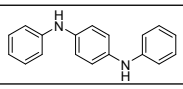
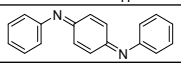
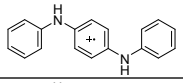
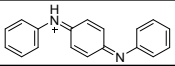
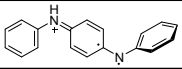
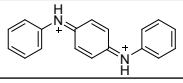
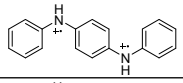
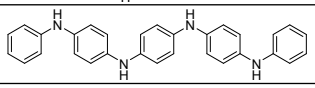
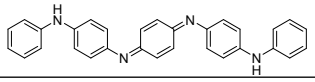
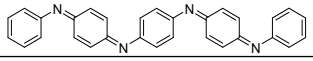
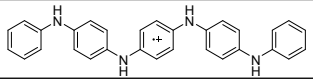
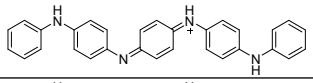
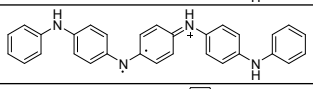
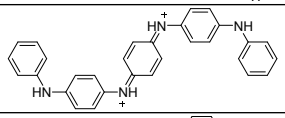
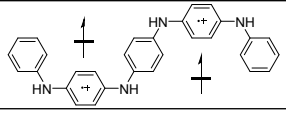
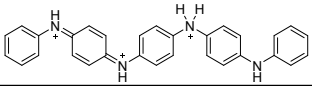
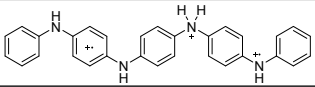
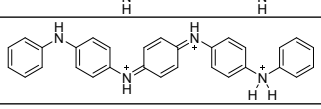
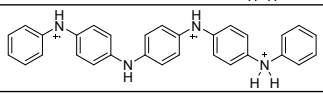


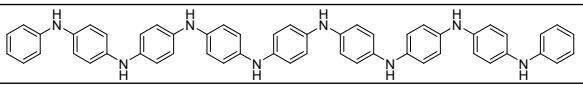
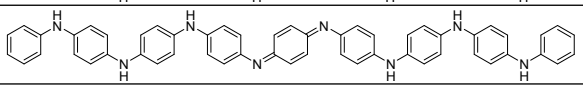
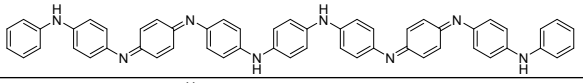
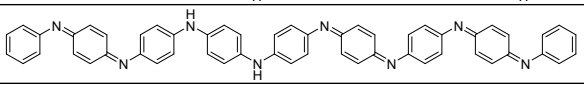
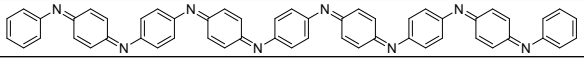
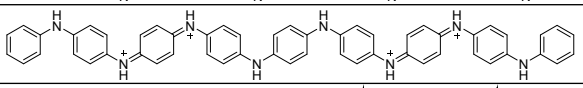
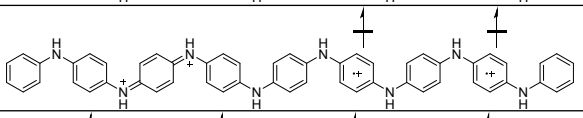
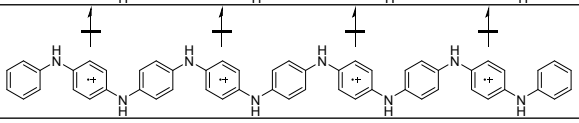
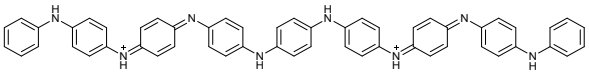
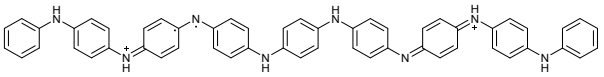
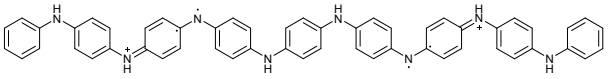
Figure S12. Spin density surfaces for OANI-^{3}ES and ^{5}ES.

Time-dependent density functional theory (TD-DFT) calculations

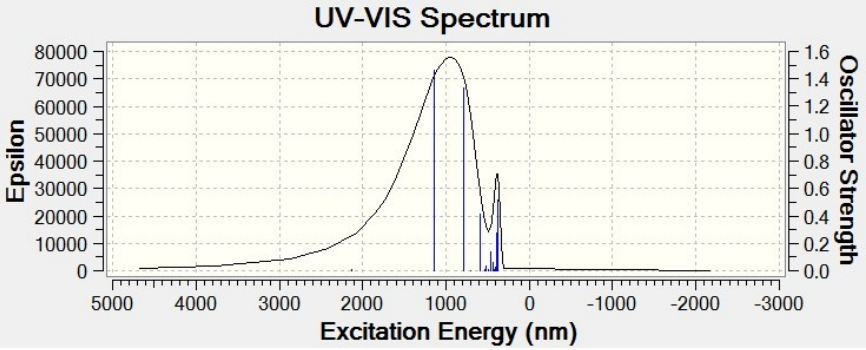
Summary of maxima

Table S7. Structures and simulated UV-vis-NIR maxima of possible oxidation states and doped forms of DPPD, TANI and OANI that were modelled by DFT and TD-DFT, alongside the corresponding experimental maxima of those species believed to have been observed (in THF solution except where specified otherwise).

Species	Structure	λ_{max} / nm		
		B3LYP	CAM-B3LYP	Experiment
DPPD-LEB		320	290	308
DPPD-PB		504	426	448
DPPD-RC		739	694	716
DPPD-^{1}MP		586	551	544
DPPD-^{3}MP		-	651	-
DPPD-^{1}ES		-	570	-
DPPD-^{3}ES		-	657	-
TANI-LEB		355	309	328
TANI-EB		672	537	571
TANI-PB		626	503	504
TANI-RC		-	1306	-
TANI-^{1}MP		-	688	-
TANI-^{3}MP		-	969	-
TANI-^{1}ES		1021	1032	1032
TANI-^{3}ES		924	812	818
TANI-^{1}TP-i		-	550	-
TANI-^{3}TP-i		-	655	-
TANI-^{1}TP-o		-	731	-
TANI-^{3}TP-o		-	799	-

Species	Structure	λ_{max} / nm		
		B3LYP	CAM-B3LYP	Experiment
OANI-LEB		374	324	338 [a]
OANI-NEB		-	568	-
OANI-EB		761	554	616 [a]
OANI-PEB		-	571	-
OANI-PB		-	567	-
OANI-^{1}ES		1628 [c]	1370	1430 [b]
OANI-^{3}ES		-	1286	-
OANI-^{5}ES		1176 [c]	938	1070 [b]
OANI-^{1}MP (most stable isomer, 2o-6i)			734	
OANI-^{3}MP (most stable isomer, 2o-6o)			952[d]	
OANI-^{5}MP (most stable isomer, 2o-6o)			1168	

[a] Dissolved in DMSO. [b] Dissolved in *meta*-cresol. [c] These B3LYP-calculated maxima appear to be anomalies in Figure 1, but their deviation from the trend line is much less pronounced in dimensions of energy, rather than wavelength, as shown in Figure S50. [d] TD-DFT predicts 2 strong peaks at 1144 and 785 nm; plot shows maximum at 952.



A range of different protonation sites were explored for the OANI-MP structures; data shown here show the protonation state lowest in energy for each electronic configuration. We note that other configurations could potentially be sufficiently low in energy to contribute. However, the OANI-ES states are generally in better agreement with the experimental data.

Example of CAM-B3LYP- and B3LYP-calculated spectra compared to experiment

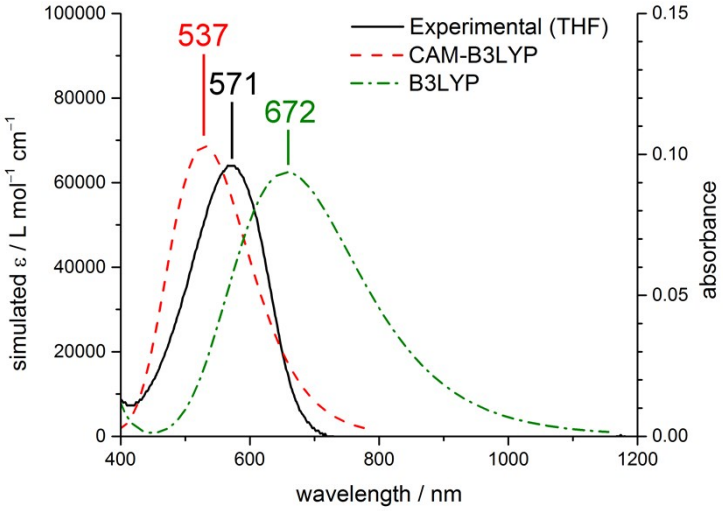


Figure S13. Comparison of TD-DFT-calculated and experimental UV-vis-NIR spectra of **TANI-EB** in THF, highlighting the quantitatively and qualitatively closer match between CAM-B3LYP and experiment compared to B3LYP.

Simulated and experimental UV-vis-NIR spectra

DPPD

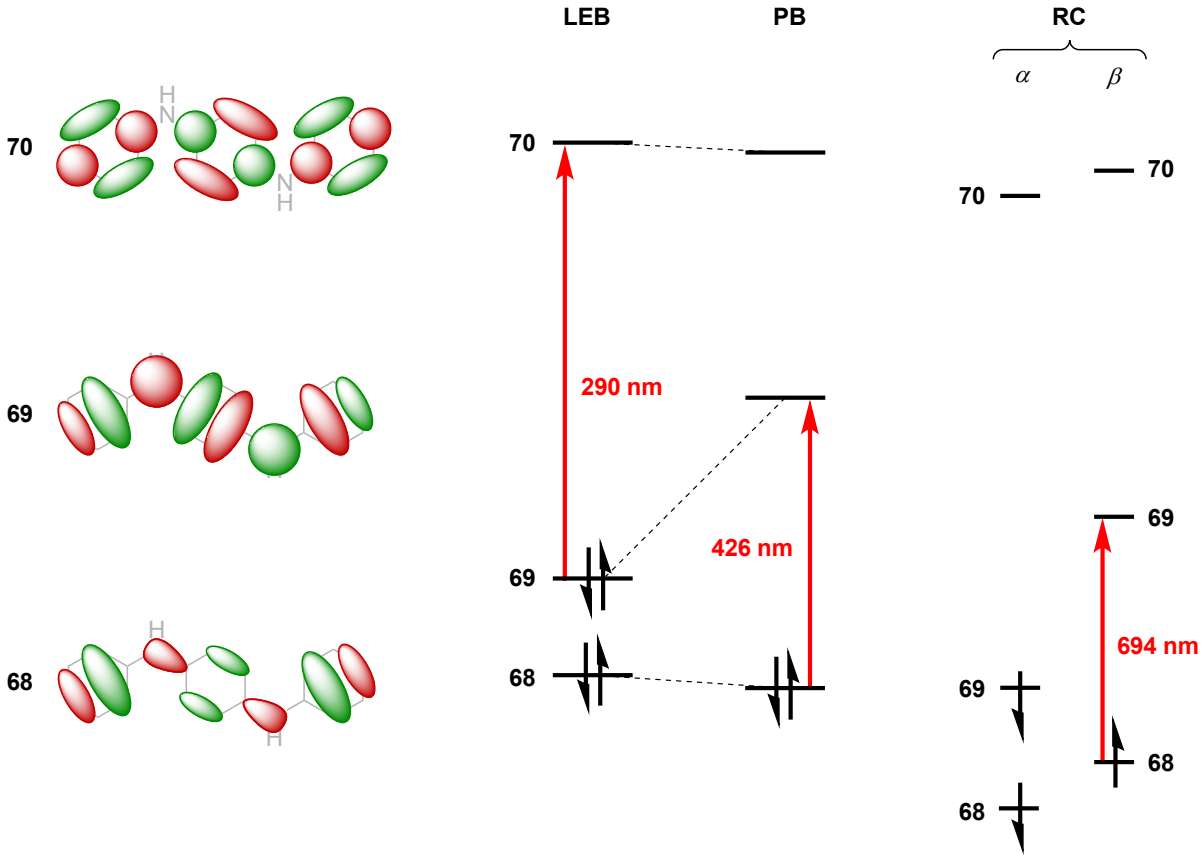


Figure S14. Approximate shapes of the DFT-calculated frontier molecular orbitals of **DPPD**-LEB, PB and RC compared, alongside the corresponding energy levels and characteristic TD-DFT-calculated optical transitions.

DPPD-LEB

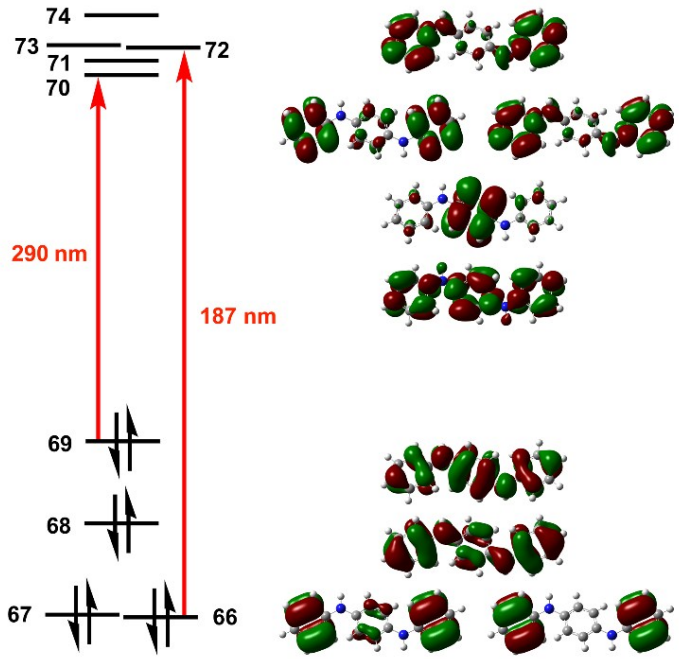


Figure S15. Frontier molecular orbitals of **DPPD**-LEB calculated by DFT.

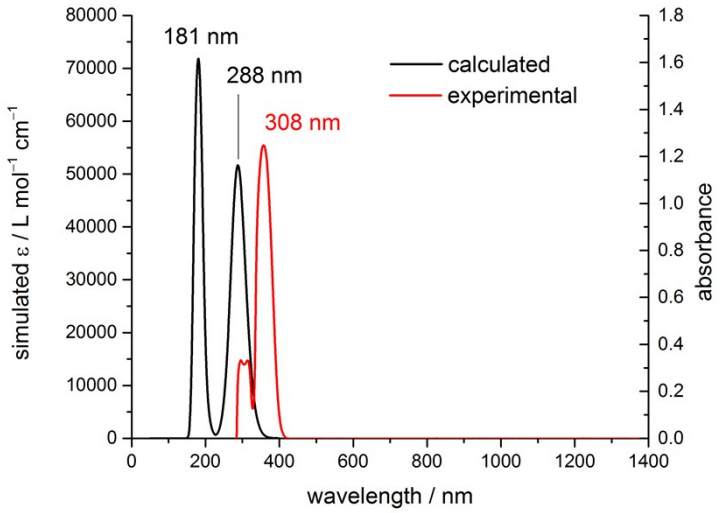


Figure S16. Simulated and experimental (THF) UV-vis-NIR spectra of **DPPD**-LEB.

Table S8. Main optical transitions (*f* > 0.5) of **DPPD**-LEB simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
4.27	290	0.94	69 (HOMO) → 70 (LUMO) (82%)
6.62	187	0.67	66 (HOMO−3) → 72 (LUMO+2) (25%)
7.17	173	0.57	68 (HOMO−1) → 74 (LUMO+4) (53%)

DPPD-PB

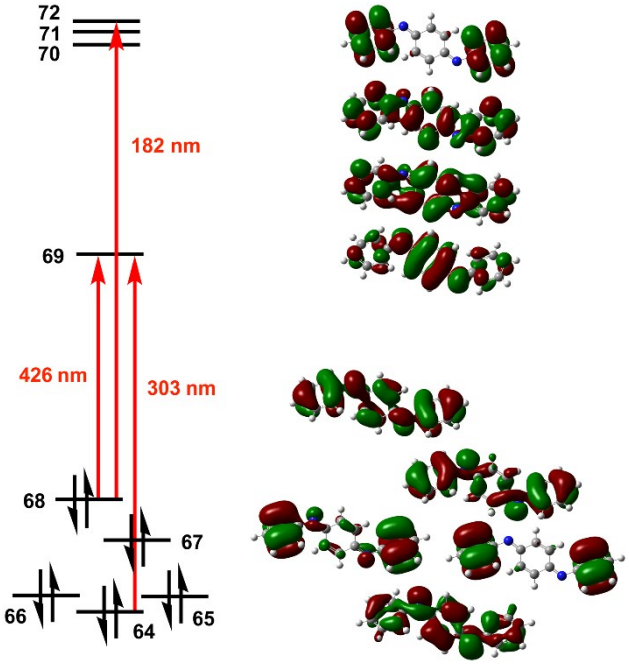


Figure S17. Frontier molecular orbitals of **DPPD**-PB calculated by DFT.

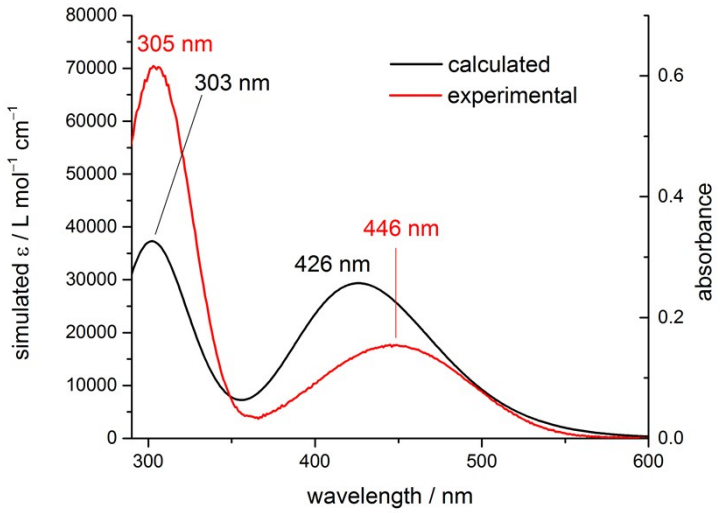


Figure S18. Simulated and experimental (THF) UV-vis-NIR spectra of **DPPD**-PB.

Table S9. Main optical transitions (*f* > 0.4) of **DPPD**-LEB simulated by TD-DFT.

Energy / eV	**Wavelength / nm**	**Oscillator strength, *f***	**Major MO contributions**
2.91	426	0.72	68 (HOMO) → 69 (LUMO) (85%)
4.10	303	0.91	64 (HOMO−4) → 69 (LUMO) (62%)
6.82	182	0.46	68 (HOMO) → 72 (LUMO+3) (27%) 65 (HOMO−3) → 70 (LUMO+1) (24%)

DPPD-RC

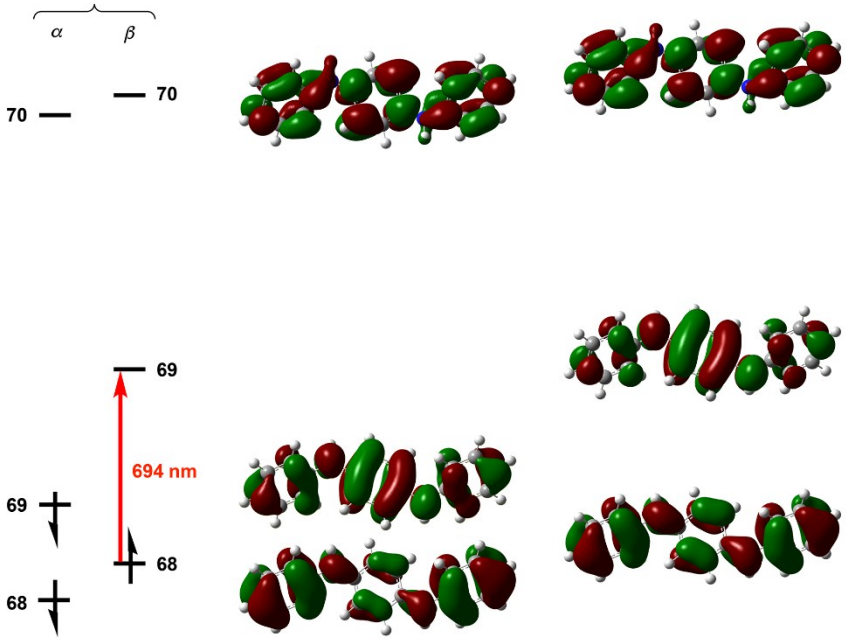


Figure S19. Frontier molecular orbitals of **DPPD**-RC calculated by DFT.

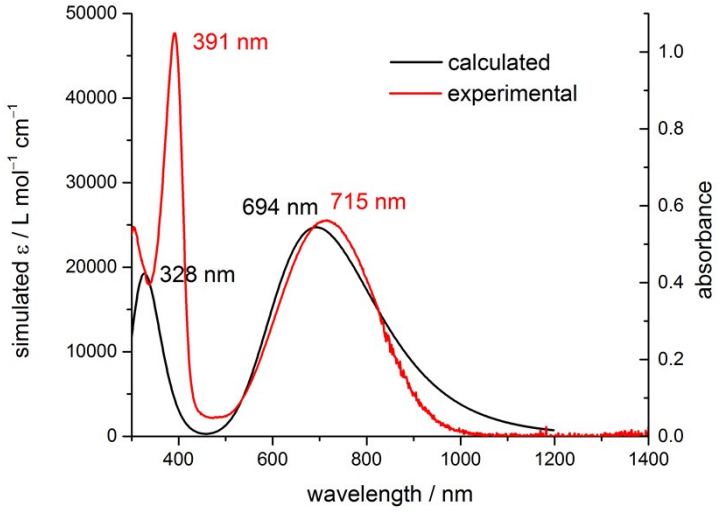


Figure S20. Simulated and experimental (THF, $HClO_4$) UV-vis-NIR spectra of **DPPD**-RC.

Table S10. Main optical transitions (f > 0.3) of **DPPD**-RC simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
1.79	694	0.61	68B (β HOMO) → 69B (LUMO) (95%)
3.84	323	0.36	69A (HOMO) → 70A (α LUMO) (53%)

TANI

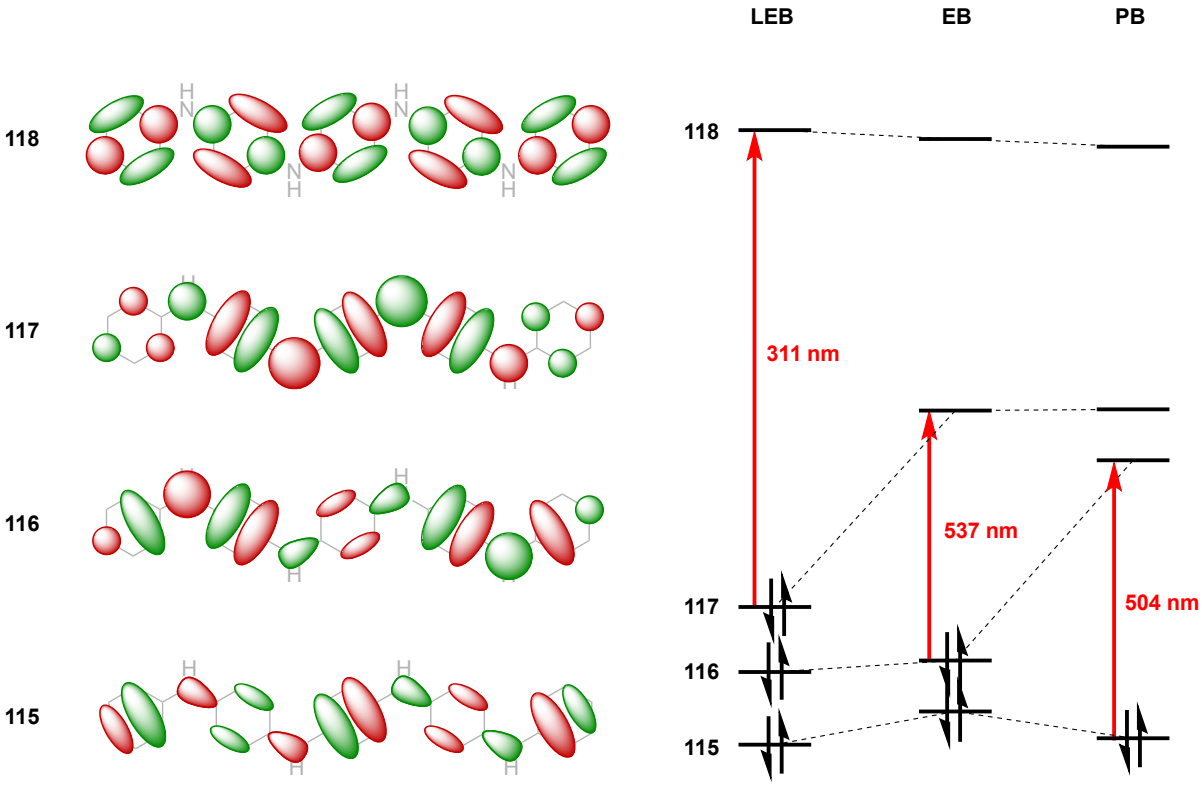


Figure S21. Approximate shapes of the DFT-calculated frontier molecular orbitals of **TANI**-LEB, EB and PB compared, alongside the corresponding energy levels and characteristic TD-DFT-calculated optical transitions.

Conformational isomerism

Table S11. Simulated UV-vis-NIR maxima of linear and sigmoid conformers of **TANI** in six different oxidation states, calculated with TD-DFT (CAM-B3LYP/6-31G*).

Oxidation state	Simulated λ_{max}(linear) / nm	Simulated λ_{max}(sigmoid) / nm
LEB	309	310
EB	537	538
PB	503	503
RC	1256	1306
^{1}ES	1021	1032
^{3}ES	798	812

TANI-LEB

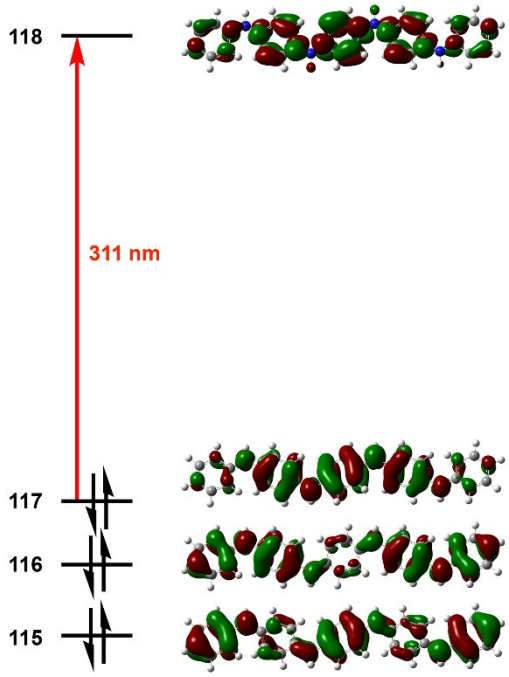


Figure S22. Frontier molecular orbitals of **TANI**-LEB calculated by DFT.

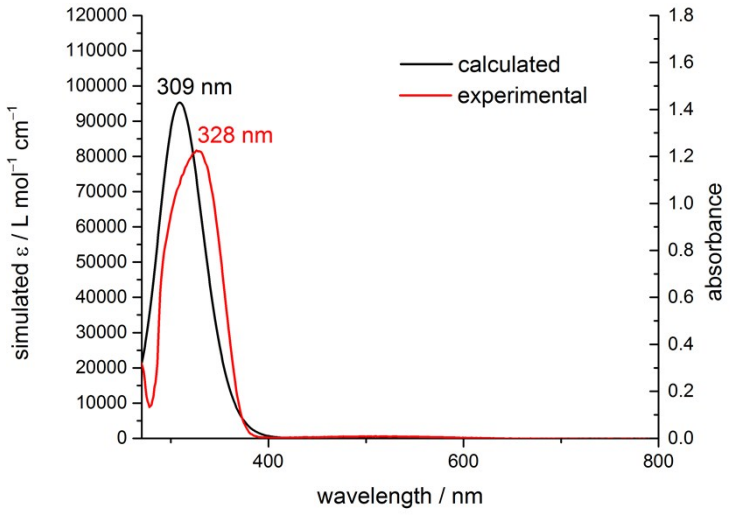


Figure S23. Simulated and experimental (THF) UV-vis-NIR spectra of **TANI**-LEB.

Table S12. Main optical transitions (*f* > 0.3) of **TANI**-LEB simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
3.98	311	2.08	117 (HOMO) → 118 (LUMO) (77%)

TANI-EB

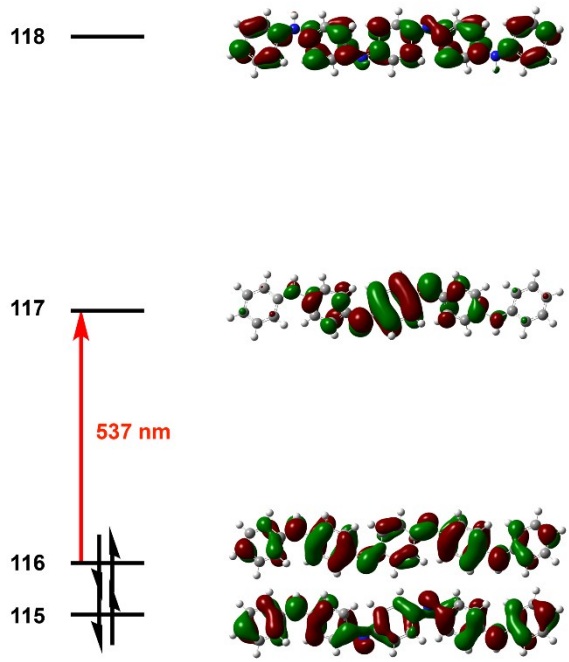


Figure S24. Frontier molecular orbitals of **TANI**-EB calculated by DFT.

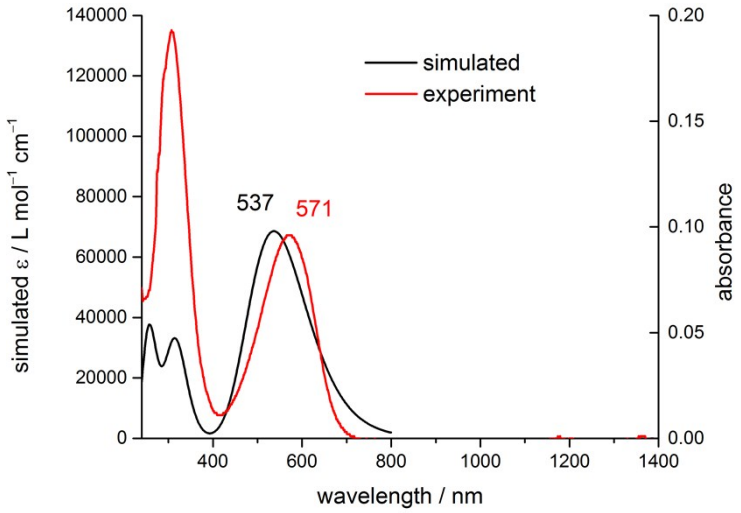


Figure S25. Simulated and experimental (THF) UV-vis-NIR spectra of **TANI**-EB.

Table S13. Main optical transitions (*f* > 0.3) of **TANI**-EB simulated by TD-DFT.

Energy / eV	**Wavelength / nm**	**Oscillator strength, *f***	**Major MO contributions**
2.31	537	1.69	116 (HOMO) → 117 (LUMO) (90%)
3.91	317	0.76	116 (HOMO) → 117 (LUMO) (54%) 105 (HOMO−11) → 117 (LUMO) (19%)
4.85	256	0.38	116 (HOMO) → 121 (LUMO+4) (20%)

TANI-PB

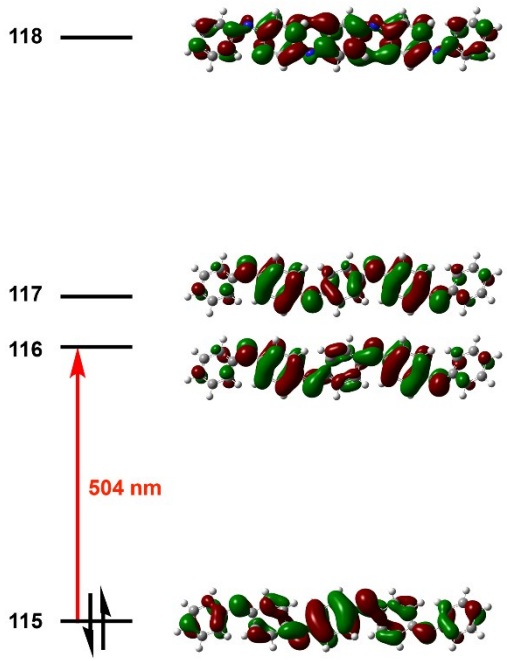


Figure S26. Frontier molecular orbitals of **TANI**-PB calculated by DFT.

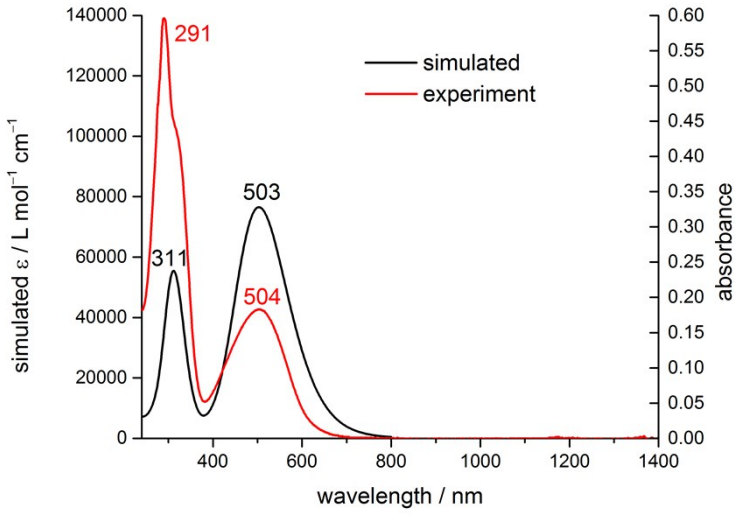


Figure S27. Simulated and experimental (THF) UV-vis-NIR spectra of **TANI**-PB.

Table S14. Main optical transitions ($f > 0.2$) of **TANI**-PB simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
2.46	504	1.88	115 (HOMO) → 116 (LUMO) (86%)
3.97	313	1.34	108 (HOMO−7) → 116 (LUMO) (32%)

TANI-ES

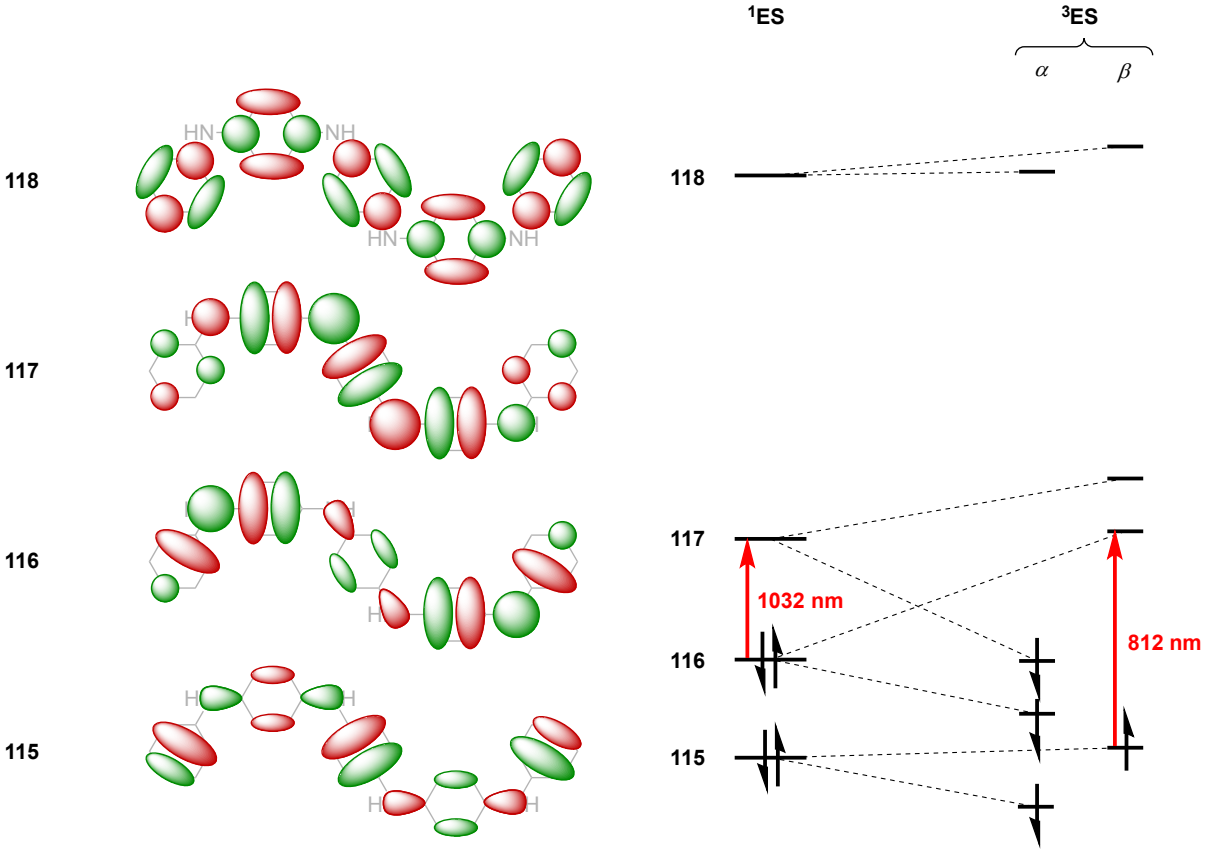


Figure S28. Approximate shapes of the DFT-calculated frontier molecular orbitals of **TANI**-^{1}ES and ^{3}ES (sigmoid conformation) compared, alongside the corresponding energy levels and characteristic TD-DFT-calculated optical transitions.

TANI-^{1}ES

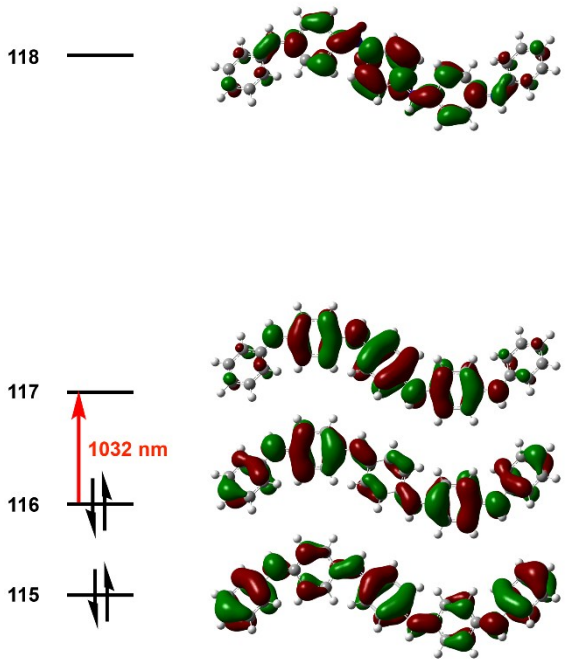


Figure S29. Frontier molecular orbitals of **TANI**-^{1}ES calculated by DFT.

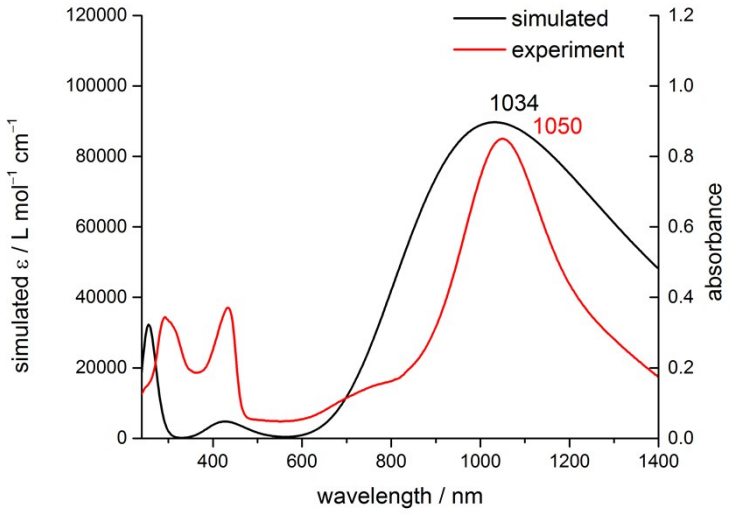


Figure S30. Simulated and experimental (THF, 1.1 mM $HClO_4$) UV-vis-NIR spectra of **TANI**-^{1}ES (0.5 mM).

Table S15. Main optical transitions (f > 0.2) of **TANI**-^{1}ES simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, f	Major MO contributions
1.20	1032	2.21	116 (HOMO) → 117 (LUMO) (96%)
4.86	255	0.72	116 (HOMO) → 122 (LUMO+5) (68%) 115 (HOMO−1) → 118 (LUMO+1) (20%)

TANI-^{3}ES

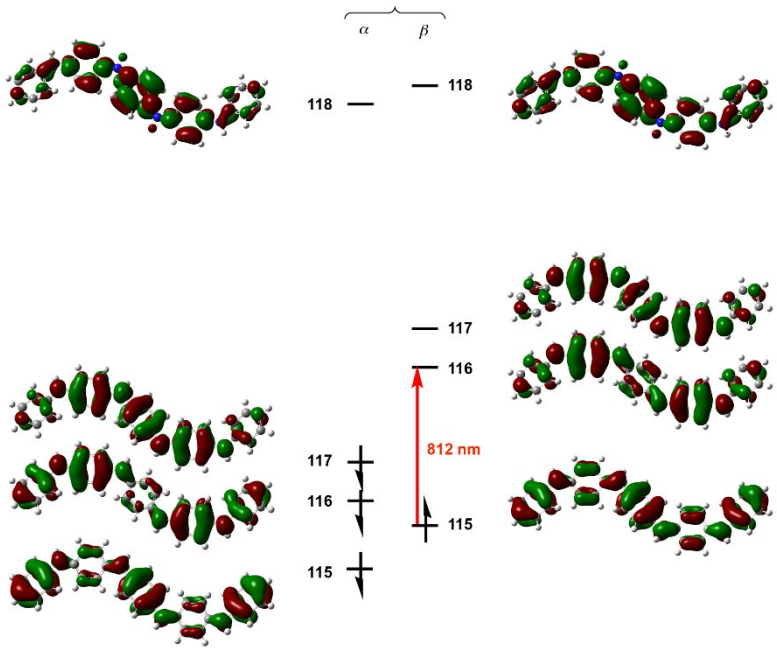


Figure S31. Frontier molecular orbitals of **TANI**-^{3}ES calculated by DFT.

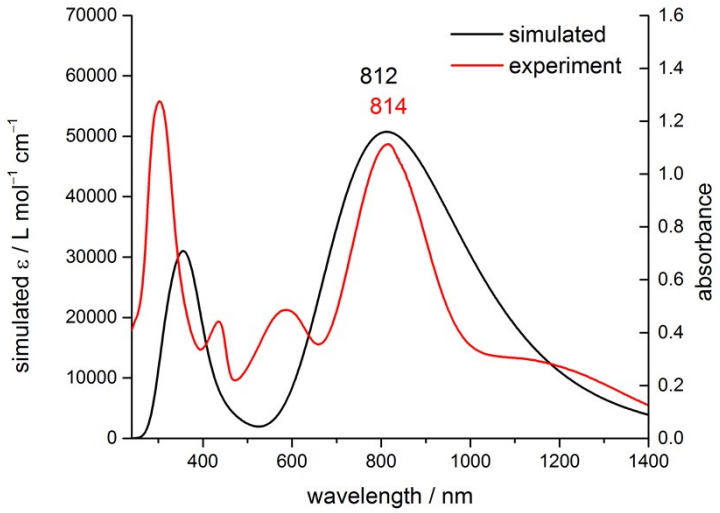


Figure S32. Simulated and experimental (THF, 0.4 mM $HClO_4$) UV-vis-NIR spectra of **TANI**-^{3}ES (0.5 mM).

Table S16. Main optical transitions (*f* > 0.2) of **TANI**-^{1}ES simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
1.53	812	1.25	115B (β HOMO) → 116B (LUMO) (80%)
3.35	370	0.56	117A (HOMO) → 118A (α LUMO) (39%)

OANI

OANI-LEB

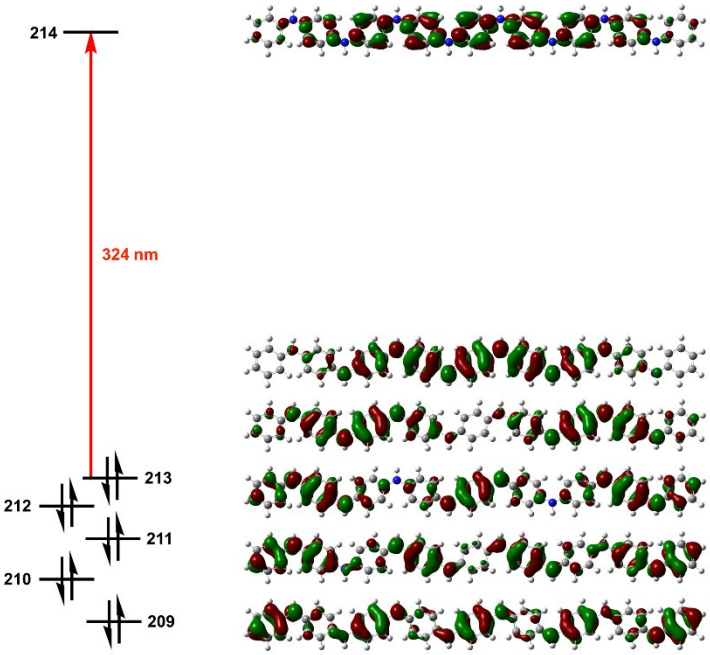


Figure S33. Frontier molecular orbitals of **OANI**-LEB calculated by DFT.

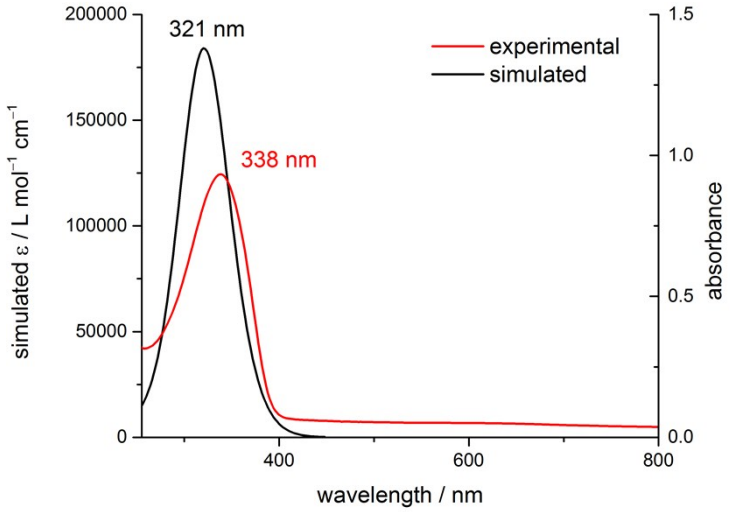


Figure S34. Simulated and experimental (DMSO) UV-vis-NIR spectra of **OANI**-LEB.

Table S17. Main optical transitions (*f* > 0.4) of **OANI**-LEB simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
3.82	324	4.06	213 (HOMO) → 214 (LUMO) (56%) 212 (HOMO−1) → 215 (LUMO+1) (17%)

OANI-EB

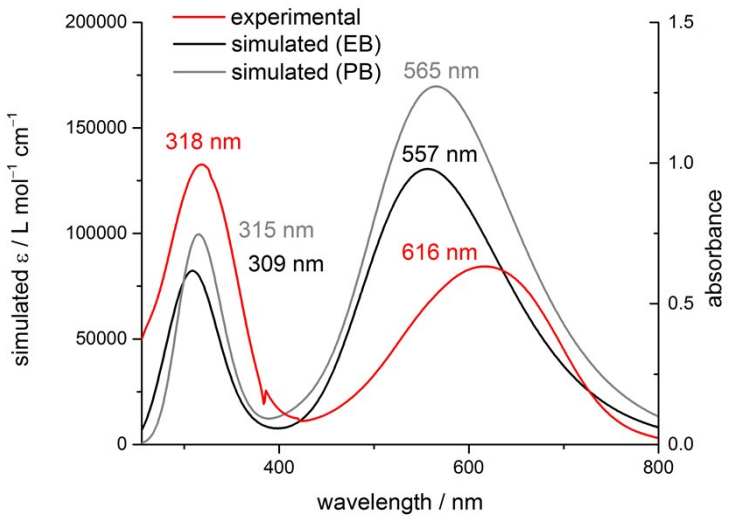


Figure S35. Experimental (DMSO) UV-vis-NIR spectrum of **OANI**-EB with simulated spectra of **OANI**-EB and PB.

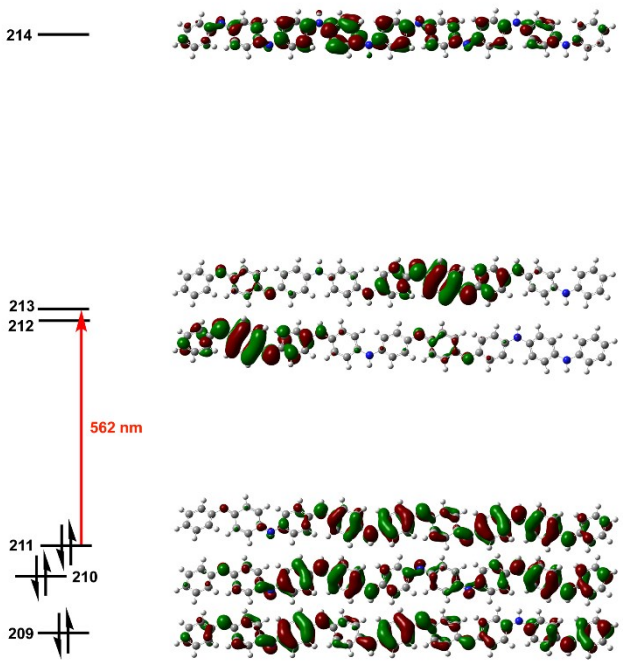


Figure S36. Frontier molecular orbitals of **OANI**-EB calculated by DFT.

Table S18. Main optical transitions (*f* > 0.4) of **OANI**-EB simulated by TD-DFT.

Energy / eV	**Wavelength / nm**	**Oscillator strength, *f***	**Major MO contributions**
2.21	562	2.87	211 (HOMO) → 213 (LUMO+1) (45%) 211 (HOMO) → 212 (LUMO) (29%)

OANI-PB

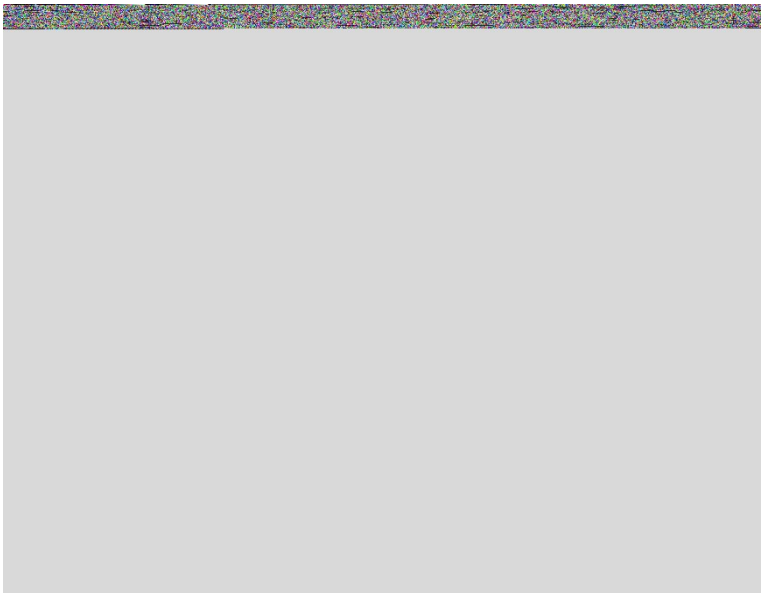


Figure S37. Experimental (DMSO) UV-vis-NIR spectrum of **OANI**-EB with simulated spectra of **OANI**-EB and PB.

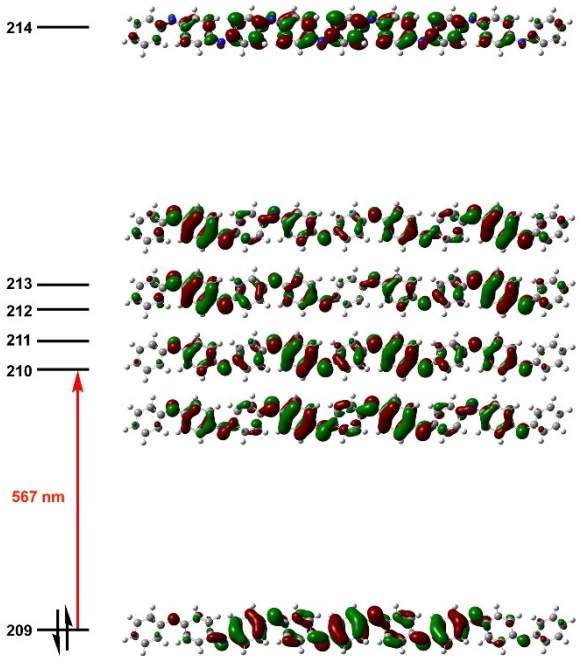


Figure S38. Frontier molecular orbitals of **OANI**-PB calculated by DFT.

Table S19. Main optical transitions (f > 0.4) of **OANI**-PB simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, f	Major MO contributions
2.19	567	4.14	209 (HOMO) → 210 (LUMO) (69%) 208 (HOMO−1) → 211 (LUMO+1) (16%)
3.88	319	1.56	196 (HOMO−13) → 210 (LUMO) (18%) 193 (HOMO−16) → 213 (LUMO+3) (12%)
4.02	308	0.79	208 (HOMO−1) → 211 (LUMO+1) (34%) 209 (HOMO) → 210 (LUMO) (18%)

OANI-^{1}ES

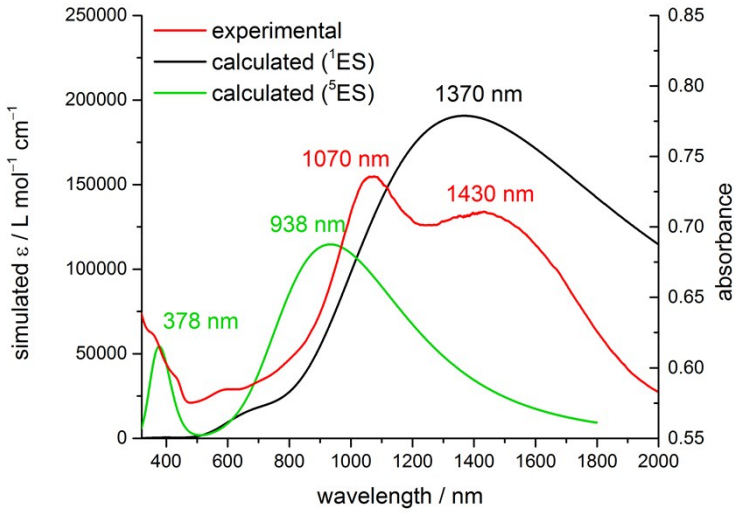


Figure S39. Experimental UV-vis-NIR spectrum of **OANI**-ES (*m*-cresol, **CSA**) with simulated spectra of **OANI**-^{1}ES and ^{5}ES.

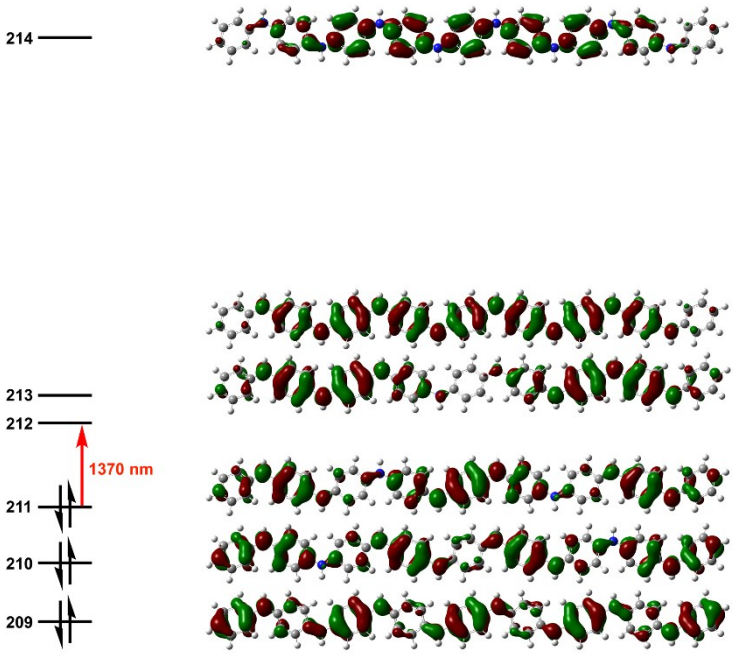


Figure S40. Frontier molecular orbitals of **OANI**-^{1}ES calculated by DFT.

Table S20. Main optical transitions (f > 0.3) of **OANI**-^{1}ES simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, f	Major MO contributions
0.90	1370	4.70	211 (HOMO) → 212 (LUMO) (90%)
1.73	716	0.39	210 (HOMO−1) → 213 (LUMO+1) (72%)

OANI-^{5}ES

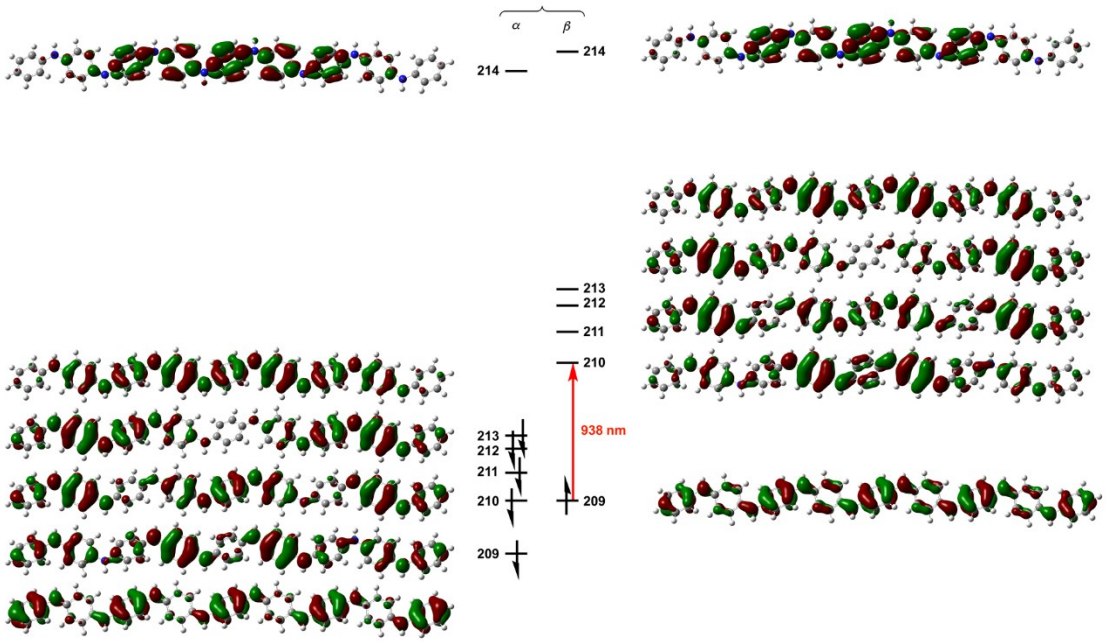


Figure S41. Frontier molecular orbitals of **OANI**-^{5}ES calculated by DFT.

Table S21. Main optical transitions (*f* > 0.4) of **OANI**-^{5}ES simulated by TD-DFT.

Energy / eV	Wavelength / nm	Oscillator strength, *f*	Major MO contributions
1.32	938	2.80	209B (β HOMO) → 210B (LUMO) (62%)
3.30	375	0.91	213A (HOMO) → 214A (α LUMO) (23%) 209B (β HOMO) → 210B (LUMO) (19%) 208B (β HOMO−1) → 211B (LUMO+1) (11%) 212A (HOMO−1) → 215A (α LUMO+1) (11%)

Experimental spectra

Ultraviolet-visible-near-infrared (UV-vis-NIR) spectroscopy

DPPD doping

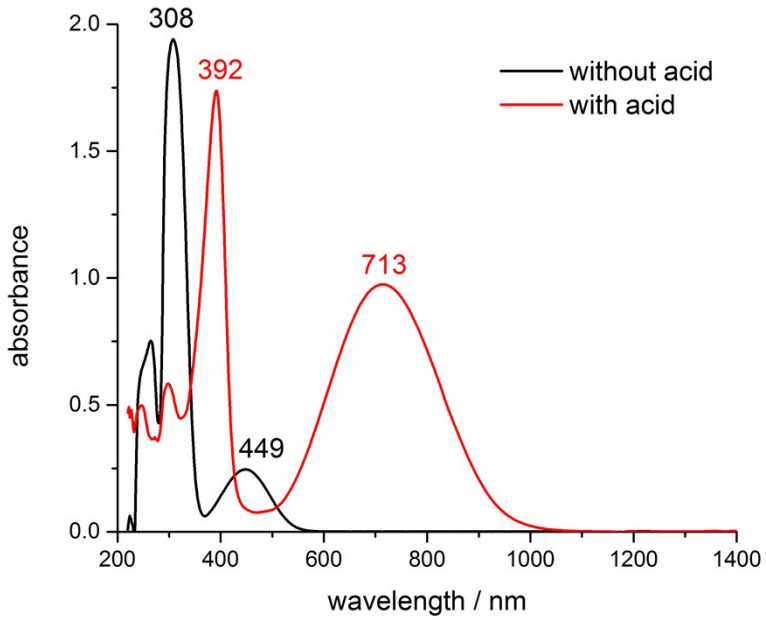


Figure S42. Experimental UV-vis-NIR spectra of an equimolar mixture of **DPPD-LEB** and **DPPD-PB** (43 µM) dissolved in THF, before and after the addition of a drop of concentrated $HClO_4$(aq).

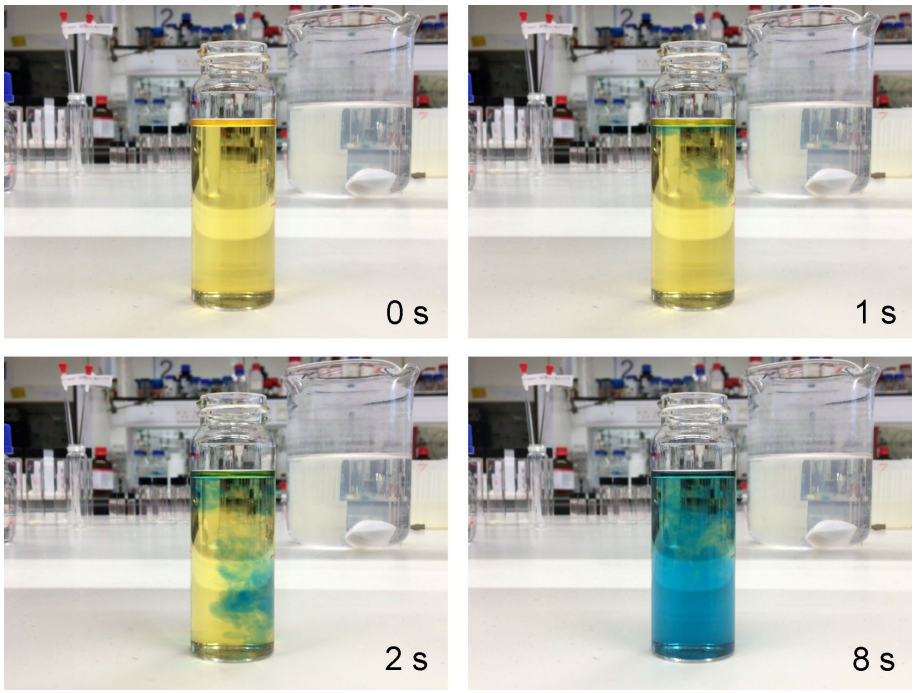


Figure S43. Frames from a video showing the rapid color change upon the addition of a drop of concentrated $HClO_4$(aq) to an equimolar mixture of **DPPD-LEB** and **DPPD-PB** (43 µM) dissolved in THF, associated with the formation of **DPPD-RC**.

TANI doping

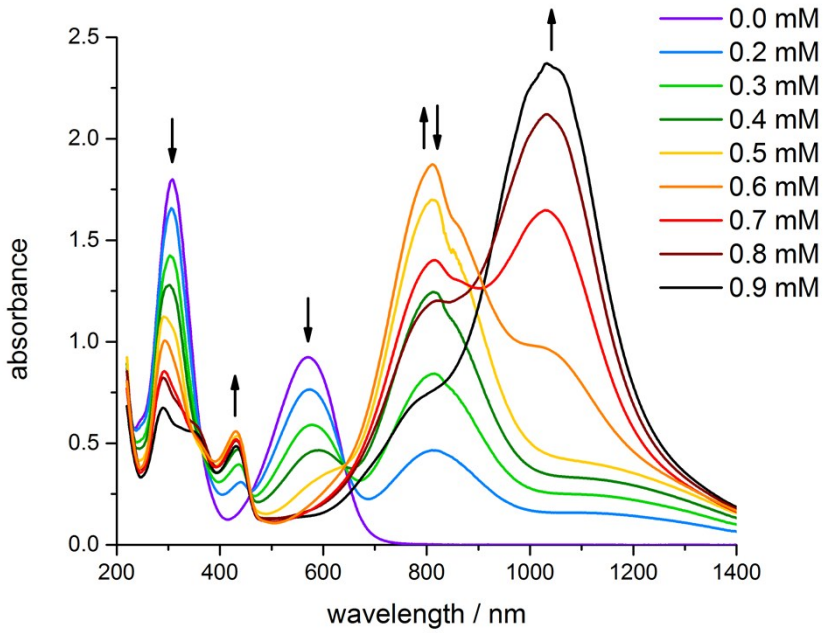


Figure S44. Experimental UV-vis-NIR spectra of solutions of **TANI**-EB (0.5 mM) in THF, at different concentrations of $HClO_4$. Optical path length = 1 mm.

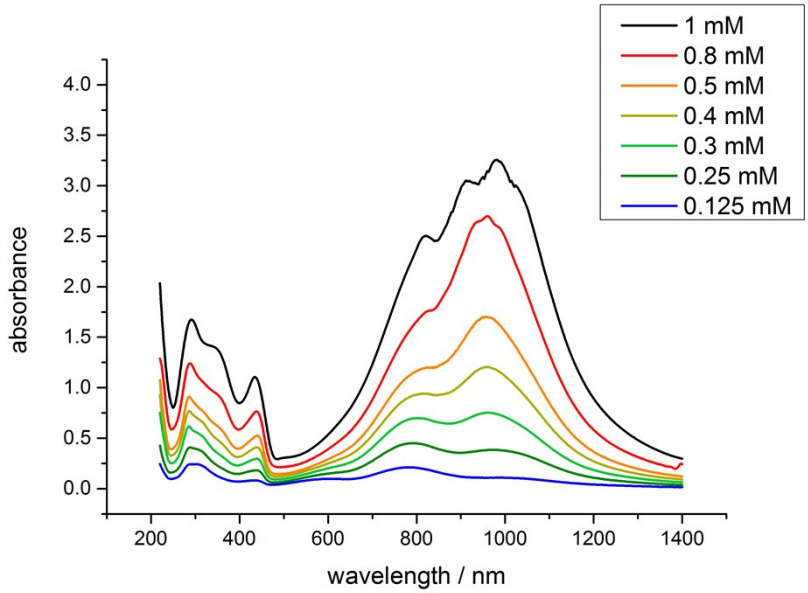


Figure S45. Experimental UV-vis-NIR spectra of solutions of **TANI**-EB in THF at different concentrations, doped with 2 equivalents of camphor-10-sulfonic acid (CSA) in each case. Optical path length = 1 cm.

Electron spin resonance (ESR) spectroscopy

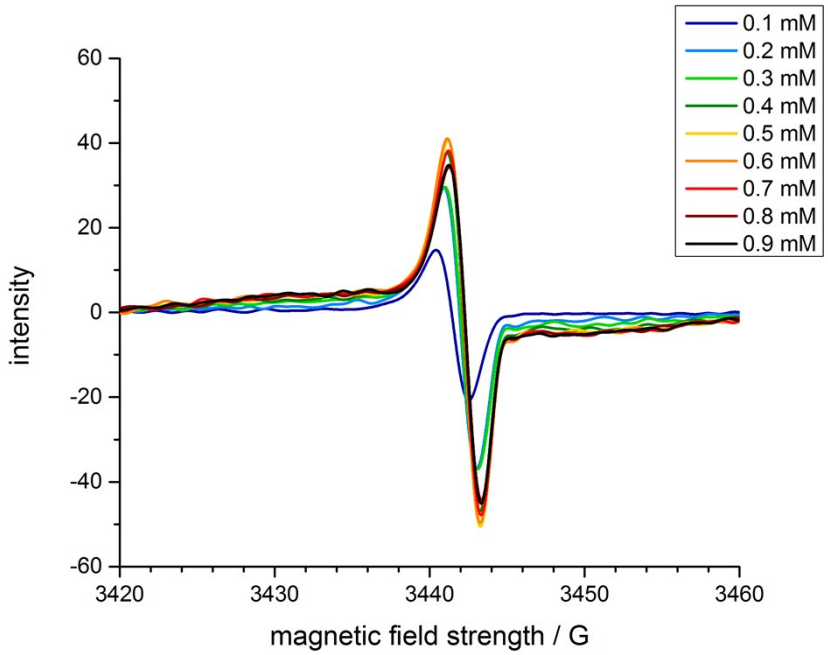


Figure S46. Experimental ESR spectra of solutions of **TANI**-EB (0.5 mM) in THF, at different concentrations of $HClO_4$.

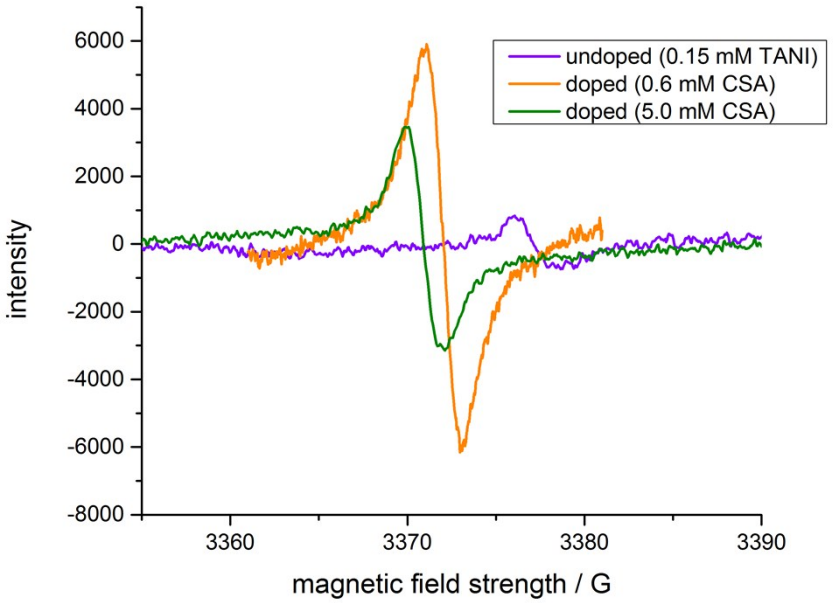


Figure S47. Experimental ESR spectra of solutions of **TANI**-EB (0.15 mM) in THF, at different concentrations of camphor-10-sulfonic acid (CSA).

Crystal structure of $HClO_4$-doped TANI

A solution of **TANI**-EB (0.5 mM) in THF was prepared and doped with $HClO_4$ (1.0 mM) in preparation for UV-vis-NIR analysis. After the green solution was left to stand for several days, it was found to contain red crystals with a metallic lustre that were examined by single-crystal X-ray diffraction. Single crystal X-ray diffraction of **TANI**-ES was carried out at 100(2) K on a Bruker Microstar rotating anode CCD diffractometer using Cu-Kα radiation (λ = 1.54184 Å). Intensities were integrated[19] and absorption corrections were based on equivalent reflections using SADABS.[20] The structure was solved using Superflip[21, 22] and refined against F^2 in SHELXL[23, 24] using Olex2.[25] All of the non-hydrogen atoms were refined anisotropically. Hydrogen atoms on heteroatoms were found by difference map, all other hydrogen atoms were located geometrically and refined using a riding model. The perchlorate counterion and THF solvent molecule were disordered and modelled in two positions with refined occupancies of 88% and 12%, and 53% and 47%, respectively. Equivalent atom distances, in the major and minor component, have been restrained to be the same and atoms in close proximity have been restrained to have the same ADP. CCDC 1562964, crystal structure and refinement data are given in Table S22. Two similar structures have been reported previously.[26, 27] Those earlier crystals, [**TANI**-ES]·2ClO_4·MeCN and [**TANI**-ES]·2BF_4·MeCN, contained one solvent molecule per **TANI** molecule rather than two and the solvent was acetonitrile rather than THF. More importantly, the full crystallographic details including the atomic coordinates were never published.

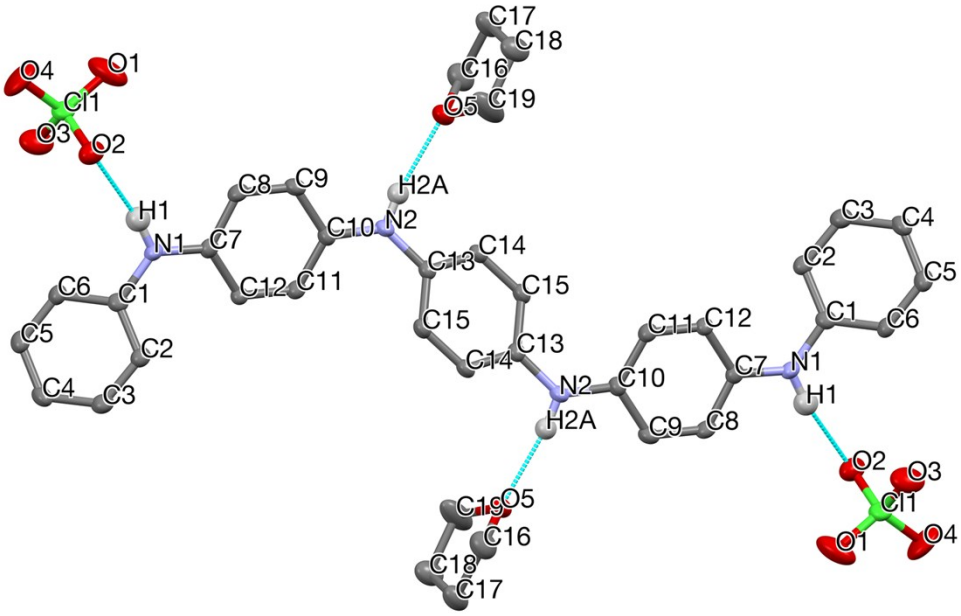


Figure S48. Mercury representation of [**TANI**-ES]·2ClO_4·2THF (CCDC 1562964); thermal ellipsoids shown at 50% probability, disordered counterion and solvent atoms and hydrogen atoms, except those on heteroatoms, omitted for clarity. The symmetry generated half of the structure, i, is related by −X, 1−Y, 1−Z.

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Table S22. Crystal data and structure refinement for [**TANI**-ES]·2ClO$_4$·2THF.

Identification code	[TANIES][2ClO4][2THF]
Empirical formula	$C_{38}H_{42}Cl_2N_4O_{10}$
Formula weight	785.65
Temperature / K	100
Crystal system	monoclinic
Space group	$P2_1/n$
a / Å	7.6212(7)
b / Å	16.5016(16)
c / Å	14.1509(14)
α / °	90
β / °	92.261(6)
γ / °	90
Volume / Å^3	1778.3(3)
Z	2
ρ_{calc}g / cm^3	1.467
μ / mm^{-1}	2.211
F(000)	824.0
Crystal size / mm^3	0.2 × 0.07 × 0.04
Radiation	Cu Kα (λ = 1.54178)
2ϑ range for data collection / °	8.234 to 133.102
Index ranges	−9 ≤ h ≤ 7, -19 ≤ k ≤ 19, −15 ≤ l ≤ 16
Reflections collected	26784
Independent reflections	3117 [R_{int} = 0.0955, R_{sigma} = 0.0519]
Data/restraints/parameters	3117/360/344
Goodness-of-fit on F^2	1.065
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0540, wR_2 = 0.1291
Final R indexes [all data]	R_1 = 0.0686, wR_2 = 0.1384
Largest diff. peak/hole / e Å^{-3}	0.43/−0.35

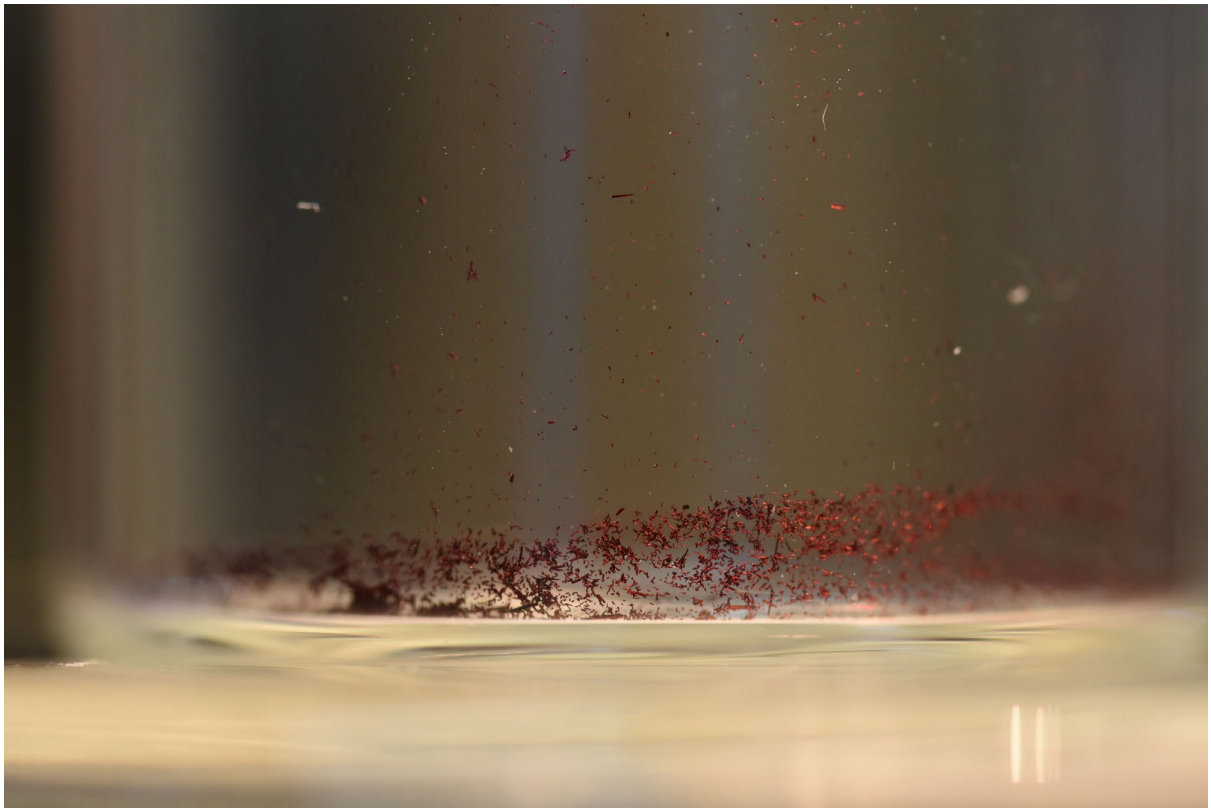

Figure S49. Lustrous red crystals of [**TANI**-ES]·2ClO_4·2THF.

Comparison of calculated and experimental transitions

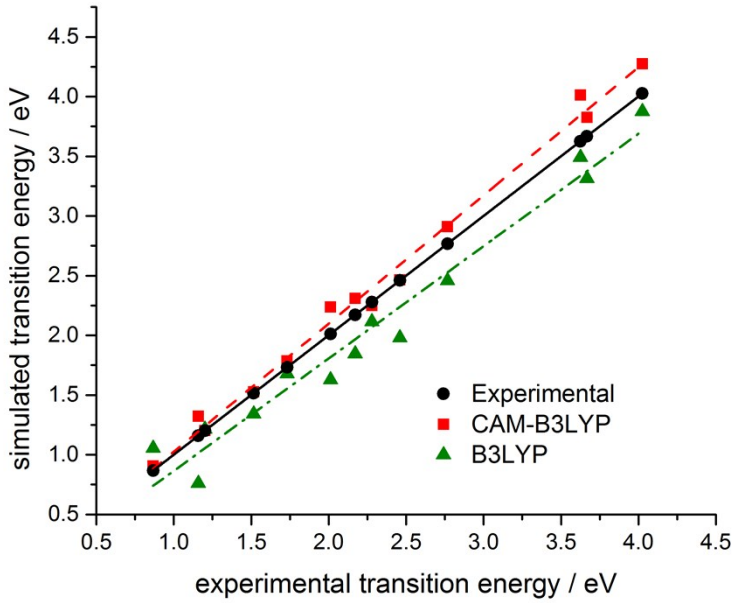

*Figure S50. C*omparison of the energies of simulated and experimental UV-vis-NIR maxima associated with electronic transitions in the LEB, EB, PB, RC and ES states of **DPPD**, **TANI** and **OANI**.

Table S23. Comparison of functional effects on TANI-EB main absorptions predicted by TD-DFT. Geometries optimised with B3LYP/6-31G(d), PCM solvation, TD-DFT calculation with functional as shown, PCM solvation. (All functionals as implemented in Gaussian09, see documentation for full references.

Approach	Absorption 1 (nm)	Absorption 2 (nm)
Experiment	571	308
B3LYP	674	343
CAM-B3LYP (used here)	537	321
CAM-B3LYP/6-311G(d)//B3LYP/6-311G(d)	545	322
ωB97XD	524	321
M06	651	338
PBE0	648	334

Also note the following recent evaluation of functionals for a broader range of compounds: T. M. Maier, H. Bahmann, A. V. Arbuznikov, M. Kaupp, *J. Chem. Phys.* **2016**, *144*, 074106, http://dx.doi.org/10.1063/1.4941919.

Cartesian coordinates of DFT models

Cartesian atomic coordinates (in Å) of phenyl-capped oligo(aniline)s at the B3LYP/6-31G* level.

DPPD-LEB	x	y	z
H	3.09162000	4.40214200	0.46632000
C	3.05133000	3.89719000	1.42888600
C	2.93698000	2.61527700	3.89398400
C	2.39002300	2.65566600	1.52624400
C	3.64455700	4.47749100	2.54634700
C	3.58711600	3.84698100	3.79336500
C	2.34898400	2.01555400	2.77969600
H	4.14922400	5.43457300	2.44112000
H	4.04223200	4.30535700	4.66637100
H	1.87995900	1.04345800	2.87895700
H	2.89336100	2.10025700	4.85049300
N	1.84355200	2.10782600	0.36479200
H	2.23066600	2.46154600	-0.49953200
C	0.93441800	1.04778300	0.22265500
C	-0.93441800	-1.04778300	-0.22265500
C	1.00104200	0.24338100	-0.92749100
C	-0.08996500	0.78524900	1.14871200
C	-1.00104200	-0.24338100	0.92749100
C	0.08996500	-0.78524900	-1.14871200
H	1.79230100	0.41667200	-1.65308200
H	-0.19915100	1.40607200	2.03102000
H	-1.79230100	-0.41667200	1.65308200
H	0.19915100	-1.40607200	-2.03102000
N	-1.84355200	-2.10782600	-0.36479200
H	-2.23066600	-2.46154600	0.49953200
C	-2.39002300	-2.65566600	-1.52624400
C	-3.58711600	-3.84698100	-3.79336500
C	-2.34898400	-2.01555400	-2.77969600
C	-3.05133000	-3.89719000	-1.42888600
C	-3.64455700	-4.47749100	-2.54634700
C	-2.93698000	-2.61527700	-3.89398400
H	-1.87995900	-1.04345800	-2.87895700
H	-3.09162000	-4.40214200	-0.46632000
H	-4.14922400	-5.43457300	-2.44112000
H	-2.89336100	-2.10025700	-4.85049300

DPPD-PB	x	y	z
C	-4.02868500	-0.84863600	0.63298400
C	-5.31117900	-1.35321600	0.41851900
C	-6.29117400	-0.56492100	-0.18926100
C	-5.98594000	0.74950700	-0.55961700
C	-4.71767500	1.27159900	-0.32200700
C	-3.70971300	0.47033600	0.25012000
H	-3.27966200	-1.45659300	1.13141700
H	-5.54393000	-2.36777200	0.73070100
H	-7.28695800	-0.96406600	-0.35909400
H	-6.74482500	1.37475200	-1.02223500
H	-4.47862200	2.29696700	-0.58833700
N	-2.47373600	1.07122200	0.51684900
C	-1.32995000	0.51183700	0.24389200
C	-0.13093900	1.19625200	0.73219900
H	-0.29790800	2.09784800	1.31411600
C	-1.11433400	-0.71981100	-0.52070000
H	-1.97470500	-1.22953600	-0.93905600
C	0.13096200	-1.19644100	-0.73198000
H	0.29793700	-2.09804100	-1.31388900
C	1.11435900	0.71961500	0.52092900
H	1.97472700	1.22931800	0.93931900
C	1.32997400	-0.51202700	-0.24367300
N	2.47376400	-1.07133700	-0.51674000
C	3.70972900	-0.47035700	-0.25009600
C	4.71774200	-1.27143500	0.32217100
C	4.02860600	0.84856200	-0.63323900
C	5.98598900	-0.74920800	0.55962100
H	4.47877600	-2.29676200	0.58873900
C	5.31107200	1.35327000	-0.41892000
H	3.27951300	1.45635800	-1.13176000
C	6.29113600	0.56515400	0.18898500
H	6.74492000	-1.37431700	1.02235000
H	5.54375600	2.36777800	-0.73131000
H	7.28690100	0.96439600	0.35870500

H	-4.04223200	-4.30535700	-4.66637100

DPPD-^{1}ES	x	y	z
C	4.07259700	-0.93890800	-0.44019900
C	5.36777400	-1.42276000	-0.31041600
C	6.40373700	-0.57698800	0.10490200
C	6.15010600	0.77442700	0.37098100
C	4.86493900	1.27916400	0.23846000
C	3.81786400	0.41306900	-0.13660600
H	3.29305300	-1.57884100	-0.83469200
H	5.57572900	-2.45825600	-0.55760700
H	7.41245500	-0.96594200	0.19838200
H	6.95615300	1.43236100	0.67730800
H	4.65602600	2.32344600	0.44968900
N	2.54122300	0.98793800	-0.25027400
C	1.32115300	0.47562700	-0.10542300
C	0.20381800	1.29816900	-0.51417700
H	0.40153300	2.27124900	-0.95183200
C	1.06829700	-0.83874300	0.43147800
H	1.88373500	-1.43432300	0.81872700
C	-0.20382500	-1.29818000	0.51421100
H	-0.40154000	-2.27125900	0.95186900
C	-1.06830400	0.83873300	-0.43144300
H	-1.88374500	1.43431500	-0.81868600
C	-1.32116000	-0.47564000	0.10545000
N	-2.54123000	-0.98795100	0.25029200
C	-3.81786700	-0.41307500	0.13660500
C	-4.86494700	-1.27916400	-0.23845700
C	-4.07258600	0.93891100	0.44017300
C	-6.15010700	-0.77441500	-0.37099300
H	-4.65604400	-2.32345100	-0.44966900
C	-5.36775700	1.42277400	0.31037500
H	-3.29303400	1.57884200	0.83465600
C	-6.40372600	0.57700700	-0.10493600
H	-6.95616000	-1.43234500	-0.67731600
H	-5.57570100	2.45827700	0.55754600
H	-7.41244000	0.96597000	-0.19843000
H	2.56092100	1.98198700	-0.47887400
H	-2.56093400	-1.98199800	0.47889800

DPPD-^{3}ES	x	y	z
C	3.96313200	0.92588000	0.33218800
C	5.23019200	1.46977200	0.33379400
C	6.35383000	0.67111800	0.04079200
C	6.20184600	-0.70139500	-0.23816200
C	4.94755200	-1.27083200	-0.23821500
C	3.80067900	-0.45874300	0.02466600
H	3.10792100	1.52845100	0.61031300
H	5.36294300	2.51680600	0.58301200
H	7.34436600	1.11340900	0.04653400
H	7.07226800	-1.31097300	-0.45396300
H	4.81394900	-2.32496200	-0.46072200
N	2.58590900	-1.06917400	0.00831700
C	1.29711400	-0.50326200	0.00518300
C	0.27418900	-1.19733100	0.67382900
H	0.49781000	-2.10785700	1.21951100
C	1.01596500	0.69074000	-0.68259300
H	1.78309600	1.19210200	-1.25983400
C	-0.27415800	1.19726600	-0.67379300
H	-0.49777500	2.10780100	-1.21946000
C	-1.01593500	-0.69080600	0.68262800
H	-1.78305400	-1.19215400	1.25989500
C	-1.29708900	0.50318900	-0.00516100
N	-2.58587700	1.06911500	-0.00829900
C	-3.80067000	0.45872400	-0.02466100
C	-4.94750500	1.27085200	0.23826000
C	-3.96319300	-0.92587600	-0.33225500
C	-6.20182700	0.70147400	0.23818900
H	-4.81385300	2.32496600	0.46081300
C	-5.23027800	-1.46970900	-0.33387800
H	-3.10801800	-1.52847300	-0.61042800
C	-6.35387700	-0.67101800	-0.04082700
H	-7.07221800	1.31108400	0.45402400
H	-5.36308100	-2.51672300	-0.58315000
H	-7.34443400	-1.11326200	-0.04658600
H	2.60797500	-2.08740600	0.00178800
H	-2.60792100	2.08734700	-0.00177000

DPPD-^{1}MP	x	y	z
C	-4.07366400	-0.88177200	0.55680500
C	-5.35667500	-1.37058700	0.31520600
C	-6.32561800	-0.55474400	-0.27364800
C	-6.01354000	0.76441200	-0.61566800
C	-4.73505800	1.26507600	-0.38437100
C	-3.76264400	0.43320400	0.18621200
H	-3.33863600	-1.50069100	1.05940700
H	-5.60097500	-2.38763500	0.60540000
H	-7.32387700	-0.94115300	-0.45447000
H	-6.76507600	1.40544800	-1.06567000
H	-4.48310600	2.28576100	-0.65665000
N	-2.47759500	0.99381600	0.43581100
C	-1.26644000	0.45953200	0.26151500
C	-0.12790600	1.20258500	0.74657100
H	-0.30425300	2.13173500	1.28007700
C	-1.05654600	-0.81262400	-0.37566100
H	-1.90162800	-1.36426400	-0.76612700
C	0.20541400	-1.29651500	-0.50600600
H	0.38947800	-2.24542600	-0.99790800
C	1.13248200	0.72750200	0.59118500
H	1.96740600	1.26744300	1.02097900
C	1.37288800	-0.54382200	-0.07747300
N	2.53449900	-1.10434400	-0.31101500
C	3.75515800	-0.47031300	-0.19434600
C	4.84930200	-1.28474600	0.18516200
C	3.99104300	0.88775800	-0.52553400
C	6.11656800	-0.73611400	0.32309200
H	4.66247500	-2.33244000	0.39702700
C	5.27415900	1.41284700	-0.42692800
H	3.18574800	1.49393600	-0.92646200
C	6.33405600	0.61344500	0.01616600
H	6.94333900	-1.36041700	0.64758300
H	5.45305000	2.44650600	-0.70682400
H	7.33213200	1.03351400	0.09559800
H	-2.49227700	1.95064600	0.78079000

DPPD-^{3}MP	x	y	z
C	-3.92080900	-0.90872900	0.55522400
C	-5.09017400	-1.63200900	0.33664100
C	-6.10615900	-1.11398500	-0.47170800
C	-5.95556300	0.14793300	-1.05692100
C	-4.79293000	0.88173100	-0.85057800
C	-3.76170700	0.34647300	-0.05811900
H	-3.16337800	-1.29111600	1.22946200
H	-5.21451100	-2.59712900	0.81770000
H	-7.01602400	-1.68354800	-0.63319400
H	-6.74468700	0.56037300	-1.67770900
H	-4.66713900	1.85633400	-1.31312800
N	-2.61497000	1.13801100	0.14078500
C	-1.31955500	0.77012000	0.34207300
C	-0.40040400	1.77171300	0.77408500
H	-0.75802100	2.78292200	0.94479200
C	-0.83888000	-0.54914900	0.10097100
H	-1.50381600	-1.30490800	-0.29724500
C	0.48232700	-0.85430500	0.31961700
H	0.85204900	-1.85539600	0.12689400
C	0.91691400	1.46359100	0.99886300
H	1.60914900	2.22076700	1.34980900
C	1.39778100	0.14079100	0.77087000
N	2.67672600	-0.18999100	1.08427000
C	3.76570400	-0.20856500	0.31559100
C	5.00417600	-0.61823400	0.90980500
C	3.75495400	0.16212500	-1.07134600
C	6.15951400	-0.65419300	0.15411700
H	5.00044700	-0.89492600	1.95878400
C	4.92368400	0.11741900	-1.80563600
H	2.81941000	0.47419000	-1.52411700
C	6.12925400	-0.28880600	-1.20385900
H	7.09465200	-0.96543600	0.60894000
H	4.91254600	0.39769900	-2.85450400
H	7.04100200	-0.31971900	-1.79205300
H	-2.78274500	2.14022800	0.12204900

DPPD-RC	x	y	z
H	3.01326500	4.27282700	0.41798300
C	3.00153400	3.81147500	1.40149100
C	2.95203000	2.61642400	3.92545200
C	2.47990000	2.51621700	1.55735700
C	3.48254500	4.50243200	2.50935600
C	3.45235500	3.91246400	3.77680900
C	2.47328900	1.90959200	2.82398200
H	3.87788300	5.50560000	2.38230900
H	3.82721000	4.45434200	4.63960600
H	2.13828200	0.88537200	2.94101100
H	2.94985400	2.14107300	4.90162200
N	2.03606100	1.84468800	0.39847000
H	2.53667100	2.08748600	-0.45034400
C	1.03063600	0.93895300	0.24002900
C	-1.03063600	-0.93895300	-0.24002900
C	0.94739300	0.23858000	-0.99822900
C	0.04554500	0.67832200	1.23377800
C	-0.94739300	-0.23858000	0.99822900
C	-0.04554500	-0.67832200	-1.23377800
H	1.70652800	0.41175700	-1.75549800
H	0.05132500	1.22997200	2.16492300
H	-1.70652800	-0.41175700	1.75549800
H	-0.05132500	-1.22997200	-2.16492300
N	-2.03606100	-1.84468800	-0.39847000
H	-2.53667100	-2.08748600	0.45034400
C	-2.47990000	-2.51621700	-1.55735700
C	-3.45235500	-3.91246400	-3.77680900
C	-2.47328900	-1.90959200	-2.82398200
C	-3.00153400	-3.81147500	-1.40149100
C	-3.48254500	-4.50243200	-2.50935600
C	-2.95203000	-2.61642400	-3.92545200
H	-2.13828200	-0.88537200	-2.94101100
H	-3.01326500	-4.27282700	-0.41798300
H	-3.87788300	-5.50560000	-2.38230900
H	-2.94985400	-2.14107300	-4.90162200
H	-3.82721000	-4.45434200	-4.63960600

TANI-LEB	x	y	z
H	2.04700000	10.05700000	-1.09100000
C	2.29700000	9.97300000	-0.03600000
C	2.92800000	9.76600000	2.66400000
C	2.16200000	8.72400000	0.60600000
C	2.74200000	11.09000000	0.66500000
C	3.05600000	11.00100000	2.02600000
C	2.49400000	8.63500000	1.97100000
H	2.83800000	12.03800000	0.14300000
H	3.39400000	11.87600000	2.57400000
H	2.43200000	7.68300000	2.48500000
H	3.18000000	9.67000000	3.71700000
N	1.73100000	7.63700000	-0.15500000
H	1.86200000	7.73600000	-1.15300000
C	1.37000000	6.34600000	0.27300000
C	0.56800000	3.71200000	0.98900000
C	1.70700000	5.23900000	-0.52200000
C	0.61600000	6.11100000	1.43600000
C	0.23000000	4.82200000	1.78600000
C	1.31500000	3.94800000	-0.17800000
H	2.30000000	5.39000000	-1.42100000
H	0.30300000	6.94400000	2.05700000
H	-0.36200000	4.67100000	2.68500000
H	1.62200000	3.11900000	-0.80600000
N	0.17700000	2.43700000	1.41500000
H	0.03700000	2.34000000	2.41100000
C	0.11300000	1.24300000	0.68300000
C	-0.11300000	-1.24300000	-0.68300000
C	-0.20700000	1.19600000	-0.68500000
C	0.31500000	0.02200000	1.34900000
C	0.20700000	-1.19600000	0.68500000
C	-0.31500000	-0.02200000	-1.34900000
H	-0.40400000	2.11300000	-1.23000000
H	0.57800000	0.02900000	2.40500000
H	0.40400000	-2.11300000	1.23000000
H	-0.57800000	-0.02900000	-2.40500000
N	-0.17700000	-2.43700000	-1.41500000
H	-0.03700000	-2.34000000	-2.41100000
C	-0.56800000	-3.71200000	-0.98900000
C	-1.37000000	-6.34600000	-0.27300000
C	-0.23000000	-4.82200000	-1.78600000
C	-1.31500000	-3.94800000	0.17800000
C	-1.70700000	-5.23900000	0.52200000
C	-0.61600000	-6.11100000	-1.43600000
H	0.36200000	-4.67100000	-2.68500000
H	-1.62200000	-3.11900000	0.80600000
H	-2.30000000	-5.39000000	1.42100000
H	-0.30300000	-6.94400000	-2.05700000
N	-1.73100000	-7.63700000	0.15500000
H	-1.86200000	-7.73600000	1.15300000
C	-2.16200000	-8.72400000	-0.60600000
C	-3.05600000	-11.00100000	-2.02600000
C	-2.49400000	-8.63500000	-1.97100000
C	-2.29700000	-9.97300000	0.03600000
C	-2.74200000	-11.09000000	-0.66500000
C	-2.92800000	-9.76600000	-2.66400000
H	-2.43200000	-7.68300000	-2.48500000
H	-2.04700000	-10.05700000	1.09100000
H	-2.83800000	-12.03800000	-0.14300000
H	-3.18000000	-9.67000000	-3.71700000
H	-3.39400000	-11.87600000	-2.57400000

TANI-EB	x	y	z
C	0.11528700	1.34195600	-0.39224600
H	0.26129700	2.36386000	-0.73048100
C	-1.12765600	0.81566300	-0.28217800
H	-1.99281200	1.41204600	-0.54833500
C	-1.32611000	-0.56857600	0.13914700
C	-0.11530900	-1.34183900	0.39267900
H	-0.26131800	-2.36375600	0.73087500
C	1.12763600	-0.81554200	0.28264100
H	1.99279300	-1.41193800	0.54876800
C	1.32609600	0.56870500	-0.13867300
N	-2.46502100	-1.19899200	0.29269500
N	2.46500400	1.19911600	-0.29219200
C	-3.71068200	-0.58329700	0.28001600
C	-6.36816400	0.44721700	0.28908200
C	-4.79137900	-1.31611900	-0.25740800
C	-4.00841800	0.67212000	0.86129600
C	-5.30409800	1.16483100	0.87577900
C	-6.08163400	-0.80789600	-0.28778700
H	-4.58512000	-2.28947300	-0.69288100
H	-3.22540700	1.23583700	1.35812100
H	-5.50987400	2.11720400	1.35855300
H	-6.86638800	-1.37945600	-0.76884200
C	3.71066100	0.58334900	-0.27935600
C	6.36803600	-0.44736900	-0.28820900
C	4.00838100	-0.67194500	-0.86086500
C	4.79129900	1.31596800	0.25845500
C	6.08150100	0.80761600	0.28894000
C	5.30403800	-1.16476700	-0.87524600
H	3.22539500	-1.23548600	-1.35793000
H	4.58503700	2.28922500	0.69414400
H	6.86622300	1.37894700	0.77032800
H	5.50981100	-2.11704800	-1.35820200
N	7.63155400	-1.02828600	-0.28559400
N	-7.63171100	1.02802600	0.28674800
H	7.64126100	-2.03100900	-0.41883500
C	8.88851200	-0.44963000	-0.06230100
C	11.48144400	0.57937800	0.34773000
C	9.18258300	0.88980200	-0.37489900
C	9.91644300	-1.26868900	0.44145100
C	11.19739700	-0.75870600	0.63647300
C	10.46590100	1.39304700	-0.15907100
H	8.42136200	1.52688400	-0.81055600
H	9.69916900	-2.30654000	0.68269200
H	11.97497000	-1.41058800	1.02574600
H	10.67269800	2.43079500	-0.40726800
H	12.47839200	0.97844500	0.50943800
H	-7.64142700	2.03077000	0.41985300
C	-8.88854100	0.44950700	0.06222500
C	-11.48117700	-0.57924100	-0.35014400
C	-9.91588900	1.26863600	-0.44260400
C	-9.18305600	-0.88983700	0.37472700
C	-10.46622800	-1.39297300	0.15771500
C	-11.19671200	0.75878700	-0.63877800
H	-9.69823600	2.30642800	-0.68376000
H	-8.42232700	-1.52694500	0.81121200
H	-10.67337900	-2.43066800	0.40583400
H	-11.97385200	1.41069600	-1.02886900
H	-12.47802100	-0.97820400	-0.51275100

TANI-PB	x	y	z
H	8.31783200	1.35429800	-1.23831400
C	9.06000200	0.79181700	-0.67991200
C	11.00269200	-0.69763600	0.66720500
C	8.73425100	-0.48810900	-0.18534300
C	10.34145100	1.31160300	-0.49873700
C	11.31418100	0.57857700	0.18517800
C	9.73551900	-1.23692400	0.46484600
H	10.57941700	2.29426900	-0.89707000
H	12.30926900	0.98973500	0.32830700
H	9.49185300	-2.23443100	0.81844100
H	11.75599500	-1.28070900	1.19008700
N	7.50058200	-1.10868100	-0.41123800
C	6.35441100	-0.52267900	-0.20869700
C	5.16094200	-1.24201500	-0.65598100
H	5.33220200	-2.19034600	-1.15658300
C	3.91438500	-0.74251900	-0.50967500
H	3.05999200	-1.28082500	-0.90384300
C	6.13248200	0.77304700	0.43734900
H	6.98812500	1.31466300	0.82404700
C	4.88579300	1.27290000	0.58130900
H	4.71443800	2.22418400	1.07629000
C	3.69316700	0.55023100	0.14055500
N	2.54575800	1.13691700	0.34599500
C	1.31044700	0.52491700	0.15251000
C	-1.31048700	-0.52465500	-0.15373800
C	0.28154400	1.29648600	-0.42723000
C	0.99474100	-0.78061400	0.59490200
C	-0.28158500	-1.29623000	0.42600000
C	-0.99478800	0.78087600	-0.59612200
H	0.51525700	2.30165800	-0.76534600
H	1.75203600	-1.37484400	1.09647500
H	-0.51530600	-2.30139700	0.76412200
H	-1.75210300	1.37511300	-1.09765700
N	-2.54581400	-1.13662700	-0.34720300
C	-3.69319300	-0.55000400	-0.14145200
C	-4.88589600	-1.27259900	-0.58212100
H	-4.71462600	-2.22375200	-1.07738200
C	-3.91429100	0.74264800	0.50902000
H	-3.05981200	1.28094400	0.90301300
C	-6.13257100	-0.77285300	-0.43768700
H	-6.98829600	-1.31441700	-0.82427700
C	-5.16083100	1.24205400	0.65576200
H	-5.33200100	2.19030000	1.15655800
C	-6.35439300	0.52269800	0.20875100
N	-7.50054300	1.10857100	0.41177600
C	-8.73422900	0.48791500	0.18614800
C	-11.31416700	-0.57898500	-0.18364800
C	-9.05966300	-0.79213100	0.68061500
C	-9.73579600	1.23673100	-0.46357000
C	-11.00298400	0.69733900	-0.66557400
C	-10.34112000	-1.31202400	0.49980100
H	-8.31722900	-1.35462600	1.23865100
H	-9.49236400	2.23432400	-0.81708600
H	-11.75653100	1.28041600	-1.18809900
H	-10.57884200	-2.29478400	0.89804900
H	-12.30926400	-0.99022200	-0.32649300

TANI-RC	x	y	z
H	1.84301000	9.83764000	-1.11946400
C	2.08294900	9.87304600	-0.05979400
C	2.67651100	9.95644200	2.66081500
C	2.29365000	8.67187400	0.64022200
C	2.17088900	11.09705000	0.59857500
C	2.45782700	11.14789900	1.96573400
C	2.60799500	8.72500100	2.00904500
H	2.00470000	12.01438400	0.04057200
H	2.51756300	12.10265100	2.47955800
H	2.82712300	7.81371400	2.55409400
H	2.92104000	9.98025700	3.71925100
N	2.24121100	7.46647600	-0.08102900
H	2.46615300	7.54684800	-1.06449200
C	1.85677900	6.20384800	0.33375800
C	1.05260700	3.57677200	1.02529700
C	2.15919800	5.10191000	-0.49826200
C	1.14810900	5.95611700	1.53007800
C	0.76270600	4.66880100	1.86558900
C	1.77189000	3.81622300	-0.16225700
H	2.73045900	5.26334100	-1.40850000
H	0.86924100	6.77617000	2.17991000
H	0.19955800	4.50524800	2.78048300
H	2.06955700	2.99205100	-0.79981900
N	0.65817500	2.29956900	1.43753700
H	0.57539300	2.18311100	2.44166700
C	0.34421300	1.18501600	0.69697900
C	-0.34421300	-1.18501600	-0.69697900
C	0.06322400	1.21970500	-0.69193900
C	0.26548500	-0.06355900	1.36506500
C	-0.06322400	-1.21970500	0.69193900
C	-0.26548500	0.06355900	-1.36506500
H	0.06333200	2.16091100	-1.22688400
H	0.49942400	-0.11325000	2.42467200
H	-0.06333200	-2.16091100	1.22688400
H	-0.49942400	0.11325000	-2.42467200
N	-0.65817500	-2.29956900	-1.43753700
H	-0.57539300	-2.18311100	-2.44166700
C	-1.05260700	-3.57677200	-1.02529700
C	-1.85677900	-6.20384800	-0.33375800
C	-0.76270600	-4.66880100	-1.86558900
C	-1.77189000	-3.81622300	0.16225700
C	-2.15919800	-5.10191000	0.49826200
C	-1.14810900	-5.95611700	-1.53007800
H	-0.19955800	-4.50524800	-2.78048300
H	-2.06955700	-2.99205100	0.79981900
H	-2.73045900	-5.26334100	1.40850000
H	-0.86924100	-6.77617000	-2.17991000
N	-2.24121100	-7.46647600	0.08102900
H	-2.46615300	-7.54684800	1.06449200
C	-2.29365000	-8.67187400	-0.64022200
C	-2.45782700	-11.14789900	-1.96573400
C	-2.60799500	-8.72500100	-2.00904500
C	-2.08294900	-9.87304600	0.05979400
C	-2.17088900	-11.09705000	-0.59857500
C	-2.67651100	-9.95644200	-2.66081500
H	-2.82712300	-7.81371400	-2.55409400
H	-1.84301000	-9.83764000	1.11946400
H	-2.00470000	-12.01438400	-0.04057200
H	-2.92104000	-9.98025700	-3.71925100
H	-2.51756300	-12.10265100	-2.47955800

TANI-^{1}MP	x	y	z
C	-0.20320000	-1.25598600	-0.00546600
H	-0.37510600	-2.30117400	-0.24060200
C	1.06876000	-0.75260100	0.01856500
H	1.91089300	-1.39395000	-0.20769800
C	1.28162600	0.62724100	0.31473500
C	0.14322000	1.45467700	0.57766900
H	0.30525300	2.48938100	0.86668400
C	-1.12628900	0.95259100	0.51861500
H	-1.95649100	1.59111800	0.79520100
C	-1.36303100	-0.43100400	0.19520700
N	2.50740200	1.19725700	0.36602100
N	-2.54225800	-1.05565300	0.11106400
C	3.78684200	0.59833300	0.33798800
C	6.40560700	-0.46715600	0.29939200
C	4.82647700	1.27281100	-0.32024100
C	4.07198700	-0.61014000	0.99540000
C	5.35558000	-1.13205200	0.97002100
C	6.11218300	0.75171300	-0.34816300
H	4.61875700	2.20359700	-0.84083100
H	3.30343300	-1.12133700	1.56437400
H	5.56339100	-2.05838900	1.49862200
H	6.88085000	1.27617400	-0.90184800
C	-3.75131200	-0.47747000	-0.03427500
C	-6.42608300	0.47539000	-0.26750100
C	-4.03042900	0.83287000	-0.54639200
C	-4.87709300	-1.29636400	0.29664500
C	-6.16785200	-0.83590800	0.22080100
C	-5.31910000	1.28521700	-0.66201800
H	-3.22341900	1.44969800	-0.92341200
H	-4.67398100	-2.29453900	0.67061900
H	-6.98662700	-1.46560400	0.54476000
H	-5.51314900	2.26323900	-1.09362000
N	-7.67518900	1.00190500	-0.38058700
N	7.65715200	-1.06144800	0.28529600
H	-7.71220700	1.99739800	-0.56956800
C	-8.93670300	0.37419100	-0.23932700
C	-11.48986600	-0.74905900	0.00701400
C	-9.18550200	-0.91645500	-0.72930100
C	-9.97585800	1.10844500	0.35196200
C	-11.24519800	0.54673400	0.47003500
C	-10.45712300	-1.47302600	-0.59288900
H	-8.40376700	-1.46790400	-1.23978700
H	-9.78146100	2.11079200	0.72358100
H	-12.04240100	1.12221000	0.93129000
H	-10.64196100	-2.47249700	-0.97558500
H	-12.47876200	-1.18668400	0.10462600
H	7.66677700	-2.04811800	0.50895800
C	8.90810600	-0.51768900	-0.05188200
C	11.48084600	0.44017300	-0.67831300
C	9.88897900	-1.38302800	-0.56847100
C	9.23719200	0.83148500	0.16518500
C	10.51099500	1.29991300	-0.15841100
C	11.16238500	-0.90714200	-0.87113100
H	9.64276600	-2.42892900	-0.73414300
H	8.51381200	1.50492300	0.61090400
H	10.74770000	2.34610000	0.01584600
H	11.90561600	-1.59305800	-1.26841800
H	12.47125200	0.81205600	-0.92328500
H	2.51221200	2.21083300	0.41805400

TANI-^{3}MP	x	y	z
C	-0.29002000	-1.37516600	-0.26903100
H	-0.48963100	-2.36789100	-0.65981300
C	0.98251600	-0.83740200	-0.36285800
H	1.76414300	-1.39938800	-0.86088900
C	1.24341200	0.45016700	0.14676000
C	0.18751500	1.19000700	0.71285000
H	0.38212200	2.18244000	1.11095200
C	-1.08784100	0.65634300	0.78727800
H	-1.88077500	1.22885400	1.25685500
C	-1.36578000	-0.64566900	0.29473400
N	2.50327300	1.06089100	0.06808100
N	-2.58374200	-1.27352400	0.42942800
C	3.75541500	0.50922400	0.06978700
C	6.40467000	-0.48860500	0.07499600
C	4.85032000	1.33094600	-0.31407800
C	4.02157800	-0.82851600	0.46712700
C	5.30908300	-1.30898600	0.46239300
C	6.13778500	0.85020500	-0.31976600
H	4.65900500	2.34852900	-0.64191600
H	3.21873600	-1.46315600	0.81965800
H	5.50104400	-2.32502500	0.79439200
H	6.94204500	1.48760300	-0.66393800
C	-3.75898300	-0.66588400	0.20166900
C	-6.36849400	0.41361100	-0.25056600
C	-3.95011000	0.55660800	-0.52799900
C	-4.94495400	-1.31794000	0.67501500
C	-6.20164300	-0.79733500	0.47266800
C	-5.20682500	1.06949500	-0.74218000
H	-3.08852900	1.06868200	-0.94240100
H	-4.81923600	-2.23929900	1.23532300
H	-7.06433900	-1.30164400	0.89076500
H	-5.32491800	1.98748300	-1.31283100
N	-7.58921100	1.00635400	-0.47253200
N	7.65597700	-1.03848300	0.07593500
H	-7.55132500	1.97243100	-0.77539600
C	-8.88850900	0.49558800	-0.28283000
C	-11.52904100	-0.40082100	0.04484500
C	-9.21205600	-0.85057500	-0.51959500
C	-9.90186300	1.39188100	0.09706200
C	-11.21114300	0.94425100	0.25429300
C	-10.52419400	-1.28971600	-0.34374100
H	-8.45252600	-1.54083900	-0.86897900
H	-9.65358700	2.43471800	0.27651500
H	-11.98330800	1.64885300	0.54982600
H	-10.76197100	-2.33312100	-0.53072400
H	-12.54911400	-0.74968900	0.17460700
H	7.68492200	-2.04983300	0.15047800
C	8.91574100	-0.41490300	-0.03698200
C	11.47431100	0.70299500	-0.24817800
C	9.94853400	-1.12884100	-0.66751100
C	9.17647100	0.85138200	0.51200400
C	10.45053400	1.40410000	0.39371800
C	11.21877800	-0.56893600	-0.76958900
H	9.74622500	-2.11180000	-1.08386000
H	8.40460900	1.38163200	1.05812500
H	10.64553900	2.38197900	0.82384200
H	12.00930300	-1.12642800	-1.26296000
H	12.46523100	1.13863900	-0.33179900
H	2.48102900	2.07454400	0.01399900

TANI-^{1}ES	x	y	z
H	1.79431600	9.83199000	-1.08465900
C	2.05913200	9.86587600	-0.03159800
C	2.72229500	9.93433200	2.67918200
C	2.31312100	8.66950300	0.65916200
C	2.12997000	11.08382200	0.63837800
C	2.45251000	11.12394900	1.99824200
C	2.66491300	8.70846200	2.01800800
H	1.92659200	12.00303900	0.09727900
H	2.50411100	12.07497400	2.51934500
H	2.92808100	7.79716500	2.54298700
H	2.99869600	9.95734500	3.72906600
N	2.26449800	7.46376000	-0.07398100
H	2.54434500	7.54607100	-1.04552500
C	1.85514000	6.22233700	0.31067800
C	1.00246200	3.60625600	0.95346900
C	2.10101500	5.13063000	-0.56958600
C	1.18311800	5.96204300	1.53587500
C	0.78231000	4.68440800	1.84779000
C	1.69290900	3.85562300	-0.25871800
H	2.65341200	5.30506300	-1.48793900
H	0.95173000	6.77221400	2.21466400
H	0.25002400	4.50600600	2.77774500
H	1.96173000	3.04241800	-0.92023600
N	0.55919800	2.35810500	1.34468500
H	0.39925400	2.27570100	2.34584300
C	0.28744100	1.22208200	0.64580700
C	-0.28744100	-1.22208200	-0.64580700
C	0.12449300	1.17699300	-0.76859800
C	0.14266100	0.01326300	1.38992100
C	-0.12449300	-1.17699300	0.76859800
C	-0.14266100	-0.01326300	-1.38992100
H	0.15010500	2.08486700	-1.35579500
H	0.29801200	0.03119300	2.46419200
H	-0.15010500	-2.08486700	1.35579500
H	-0.29801200	-0.03119300	-2.46419200
N	-0.55919800	-2.35810500	-1.34468500
H	-0.39925400	-2.27570100	-2.34584300
C	-1.00246200	-3.60625600	-0.95346900
C	-1.85514000	-6.22233700	-0.31067800
C	-0.78231000	-4.68440800	-1.84779000
C	-1.69290900	-3.85562300	0.25871800
C	-2.10101500	-5.13063000	0.56958600
C	-1.18311800	-5.96204300	-1.53587500
H	-0.25002400	-4.50600600	-2.77774500
H	-1.96173000	-3.04241800	0.92023600
H	-2.65341200	-5.30506300	1.48793900
H	-0.95173000	-6.77221400	-2.21466400
N	-2.26449800	-7.46376000	0.07398100
H	-2.54434500	-7.54607100	1.04552500
C	-2.31312100	-8.66950300	-0.65916200
C	-2.45251000	-11.12394900	-1.99824200
C	-2.66491300	-8.70846200	-2.01800800
C	-2.05913200	-9.86587600	0.03159800
C	-2.12997000	-11.08382200	-0.63837800
C	-2.72229500	-9.93433200	-2.67918200
H	-2.92808100	-7.79716500	-2.54298700
H	-1.79431600	-9.83199000	1.08465900
H	-1.92659200	-12.00303900	-0.09727900
H	-2.99869600	-9.95734500	-3.72906600
H	-2.50411100	-12.07497400	-2.51934500

TANI-^{3}ES	x	y	z
H	1.97346500	9.79480100	-1.12497700
C	2.19585200	9.82633800	-0.06202800
C	2.75615700	9.88753100	2.67426800
C	2.31538900	8.62625800	0.66078100
C	2.34217500	11.04518400	0.59147200
C	2.61362700	11.08207200	1.96314500
C	2.61787400	8.65885400	2.03275000
H	2.24053400	11.96816700	0.02909100
H	2.72711700	12.03492500	2.47069700
H	2.78781400	7.73989900	2.58129400
H	2.99608800	9.90826500	3.73285900
N	2.18476100	7.42062900	-0.05558100
H	2.46915300	7.47529900	-1.02892400
C	1.71488400	6.20443100	0.34131800
C	0.75825700	3.63110600	1.01686100
C	1.91788300	5.09364400	-0.52761100
C	1.00722100	5.99423900	1.55822900
C	0.55173900	4.74157900	1.88402100
C	1.46212000	3.84123500	-0.20122000
H	2.47380500	5.23761800	-1.44941300
H	0.78691600	6.82779000	2.21225700
H	-0.00729300	4.59755900	2.80383700
H	1.67645100	3.00881500	-0.85911300
N	0.29168500	2.41052300	1.41202700
H	0.01076000	2.34508300	2.38511700
C	0.16175300	1.21751200	0.67544100
C	-0.16175300	-1.21751200	-0.67544100
C	-0.20228500	1.20695300	-0.68132100
C	0.35277600	0.00037800	1.34903500
C	0.20228500	-1.20695300	0.68132100
C	-0.35277600	-0.00037800	-1.34903500
H	-0.41167200	2.13288700	-1.20376000
H	0.65427100	0.00288200	2.39195000
H	0.41167200	-2.13288700	1.20376000
H	-0.65427100	-0.00288200	-2.39195000
N	-0.29168500	-2.41052300	-1.41202700
H	-0.01076000	-2.34508300	-2.38511700
C	-0.75825700	-3.63110600	-1.01686100
C	-1.71488400	-6.20443100	-0.34131800
C	-0.55173900	-4.74157900	-1.88402100
C	-1.46212000	-3.84123500	0.20122000
C	-1.91788300	-5.09364400	0.52761100
C	-1.00722100	-5.99423900	-1.55822900
H	0.00729300	-4.59755900	-2.80383700
H	-1.67645100	-3.00881500	0.85911300
H	-2.47380500	-5.23761800	1.44941300
H	-0.78691600	-6.82779000	-2.21225700
N	-2.18476100	-7.42062900	0.05558100
H	-2.46915300	-7.47529900	1.02892400
C	-2.31538900	-8.62625800	-0.66078100
C	-2.61362700	-11.08207200	-1.96314500
C	-2.61787400	-8.65885400	-2.03275000
C	-2.19585200	-9.82633800	0.06202800
C	-2.34217500	-11.04518400	-0.59147200
C	-2.75615700	-9.88753100	-2.67426800
H	-2.78781400	-7.73989900	-2.58129400
H	-1.97346500	-9.79480100	1.12497700
H	-2.24053400	-11.96816700	-0.02909100
H	-2.99608800	-9.90826500	-3.73285900
H	-2.72711700	-12.03492500	-2.47069700

TANI-^{1}TP-i	x	y	z
H	-8.81656900	2.78939100	1.12399400
C	-9.23287700	2.00722400	0.49461800
C	-10.28619700	-0.00018100	-1.12875600
C	-8.50428000	0.82061800	0.29298700
C	-10.47146400	2.18192900	-0.11512100
C	-11.00235300	1.18439100	-0.93899300
C	-9.05053600	-0.19364100	-0.51327800
H	-11.02038900	3.10477600	0.04849400
H	-11.96600000	1.32508200	-1.41889200
H	-8.53330400	-1.13910100	-0.63001900
H	-10.69819900	-0.79261300	-1.74694900
N	-7.28079200	0.67827800	0.96887400
H	-7.20450000	1.20998400	1.82727500
C	-6.15156100	-0.03282800	0.61808600
C	-3.80196000	-1.41287300	0.02743200
C	-5.16348500	-0.24286800	1.61043300
C	-5.91475400	-0.51953200	-0.68576800
C	-4.74437300	-1.21100900	-0.97617900
C	-3.99464300	-0.92529200	1.32096600
H	-5.32939400	0.12880400	2.61699900
H	-6.62720800	-0.33603500	-1.47925700
H	-4.57713800	-1.57547000	-1.98585300
H	-3.24986300	-1.07733000	2.09581100
N	-2.55602900	-2.16316500	-0.28759700
H	-2.61276500	-2.49868800	-1.25882400
C	-1.28478200	-1.40552000	-0.11961800
C	1.08723900	-0.02891900	0.12680800
C	-1.20131600	-0.11382700	-0.63646300
C	-0.22227600	-2.01090400	0.54268500
C	0.97641700	-1.31504600	0.67348300
C	-0.00821900	0.58150500	-0.50599800
H	-2.04863100	0.34679300	-1.13151900
H	-0.31341800	-3.00421300	0.96978100
H	1.79026700	-1.75407300	1.23793800
H	0.08089700	1.58168600	-0.91538700
N	2.27659400	0.72741600	0.24329700
H	2.12983000	1.72152500	0.41381900
C	3.55066100	0.34577500	0.13717300
C	6.28131600	-0.30957500	-0.06931300
C	4.56869800	1.31230700	0.47491000
C	3.94513700	-0.96876300	-0.29889600
C	5.26243900	-1.28445900	-0.38058900
C	5.88572700	0.99720000	0.39017900
H	4.26621200	2.28476700	0.84953100
H	3.19810000	-1.68978400	-0.60300500
H	5.56319100	-2.26367300	-0.73891300
H	6.63171900	1.70762800	0.71988400
N	7.55370200	-0.68510000	-0.21663700
H	7.68677000	-1.68463900	-0.37386200
C	8.74812700	0.04573700	-0.19192300
C	11.19174900	1.36920700	-0.11577300
C	8.81827700	1.39693100	-0.59011800
C	9.91083900	-0.65408600	0.19563900
C	11.12278500	0.01728000	0.24557700
C	10.04290100	2.04780100	-0.54314600
H	7.95042500	1.90265900	-0.99510400
H	9.84647800	-1.69933700	0.48202000
H	12.01592000	-0.51047000	0.56196400
H	10.10916100	3.08132100	-0.86539200
H	12.14462400	1.88759100	-0.08754400
H	-2.51396200	-3.02007800	0.28118400

TANI-^{3}TP-i	x	y	z
H	-8.78010300	3.09752400	0.80230400
C	-9.23796700	2.16238200	0.49473100
C	-10.37133900	-0.28422800	-0.29949100
C	-8.43230300	0.98970200	0.38512900
C	-10.57864200	2.10302600	0.17737100
C	-11.15276900	0.88459400	-0.22960700
C	-9.02551500	-0.24881700	0.00574600
H	-11.18904100	2.99689700	0.24235300
H	-12.20946400	0.84043300	-0.47133700
H	-8.44347500	-1.16125300	0.01270300
H	-10.83306900	-1.22672100	-0.57277900
N	-7.11011000	1.11364000	0.70014600
H	-6.86292900	1.97281700	1.18859900
C	-6.03298500	0.25424400	0.46288000
C	-3.81721700	-1.34126500	0.06019100
C	-4.93828700	0.33302300	1.34794500
C	-5.99038700	-0.61162800	-0.64459000
C	-4.87554600	-1.41999100	-0.83913800
C	-3.82675400	-0.47010400	1.14950500
H	-4.97285200	1.00679900	2.19752100
H	-6.78627000	-0.61954300	-1.37807100
H	-4.83945500	-2.08235300	-1.69787000
H	-2.98726600	-0.41114600	1.83321400
N	-2.62556900	-2.20862600	-0.15358900
H	-2.78596200	-2.79683300	-0.98221400
C	-1.32657900	-1.49057000	-0.30184500
C	1.09062300	-0.17185000	-0.58304100
C	-1.16159200	-0.61086300	-1.36921800
C	-0.32287300	-1.71660800	0.63147300
C	0.89033200	-1.04582700	0.49643600
C	0.05321600	0.04630900	-1.50770200
H	-1.95536500	-0.43974000	-2.08847000
H	-0.47498200	-2.38802700	1.47093500
H	1.65396100	-1.17930900	1.25245500
H	0.20402800	0.72316300	-2.34237400
N	2.28003900	0.55768400	-0.74844400
H	2.16427000	1.47291800	-1.17122900
C	3.56715900	0.21870600	-0.43580800
C	6.27564300	-0.34222000	0.14021300
C	4.54831700	1.25012600	-0.45008600
C	3.97729900	-1.10782800	-0.13011700
C	5.29252500	-1.37351800	0.15706400
C	5.86354600	0.98617200	-0.16400300
H	4.23898700	2.27029400	-0.65580600
H	3.26615600	-1.92325700	-0.16171000
H	5.60029000	-2.39354300	0.36595600
H	6.57536000	1.80050900	-0.12691200
N	7.55880400	-0.67786100	0.44753800
H	7.67716400	-1.60001400	0.85737000
C	8.74902100	0.06168400	0.30768100
C	11.17472900	1.43054800	0.09273900
C	8.95184300	0.96252900	-0.75212900
C	9.77516300	-0.17531600	1.23933300
C	10.97891600	0.51207800	1.12960900
C	10.16184600	1.64531300	-0.84625100
H	8.19489100	1.09230900	-1.51687200
H	9.61531900	-0.87997900	2.05044800
H	11.76467800	0.33276900	1.85673200
H	10.31915800	2.33430200	-1.67024600
H	12.11612700	1.96450000	0.00922500
H	-2.54885300	-2.87619300	0.62637800

TANI-^{1}TP-o	x	y	z
H	9.45093700	-0.65874700	-2.12353700
C	9.67344200	-0.24937900	-1.14223900
C	10.24333400	0.78736400	1.39952600
C	8.88150300	-0.54997900	-0.03974300
C	10.77286600	0.59256600	-0.95693800
C	11.05626200	1.10818300	0.30839500
C	9.13958000	-0.04832000	1.23281500
H	11.40439100	0.83801100	-1.80439100
H	11.91322300	1.75979100	0.44687500
H	8.50236800	-0.29911800	2.07522600
H	10.46617200	1.18522400	2.38415900
N	7.70231200	-1.44426000	-0.22652500
H	7.78997800	-1.92201300	-1.13352000
C	6.36326000	-0.78982800	-0.14487900
C	3.86055900	0.37756100	-0.03239900
C	5.36875600	-1.39845400	0.61146000
C	6.14456200	0.39914100	-0.83507300
C	4.88560000	0.98322400	-0.77646300
C	4.11011100	-0.80521000	0.67757900
H	5.56049400	-2.31231100	1.16509900
H	6.93515500	0.86793300	-1.40997500
H	4.69365600	1.90332100	-1.31843300
H	3.34908000	-1.24353000	1.31198200
N	2.61275800	1.03608500	0.02797300
H	2.66498700	2.05044400	0.03750000
C	1.36320900	0.51446200	0.04796300
C	-1.29169300	-0.42713400	0.07540900
C	1.08528700	-0.86024900	-0.20741900
C	0.27413800	1.39510100	0.33295100
C	-1.01671800	0.94135600	0.35349200
C	-0.20614900	-1.31432800	-0.17667400
H	1.88490800	-1.54305300	-0.46246700
H	0.48275000	2.43020100	0.58275900
H	-1.80607800	1.61694600	0.65489100
H	-0.41103400	-2.35694300	-0.39906300
N	-2.54901900	-0.96978800	0.06888300
H	-2.55175200	-1.98539400	0.16029300
C	-3.78828900	-0.43001900	-0.03127900
C	-6.43205800	0.54077400	-0.14587300
C	-4.89323900	-1.26745800	0.32715400
C	-4.04463700	0.90070400	-0.48646200
C	-5.32394000	1.36936500	-0.53136100
C	-6.17333600	-0.79880200	0.29075700
H	-4.70067300	-2.27270300	0.68892900
H	-3.24104200	1.51858300	-0.86341000
H	-5.51969600	2.36553100	-0.91459800
H	-6.98526500	-1.42608600	0.63313500
N	-7.66418700	1.07043400	-0.21203400
H	-7.69608000	2.07463000	-0.37239600
C	-8.93145100	0.46000900	-0.08053400
C	-11.48767800	-0.62113300	0.17348300
C	-9.19068300	-0.83262500	-0.56596800
C	-9.95882100	1.22414300	0.49885300
C	-11.22979900	0.67616700	0.62939700
C	-10.46912000	-1.36584200	-0.42848500
H	-8.42254500	-1.39150200	-1.08770200
H	-9.75039400	2.22725700	0.85908400
H	-12.02004000	1.26189600	1.08780300
H	-10.67367400	-2.36012300	-0.81233800
H	-12.48254100	-1.04362600	0.27250900
H	7.74052800	-2.20006800	0.46883600

TANI-^{3}TP-o	x	y	z
H	9.85055400	-0.22365200	-1.84351000
C	9.85682400	0.04072000	-0.79028800
C	9.86960800	0.69803800	1.93432100
C	8.86499300	-0.41226100	0.07137800
C	10.87337400	0.84299300	-0.26592200
C	10.87920900	1.17027400	1.09038900
C	8.84554600	-0.10160400	1.42817000
H	11.65707100	1.20619100	-0.92251200
H	11.67152100	1.79366900	1.49257500
H	8.05673000	-0.46736800	2.07769500
H	9.87563900	0.95055500	2.98960600
N	7.77387400	-1.27175600	-0.48166500
H	7.99455100	-1.49509800	-1.46158000
C	6.40300000	-0.69588700	-0.40751300
C	3.84849800	0.35731200	-0.30092300
C	5.41043200	-1.40018500	0.26316400
C	6.15802600	0.53729000	-1.00880600
C	4.87550900	1.06336000	-0.95364500
C	4.12541500	-0.86708300	0.32659700
H	5.62228000	-2.34615500	0.75142900
H	6.94676900	1.08401800	-1.51408000
H	4.66440300	2.01543500	-1.42921300
H	3.36539800	-1.38403300	0.89895700
N	2.57700700	0.95429200	-0.25115000
H	2.58349800	1.97063300	-0.24571300
C	1.34086200	0.38116200	-0.22832100
C	-1.28071300	-0.65794300	-0.19110700
C	1.10712200	-0.99121300	-0.52835000
C	0.22673600	1.21660500	0.07643600
C	-1.04905400	0.71383300	0.10341500
C	-0.16920400	-1.49227000	-0.50058500
H	1.92394600	-1.63467000	-0.82805200
H	0.39803800	2.25868000	0.32747700
H	-1.86764800	1.35975100	0.39311200
H	-0.34241000	-2.53264600	-0.75654500
N	-2.52321100	-1.23168700	-0.15738700
H	-2.53467200	-2.24641100	-0.11794300
C	-3.78551100	-0.62283300	-0.14294600
C	-6.36686400	0.46504200	-0.12544400
C	-4.82884100	-1.27753000	0.54148200
C	-4.04546500	0.58260600	-0.82441100
C	-5.31536200	1.12643700	-0.80078600
C	-6.10264900	-0.74219400	0.56102400
H	-4.62281300	-2.18875600	1.09338000
H	-3.27000800	1.06786800	-1.40429700
H	-5.51554200	2.04471000	-1.34382200
H	-6.86989000	-1.21990500	1.15632700
N	-7.61123200	1.07417600	-0.13240600
H	-7.58941100	2.07340400	-0.32544600
C	-8.87101500	0.56006100	0.08150200
C	-11.47828000	-0.33660400	0.52323700
C	-9.17252100	-0.82047300	-0.04104600
C	-9.90262500	1.48771200	0.38490800
C	-11.18870500	1.03436200	0.61311000
C	-10.46860700	-1.25177000	0.18523200
H	-8.41540500	-1.52211200	-0.36646300
H	-9.66668600	2.54503100	0.45980800
H	-11.97248800	1.74200200	0.86095400
H	-10.70618100	-2.30463700	0.07666100
H	-12.49021600	-0.68824700	0.69554000
H	7.77947600	-2.18116200	-0.00171200

OANI-LEB	x	y	z
H	-20.33784200	2.27188200	-0.00878700
C	-20.38337700	1.25857900	0.38426900
C	-20.50793900	-1.33494600	1.37847500
C	-19.19966300	0.49449700	0.45572000
C	-21.59931400	0.72988400	0.80695800
C	-21.67736000	-0.57565300	1.30280700
C	-19.27982100	-0.81462900	0.96816100
H	-22.49437400	1.34356400	0.74195900
H	-22.62842500	-0.98970000	1.62443500
H	-18.38341800	-1.41662400	1.06346800
H	-20.54226800	-2.34781600	1.77243200
N	-18.00731600	1.08549900	0.03701700
H	-18.00979800	2.09660300	0.03580200
C	-16.74163400	0.49181200	-0.13092000
C	-14.13948100	-0.57456200	-0.56413800
C	-15.59075000	1.20879700	0.22961200
C	-16.56790900	-0.77272900	-0.71985800
C	-15.29493200	-1.29359900	-0.92500300
C	-14.31395300	0.69377200	0.01705300
H	-15.69647500	2.18500200	0.69718800
H	-17.43148600	-1.34278200	-1.04581400
H	-15.18874300	-2.27001300	-1.39200400
H	-13.45338400	1.27132500	0.33464700
N	-12.88907600	-1.16606700	-0.77758100
H	-12.88937600	-2.17700000	-0.78322600
C	-11.61847100	-0.56977100	-0.72453400
C	-8.98434600	0.51092000	-0.70545100
C	-11.36680600	0.73157500	-1.19474400
C	-10.52646200	-1.31459600	-0.25086000
C	-9.23524300	-0.79219200	-0.24079300
C	-10.07928900	1.25705000	-1.18019200
H	-12.17638300	1.32861900	-1.60083400
H	-10.69305200	-2.31993100	0.12925000
H	-8.42728100	-1.39362600	0.16019300
H	-9.91183600	2.26242000	-1.55971800
N	-7.72092600	1.11327300	-0.68620300
H	-7.72634700	2.12308100	-0.64406900
C	-6.45794900	0.51545300	-0.56919700
C	-3.82533400	-0.55714100	-0.39223300
C	-5.41085600	1.23998000	0.02554700
C	-6.16068300	-0.76169900	-1.07770500
C	-4.87340900	-1.28229500	-0.98731000
C	-4.12223200	0.72079100	0.11419400
H	-5.61372100	2.22561000	0.43844600
H	-6.93006000	-1.34239900	-1.57484800
H	-4.67014900	-2.26778100	-1.40025500
H	-3.35261000	1.30351600	0.60806800
N	-2.56238600	-1.15344600	-0.29058200
H	-2.55710600	-2.16385900	-0.30607500
C	-1.30855500	-0.54715900	-0.13692800
C	1.30803000	0.54709700	0.12798600
C	-1.01706800	0.75149900	-0.59136600
C	-0.26351100	-1.28183400	0.45039400
C	1.01654300	-0.75155300	0.58241800
C	0.26297000	1.28178500	-0.45933000
H	-1.78443900	1.34298800	-1.07858100
H	-0.46241200	-2.28408700	0.82322300
H	1.78389500	-1.34306000	1.06963800
H	0.46187900	2.28404100	-0.83214900
N	2.56185000	1.15340500	0.28158100
H	2.55659700	2.16382500	0.29662100
C	3.82477600	0.55709300	0.38379000
C	6.45729500	-0.51551600	0.56206400
C	4.87266500	1.28242600	0.97900100
C	4.12183800	-0.72096300	-0.12217400
C	5.41042400	-1.24018000	-0.03287400
C	6.15988600	0.76184300	1.07001400
H	4.66926400	2.26804800	1.39155200
H	3.35241200	-1.30381800	-0.61619700
H	5.61339500	-2.22594200	-0.44540200
H	6.92913200	1.34268600	1.56719200
N	7.72019200	-1.11331900	0.67983300
H	7.72565100	-2.12314000	0.63801600
C	8.98357000	-0.51085800	0.70005400
C	11.61754800	0.57015000	0.72111900
C	9.23485200	0.79184000	0.23445100
C	10.07803400	-1.25640800	1.17675900
C	11.36549000	-0.73078500	1.19226200
C	10.52598200	1.31441600	0.24550300
H	8.42724700	1.39279000	-0.16799600
H	9.91026600	-2.26142900	1.55706700
H	12.17465000	-1.32736800	1.59984700
H	10.69288300	2.31941700	-0.13535800
N	12.88796800	1.16670800	0.77493000
H	12.88813700	2.17764300	0.77944500
C	14.13890600	0.57505700	0.56513000
C	16.74217600	-0.49149300	0.13916500
C	15.29345300	1.29487400	0.92737000
C	14.31486200	-0.69412600	-0.01373800
C	15.59221700	-1.20925400	-0.22272200
C	16.56695500	0.77392900	0.72577900
H	15.18606600	2.27198400	1.39263800
H	13.45509900	-1.27232300	-0.33234100
H	15.69911000	-2.18616100	-0.68856000
H	17.42973500	1.34462400	1.05272400
N	18.00837000	-1.08515700	-0.02510300
H	18.01090900	-2.09626600	-0.02275300
C	19.20113300	-0.49468500	-0.44344100
C	21.67974400	0.57443100	-1.28919900
C	19.28180400	0.81372100	-0.95762600
C	20.38481000	-1.25859300	-0.36958600
C	21.60120200	-0.73041400	-0.79160900
C	20.51036300	1.33353400	-1.36727100
H	18.38549100	1.41554700	-1.05479400
H	20.33889600	-2.27136700	0.02478800
H	22.49621400	-1.34396200	-0.72473200
H	20.54507800	2.34585300	-1.76260900
H	22.63115000	0.98809300	-1.61031200

OANI-NEB	x	y	z
H	-20.05591400	2.32659200	-1.08971300
C	-20.23185700	1.30064500	-0.77404400
C	-20.68319800	-1.32534400	0.02111900
C	-19.13932600	0.51397300	-0.35418200
C	-21.52165900	0.77788200	-0.78946300
C	-21.76117300	-0.54367100	-0.39938000
C	-19.38642200	-0.81102300	0.05310200
H	-22.34475900	1.40852600	-1.11595600
H	-22.76682600	-0.95304900	-0.42041300
H	-18.57289600	-1.42998500	0.41355600
H	-20.84822400	-2.35085700	0.34237100
N	-17.87430000	1.10261100	-0.33169100
H	-17.87278400	2.11306000	-0.29864200
C	-16.61617600	0.49718600	-0.17639200
C	-14.00007100	-0.58762300	0.07932500
C	-15.59958700	1.19559200	0.49566600
C	-16.29817300	-0.75799300	-0.72363800
C	-15.01775500	-1.28662100	-0.59347800
C	-14.31742300	0.66888400	0.62427700
H	-15.82201900	2.16296800	0.93986500
H	-17.04389000	-1.31297900	-1.28224500
H	-14.79527300	-2.25423600	-1.03711300
H	-13.57242200	1.22576000	1.18148700
N	-12.74433700	-1.19344600	0.22308100
H	-12.74290600	-2.20308000	0.17539800
C	-11.48891800	-0.60144200	0.38198500
C	-8.86882200	0.46113200	0.66963000
C	-11.19895200	0.72119000	-0.00090800
C	-10.43967800	-1.37571300	0.91235500
C	-9.15775800	-0.85754200	1.05918900
C	-9.91345200	1.23529500	0.14098300
H	-11.96945800	1.34328800	-0.44176400
H	-10.64044500	-2.39541800	1.23222900
H	-8.38686400	-1.47413600	1.50855500
H	-9.71178200	2.25476500	-0.17879100
N	-7.60284500	1.05224500	0.84668100
H	-7.61166800	2.04654500	1.03201100
C	-6.34530800	0.48050000	0.73873500
C	-3.69559300	-0.55724700	0.51467200
C	-5.23261200	1.19880600	1.23098500
C	-6.10841100	-0.78102200	0.14966800
C	-4.82130000	-1.28998400	0.07459200
C	-3.94445700	0.70285000	1.11202000
H	-5.39554800	2.15325600	1.72613000
H	-6.93369600	-1.35651700	-0.25308300
H	-4.65339000	-2.26713900	-0.36907900
H	-3.12336700	1.26734100	1.54161700
N	-2.45887900	-1.17972700	0.42433400
C	-1.32295400	-0.55633800	0.21150500
C	1.32295600	0.55652500	-0.21109200
C	-1.13243000	0.83290700	-0.19172800
C	-0.10896200	-1.34707200	0.37019700
C	1.13243500	-0.83272100	0.19213900
C	0.10896600	1.34725900	-0.36978600
H	-2.00374700	1.44595100	-0.39192300
H	-0.24500000	-2.37434400	0.69650300
H	2.00375300	-1.44576300	0.39232800
H	0.24500400	2.37453100	-0.69609100
N	2.45888100	1.17990000	-0.42395000
C	3.69557700	0.55738600	-0.51430500
C	6.34524800	-0.48045500	-0.73842900
C	4.82132000	1.29009500	-0.07427300
C	3.94437800	-0.70273500	-1.11162900
C	5.23251300	-1.19873700	-1.23062700
C	6.10841100	0.78108500	-0.14937800
H	4.65345700	2.26726400	0.36938300
H	3.12325300	-1.26720700	-1.54118200
H	5.39540200	-2.15320200	-1.72575700
H	6.93373100	1.35656100	0.25333300
N	7.60276500	-1.05224100	-0.84640200
H	7.61155500	-2.04654600	-1.03170000
C	8.86876500	-0.46114700	-0.66944700
C	11.48890600	0.60138300	-0.38201900
C	9.15770600	0.85750400	-1.05908200
C	9.91340900	-1.23530600	-0.14082500
C	11.19893200	-0.72122300	0.00095600
C	10.43964400	1.37565600	-0.91234800
H	8.38679300	1.47409600	-1.50842200
H	9.71173800	-2.25475400	0.17901300
H	11.96944600	-1.34331700	0.44180200
H	10.64041100	2.39534500	-1.23227400
N	12.74434600	1.19337100	-0.22323400
H	12.74293400	2.20300700	-0.17559300
C	14.00008600	0.58754400	-0.07952300
C	16.61621300	-0.49724700	0.17608100
C	15.01780000	1.28655500	0.59322000
C	14.31742100	-0.66896600	-0.62447700
C	15.59959500	-1.19566400	-0.49592300
C	16.29822700	0.75793500	0.72332800
H	14.79533600	2.25417600	1.03685300
H	13.57240300	-1.22585000	-1.18165600
H	15.82201100	-2.16304200	-0.94012700
H	17.04396600	1.31293400	1.28189400
N	17.87434300	-1.10267000	0.33132400
H	17.87282400	-2.11311900	0.29826400
C	19.13937200	-0.51404100	0.35380800
C	21.76123000	0.54357800	0.39900400
C	19.38647500	0.81096500	-0.05343900
C	20.23190200	-1.30073600	0.77363100
C	21.52170800	-0.77798500	0.78904900
C	20.68325700	1.32527300	-0.02145900
H	18.57295100	1.42994600	-0.41386500
H	20.05595400	-2.32669000	1.08927200
H	22.34480700	-1.40864700	1.11551200
H	20.84828700	2.35079300	-0.34268300
H	22.76688700	0.95294600	0.42003600

OANI-EB	x	y	z
H	-19.86618600	2.06998700	-0.72890300
C	-20.08106400	1.10776300	-0.27305400
C	-20.61298100	-1.34415900	0.94665200
C	-19.04446100	0.43881500	0.40871500
C	-21.34701800	0.53750900	-0.37561300
C	-21.62198300	-0.69129200	0.23452400
C	-19.33445500	-0.79302200	1.03190600
H	-22.12717200	1.05992000	-0.92303200
H	-22.61486900	-1.12667100	0.16724300
H	-18.56334200	-1.29302900	1.61041400
H	-20.82028300	-2.28885400	1.44261400
N	-17.81405800	1.09321700	0.53308700
C	-16.66635300	0.50640100	0.32432800
C	-14.00145400	-0.54675600	-0.09568800
C	-15.46493000	1.26855100	0.65958700
C	-16.45060900	-0.83228500	-0.22381700
C	-15.20073300	-1.32197800	-0.39471100
C	-14.21645300	0.78112900	0.47477500
H	-15.62529800	2.24320800	1.11124900
H	-17.31284300	-1.42138700	-0.51491400
H	-15.03944600	-2.30942300	-0.81767600
H	-13.35790400	1.35866000	0.79755600
N	-12.85512500	-1.13329400	-0.33992200
C	-11.62042900	-0.50450600	-0.30830700
C	-8.97386100	0.55417900	-0.30194500
C	-11.36042100	0.82419800	-0.72554700
C	-10.50755800	-1.29044600	0.06861900
C	-9.22236200	-0.77473700	0.10734000
C	-10.07236300	1.33179000	-0.73336800
H	-12.16869600	1.43794500	-1.10895700
H	-10.68659600	-2.31716900	0.37383500
H	-8.40941700	-1.39660500	0.46271600
H	-9.89634100	2.34247400	-1.09339700
N	-7.71861700	1.13901900	-0.28786600
C	-6.45288400	0.53855300	-0.16869700
C	-3.83271400	-0.53041200	0.02379300
C	-5.42089800	1.25545200	0.45866700
C	-6.15167200	-0.72578400	-0.70299400
C	-4.86659200	-1.24769800	-0.60275600
C	-4.13507600	0.73441800	0.55819900
H	-5.63471500	2.22883300	0.89284700
H	-6.91117200	-1.29101000	-1.23140300
H	-4.65312800	-2.22122000	-1.03686800
H	-3.37608000	1.30058700	1.08584800
N	-2.56940200	-1.12904700	0.13633200
C	-1.31150300	-0.54057500	0.19320900
C	1.33407400	0.51966100	0.28021300
C	-1.05291100	0.79120800	-0.19446000
C	-0.22491900	-1.32266800	0.63968500
C	1.06432600	-0.81385700	0.67012200
C	0.23188200	1.30806100	-0.11746800
H	-1.85599700	1.41721000	-0.56515200
H	-0.40787000	-2.33985400	0.97767100
H	1.86562100	-1.43432100	1.05813500
H	0.41624800	2.33894600	-0.40552800
N	2.57137000	1.14594700	0.36437700
C	3.71563600	0.56428200	0.09445400
C	6.37641900	-0.47048000	-0.41481600
C	4.92146000	1.30532700	0.44579200
C	3.92320600	-0.73238300	-0.54318200
C	5.17094200	-1.21353000	-0.76144800
C	6.16886300	0.82402500	0.22675600
H	4.77051000	2.25650000	0.94839000
H	3.06033100	-1.29409500	-0.88225400
H	5.32201100	-2.16652700	-1.26059200
H	7.03116300	1.38352300	0.57069100
N	7.52067100	-1.05100200	-0.69056900
C	8.75842100	-0.42857700	-0.61399500
C	11.40898400	0.62389300	-0.52429300
C	9.02821400	0.91570900	-0.96924900
C	9.86529000	-1.23166200	-0.25766400
C	11.15178600	-0.72125700	-0.18018500
C	10.31790300	1.42065700	-0.93744300
H	8.22568100	1.54900300	-1.33287900
H	9.68136800	-2.27093200	-0.00103000
H	11.95933500	-1.36130800	0.15520300
H	10.49963600	2.44679500	-1.24802200
N	12.66616100	1.20469000	-0.46579300
C	13.92279200	0.59129400	-0.30325000
C	16.52367700	-0.51104300	-0.01369000
C	14.91564700	1.25638600	0.43300100
C	14.25412000	-0.63654000	-0.90039400
C	15.52771800	-1.17514000	-0.75269500
C	16.19172500	0.72032500	0.57911600
H	14.67873700	2.20146800	0.91548200
H	13.52630000	-1.15957700	-1.51111700
H	15.76413000	-2.12064600	-1.23468300
H	16.91800500	1.24732700	1.18694300
N	17.76966000	-1.13082500	0.13936100
C	19.01863800	-0.56948000	0.41581800
C	21.60801600	0.42773000	0.94623600
C	19.33839500	0.77476700	0.14644700
C	20.02262400	-1.40654500	0.94232800
C	21.29921200	-0.91289800	1.19645100
C	20.61782900	1.25979600	0.41952700
H	18.59883000	1.43170100	-0.29700100
H	19.78888500	-2.44777100	1.15270800
H	22.05490000	-1.58106500	1.60148200
H	20.84153500	2.30126900	0.20246200
H	22.60146300	0.81401300	1.15407500
H	-7.71356200	2.14973800	-0.33142700
H	-2.57078200	-2.14052600	0.13457200
H	12.67408900	2.21607600	-0.45585800
H	17.76346100	-2.13714000	0.04232400

OANI-PEB	x	y	z
H	19.75576700	-2.21586600	-0.53466700
C	19.96558200	-1.22294300	-0.14753000
C	20.48310100	1.31173900	0.89699500
C	18.91607600	-0.49777000	0.45190700
C	21.23840900	-0.66956200	-0.25721400
C	21.50621300	0.60039000	0.26554200
C	19.19829600	0.77633200	0.98741100
H	22.02928000	-1.23677200	-0.74093300
H	22.50409900	1.02339200	0.19362300
H	18.41511000	1.32381900	1.50333800
H	20.68406600	2.29036300	1.32509400
N	17.67730900	-1.13332800	0.59133000
C	16.54078100	-0.55555600	0.31031900
C	13.89762700	0.49092300	-0.24046500
C	15.32423900	-1.28146600	0.67136000
C	16.35179900	0.73994400	-0.34208300
C	15.11178000	1.22813300	-0.57543700
C	14.08566500	-0.79643500	0.42531800
H	15.46436500	-2.22298500	1.19439500
H	17.22690800	1.29609900	-0.65837700
H	14.97033900	2.18257100	-1.07437600
H	13.21352700	-1.34127500	0.76795900
N	12.76273500	1.07306600	-0.53897100
C	11.51980500	0.46106000	-0.47220600
C	8.86431200	-0.57041500	-0.40704400
C	11.24705900	-0.88431400	-0.82009400
C	10.41633600	1.27604500	-0.13396300
C	9.12630700	0.77446300	-0.06570900
C	9.95372800	-1.37913900	-0.80096200
H	12.04986200	-1.52479700	-1.17022900
H	10.60530500	2.31523100	0.11851400
H	8.32132000	1.42126500	0.26182300
H	9.76781200	-2.40551000	-1.10756800
N	7.60305900	-1.14436100	-0.35963000
H	7.59192300	-2.15581800	-0.34002200
C	6.34446000	-0.53173400	-0.24646600
C	3.73919100	0.56596900	-0.04627600
C	5.31666600	-1.21919200	0.42084200
C	6.04437200	0.71567600	-0.82055900
C	4.76552100	1.25223800	-0.71620300
C	4.03788600	-0.68285800	0.52479000
H	5.53001600	-2.17863100	0.88506500
H	6.79851500	1.25475200	-1.38251700
H	4.55183500	2.21160100	-1.18034800
H	3.28285100	-1.22247200	1.08520100
N	2.48183800	1.18192500	0.07482500
H	2.49717100	2.19347900	0.08838700
C	1.22316900	0.60942300	0.14550900
C	-1.43071100	-0.42415600	0.26390600
C	0.95141200	-0.72844800	-0.21782400
C	0.14521700	1.40948100	0.58803000
C	-1.14620700	0.91386700	0.63531000
C	-0.33588000	-1.23063400	-0.12527800
H	1.74797600	-1.36725400	-0.58034400
H	0.34115200	2.42796200	0.91393500
H	-1.93586800	1.54528800	1.02829400
H	-0.53350300	-2.26356800	-0.39593600
N	-2.66613800	-1.04240100	0.34984100
C	-3.82007100	-0.45217200	0.14588400
C	-6.49448500	0.60774700	-0.17183900
C	-5.00737400	-1.21638100	0.50818200
C	-4.05371500	0.86814400	-0.43157600
C	-5.30778600	1.36068400	-0.56552200
C	-6.26216900	-0.72227600	0.38454500
H	-4.83273800	-2.19742200	0.94045800
H	-3.20838900	1.43730400	-0.80064700
H	-5.48285800	2.33102400	-1.02087700
H	-7.11225600	-1.30132300	0.72709800
N	-7.65028700	1.20000300	-0.33588300
C	-8.87716600	0.56256500	-0.19092700
C	-11.49194800	-0.53652000	0.02491700
C	-9.18302200	-0.70433100	-0.74230500
C	-9.91435900	1.26792100	0.45694300
C	-11.18605000	0.72886100	0.57915500
C	-10.45351800	-1.24523800	-0.61650100
H	-8.41965500	-1.24795000	-1.29010800
H	-9.68913800	2.24031900	0.88510400
H	-11.94516000	1.26924400	1.13580600
H	-10.67743300	-2.22110300	-1.03745200
N	-12.71883600	-1.17830600	0.15888500
C	-13.87632000	-0.58363500	0.04701600
C	-16.55564700	0.49421500	-0.10213200
C	-15.05157200	-1.36838500	0.42090500
C	-14.12604100	0.77353600	-0.43980100
C	-15.38048600	1.27286400	-0.49396900
C	-16.30614500	-0.86854700	0.37211300
H	-14.85993600	-2.37169000	0.78983000
H	-13.28843600	1.36400700	-0.79291900
H	-15.57269200	2.27125400	-0.87556900
H	-17.14613800	-1.46416300	0.71073700
N	-17.71093000	1.09065600	-0.19602600
C	-18.93379800	0.43709800	-0.00741600
C	-21.49706700	-0.68591300	0.31373100
C	-19.27373500	-0.77217500	-0.64852800
C	-19.91375900	1.09001500	0.76689600
C	-21.17195600	0.52107000	0.94265000
C	-20.54682200	-1.31957900	-0.49050000
H	-18.54982300	-1.25473700	-1.29823000
H	-19.66022200	2.03630500	1.23568000
H	-21.90783300	1.02806800	1.56098000
H	-20.79606400	-2.24574900	-1.00152400
H	-22.48551600	-1.11882800	0.43761500

OANI-PB	x	y	z
H	- 19.59560000	2.18757900	-0.39421500
C	-19.81010500	1.17962400	-0.05153700
C	-20.33794300	-1.39665700	0.88367900
C	-18.76713700	0.42604500	0.52321100
C	-21.08184300	0.63233200	-0.19515900
C	-21.35421400	-0.65782200	0.27320100
C	-19.05291300	-0.86833300	1.00466600
H	-21.86862900	1.21970000	-0.66075500
H	-22.35212000	-1.07567900	0.17670400
H	-18.27507900	-1.43616300	1.50622400
H	-20.54436900	-2.39075700	1.27110500
N	-17.52822800	1.05373500	0.69389300
C	-16.39012800	0.48378100	0.41476500
C	-13.74369100	-0.55834200	-0.09922900
C	-15.17987000	1.20514400	0.81082700
C	-16.19342100	-0.79476200	-0.27244300
C	-14.95259600	-1.28018800	-0.49474800
C	-13.93924500	0.72009200	0.58654100
H	-15.33111700	2.14170100	1.33925700
H	-17.06442500	-1.33485900	-0.62541300
H	-14.80095000	-2.21857700	-1.01984300
H	-13.06876000	1.25822300	0.94400700
N	-12.60418600	-1.13366800	-0.36958300
C	-11.36495700	-0.51769300	-0.22013800
C	-8.73922400	0.54471300	-0.00916200
C	-11.07401100	0.79216800	-0.66663100
C	-10.31070500	-1.28666800	0.31606400
C	-9.03196000	-0.76486400	0.43925800
C	-9.79486800	1.31338900	-0.54455100
H	-11.85445200	1.38524200	-1.13292000
H	-10.52647800	-2.29415000	0.65918100
H	-8.25481200	-1.35676000	0.91209900
H	-9.57944400	2.32190300	-0.88482500
N	-7.50347800	1.16545700	0.13819100
C	-6.35599200	0.57994800	-0.07910000
C	-3.69710100	-0.49409600	-0.43451200
C	-5.16090700	1.31565600	0.32828700
C	-6.13828500	-0.72258200	-0.70807900
C	-4.89138500	-1.22362700	-0.85541700
C	-3.91387600	0.81484700	0.18124400
H	-5.32821400	2.27621700	0.80635200
H	-6.99430300	-1.26982000	-1.08590800
H	-4.72396400	-2.18166200	-1.33847800
H	-3.05677500	1.36550500	0.55170400
N	-2.55001900	-1.08923600	-0.62388400
C	-1.31486400	-0.47380100	-0.44962500
C	1.30834000	0.58282000	-0.17574100
C	-0.99508600	0.81318300	-0.94194200
C	-0.28947900	-1.22286800	0.16586400
C	0.98648300	-0.70297700	0.31987500
C	0.28165300	1.33193000	-0.78989500
H	-1.75020500	1.38873600	-1.46805400
H	-0.52723000	-2.21210200	0.54559900
H	1.73771600	-1.27662500	0.85317800
H	0.51906000	2.32225500	-1.16699100
N	2.54132400	1.20274000	-0.00673600
C	3.69284700	0.60037400	-0.14260400
C	6.35701300	-0.50424300	-0.32508600
C	4.87445600	1.34985100	0.27841200
C	3.92814200	-0.73421100	-0.69281200
C	5.17656100	-1.24874500	-0.75844100
C	6.12314600	0.83584000	0.21245500
H	4.69346400	2.33477800	0.69840600
H	3.08569700	-1.29617000	-1.07934500
H	5.35789100	-2.23162000	-1.18305600
H	6.96693600	1.40089700	0.59166900
N	7.50650400	-1.11442400	-0.43592500
C	8.73888400	-0.49841300	-0.24360800
C	11.35892500	0.55097000	0.07730200
C	9.08715500	0.76299800	-0.78055600
C	9.73539800	-1.22644000	0.44049700
C	11.00979800	-0.70911700	0.61669200
C	10.36208500	1.27960500	-0.60546800
H	8.35731700	1.31909600	-1.36038200
H	9.47633000	-2.19686900	0.85336000
H	11.73834600	-1.26429000	1.19892700
H	10.62114900	2.25028400	-1.01776400
N	12.59278700	1.16668900	0.26473500
C	13.74057800	0.55304700	0.16665200
C	16.40000400	-0.57386500	0.04889400
C	14.92168900	1.30386100	0.59058200
C	13.97394900	-0.79701200	-0.34853900
C	15.21888500	-1.32007700	-0.38675800
C	16.16674900	0.78071700	0.55497100
H	14.74078900	2.30015000	0.98301400
H	13.13212200	-1.36198900	-0.73212500
H	15.40023100	-2.31312900	-0.78704300
H	17.01059600	1.34948200	0.92835100
N	17.54511700	-1.18973100	-0.03750600
C	18.77633300	-0.56540200	0.19119800
C	21.35325100	0.49833300	0.58925100
C	19.15008500	0.65458200	-0.40937000
C	19.72923800	-1.25901500	0.96380500
C	20.99420000	-0.71919600	1.17815200
C	20.43016900	1.17257400	-0.21362300
H	18.44732100	1.16851500	-1.05820000
H	19.44941800	-2.21308800	1.40068900
H	21.70909100	-1.25720700	1.79485000
H	20.70618900	2.10750100	-0.69391000
H	22.34725700	0.90835600	0.74281900

OANI-^{1}ES	x	y	z
H	-20.08154700	2.21036900	-0.91705200
C	-20.29442100	1.20715300	-0.55840000
C	-20.82232300	-1.37783500	0.35644400
C	-19.27296500	0.45134300	0.04103700
C	-21.56647300	0.66194900	-0.70447900
C	-21.83466400	-0.63524200	-0.25657900
C	-19.54624900	-0.84135200	0.51743100
H	-22.34862300	1.25083900	-1.17391200
H	-22.82734600	-1.05879300	-0.37378600
H	-18.78420600	-1.40552300	1.04301100
H	-21.02840600	-2.37600200	0.73089700
N	-18.01059900	1.06152900	0.20052100
H	-18.03864800	2.06614700	0.34110800
C	-16.76515400	0.51369500	0.16958400
C	-14.12187700	-0.48103000	0.11061800
C	-15.66766000	1.31423400	0.59894700
C	-16.50102000	-0.80889600	-0.28231000
C	-15.21439800	-1.29030300	-0.29668400
C	-14.38157200	0.83311000	0.57699400
H	-15.85951100	2.30819900	0.99106800
H	-17.30610800	-1.43025500	-0.65191000
H	-15.02505300	-2.29241400	-0.66958000
H	-13.58456400	1.44417300	0.98025000
N	-12.86468000	-1.04354900	0.06600100
H	-12.86887100	-2.06066800	0.04264500
C	-11.61716900	-0.49187300	0.04347900
C	-8.96997300	0.48732500	0.01629800
C	-11.35825300	0.86976500	-0.28004400
C	-10.51597600	-1.34647100	0.33982600
C	-9.22959700	-0.87440600	0.33967800
C	-10.07193700	1.34140900	-0.28171000
H	-12.16129700	1.52601900	-0.58775000
H	-10.70603300	-2.37777200	0.62076700
H	-8.42608400	-1.53160300	0.64375500
H	-9.88155500	2.37185300	-0.56536700
N	-7.72329200	1.03739700	-0.00866400
H	-7.71555000	2.05409500	0.00026100
C	-6.46262600	0.46588400	-0.04229600
C	-3.82550400	-0.53799000	-0.09785500
C	-5.37312800	1.26280700	0.38365200
C	-6.20654300	-0.84211900	-0.51715800
C	-4.91909300	-1.32961900	-0.53509600
C	-4.08509400	0.77460600	0.36958100
H	-5.55946500	2.26045400	0.76963400
H	-7.00313100	-1.44808300	-0.92900400
H	-4.73109900	-2.32225000	-0.93254600
H	-3.28411900	1.38746000	0.76190000
N	-2.57333100	-1.10056000	-0.12946800
H	-2.56306800	-2.11174100	-0.21164700
C	-1.31089500	-0.51445900	-0.05860900
C	1.31085400	0.51507600	0.05785500
C	-1.04781400	0.81202500	-0.45732700
C	-0.23932500	-1.31413900	0.38911900
C	1.04778800	-0.81141900	0.45654100
C	0.23930200	1.31474200	-0.38991300
H	-1.83458300	1.43315600	-0.86691400
H	-0.43277900	-2.32983400	0.72083800
H	1.83456900	-1.43254000	0.86612300
H	0.43275800	2.33044100	-0.72161900
N	2.57328400	1.10119800	0.12882800
H	2.56301000	2.11236800	0.21114200
C	3.82543800	0.53861700	0.09727200
C	6.46255200	-0.46528700	0.04176800
C	4.91902800	1.33022800	0.53455200
C	4.08501700	-0.77399500	-0.37014900
C	5.37303900	-1.26220400	-0.38419600
C	6.20647000	0.84271700	0.51663900
H	4.73103600	2.32286600	0.93198700
H	3.28402800	-1.38684300	-0.76245600
H	5.55937900	-2.25984400	-0.77019900
H	7.00304600	1.44868100	0.92850100
N	7.72319300	-1.03680600	0.00806500
H	7.71539600	-2.05350300	-0.00114300
C	8.96992200	-0.48682700	-0.01670000
C	11.61723800	0.49209300	-0.04354000
C	9.22969700	0.87497700	-0.33963400
C	10.07180300	-1.34113100	0.28099400
C	11.35817000	-0.86963200	0.27949000
C	10.51613000	1.34689900	-0.33961700
H	8.42627700	1.53236800	-0.64352500
H	9.88132300	-2.37166900	0.56423800
H	12.16114200	-1.52610300	0.58690600
H	10.70629600	2.37826900	-0.62022700
N	12.86479900	1.04365100	-0.06583000
H	12.86909700	2.06076100	-0.04224300
C	14.12195600	0.48099800	-0.11042800
C	16.76510600	-0.51402800	-0.16931200
C	15.21450500	1.29001400	0.29727700
C	14.38155000	-0.83303000	-0.57715300
C	15.66758300	-1.31430900	-0.59905400
C	16.50107900	0.80845000	0.28294100
H	15.02522500	2.29203600	0.67044400
H	13.58451600	-1.44388600	-0.98066800
H	15.85936900	-2.30819100	-0.99141700
H	17.30618700	1.42959300	0.65286400
N	18.01048600	-1.06205300	-0.20022300
H	18.03836600	-2.06664100	-0.34104900
C	19.27293200	-0.45219400	-0.04036100
C	21.83486300	0.63368900	0.25803800
C	19.54651100	0.84074200	-0.51593300
C	20.29423300	-1.20857900	0.55864300
C	21.56638600	-0.66373300	0.70511200
C	20.82269200	1.37685900	-0.35456300
H	18.78462700	1.40540000	-1.04122000
H	20.08113800	-2.21197900	0.91665600
H	22.34839600	-1.25308000	1.17420400
H	21.02898500	2.37521600	-0.72839600
H	22.82762200	1.05697000	0.37555800

OANI-^{3}ES	x	y	z
H	-20.09996700	2.08354400	-0.94526100
C	-20.29700500	1.08141400	-0.57502500
C	-20.78283100	-1.50210600	0.37061500
C	-19.25800300	0.33822800	0.01089300
C	-21.56550500	0.52269200	-0.69440500
C	-21.81251800	-0.77333500	-0.23048200
C	-19.50907200	-0.95352400	0.50301200
H	-22.36184200	1.09973600	-1.15430500
H	-22.80325600	-1.20677100	-0.32553400
H	-18.73215200	-1.50540600	1.01947800
H	-20.97356500	-2.49843900	0.75755600
N	-17.99890400	0.95933900	0.13938600
H	-18.03145600	1.96693600	0.26104700
C	-16.74880500	0.41786400	0.10449000
C	-14.09857700	-0.56478700	0.03621000
C	-15.65300300	1.23035800	0.51382300
C	-16.48104800	-0.90565200	-0.34378500
C	-15.19296600	-1.37942900	-0.36670100
C	-14.36502000	0.75564100	0.48903100
H	-15.84718200	2.23041000	0.88949000
H	-17.28547600	-1.53092800	-0.70875800
H	-14.99900000	-2.38137400	-0.73751600
H	-13.56367800	1.37883400	0.86439600
N	-12.84457900	-1.11283800	-0.00367200
H	-12.82279600	-2.12534200	-0.07997800
C	-11.58697600	-0.50940700	0.04991800
C	-8.98447200	0.55841100	0.13609300
C	-11.34564900	0.80891900	-0.38562100
C	-10.50648000	-1.28389600	0.51712900
C	-9.22686100	-0.76022500	0.57097900
C	-10.06568600	1.33167200	-0.33302600
H	-12.14215000	1.40553200	-0.81247200
H	-10.68591400	-2.29253200	0.87626200
H	-8.43049100	-1.35824500	0.99591300
H	-9.88586300	2.33958000	-0.69390100
N	-7.72808500	1.16230300	0.19132500
H	-7.74934000	2.17440200	0.26280000
C	-6.47220400	0.61162300	0.15544300
C	-3.82847600	-0.37111500	0.08721200
C	-5.38065800	1.41888300	0.57151000
C	-6.20688000	-0.70599100	-0.29651000
C	-4.91605700	-1.18381100	-0.31630300
C	-4.09010600	0.94190700	0.54740000
H	-5.57351800	2.41456100	0.95856600
H	-7.00685100	-1.33049900	-0.67204200
H	-4.72526800	-2.18487300	-0.69089600
H	-3.29481400	1.55885100	0.94503000
N	-2.56580000	-0.93355100	0.04652000
H	-2.56841000	-1.95070600	0.04190400
C	-1.32170400	-0.38012900	0.00981700
C	1.32364100	0.60231100	-0.04111300
C	-1.06683700	0.98138100	-0.32139600
C	-0.21621900	-1.23245100	0.30250800
C	1.06866800	-0.75914600	0.28998400
C	0.21833100	1.45496200	-0.33315200
H	-1.87324800	1.63545000	-0.62464300
H	-0.40330500	-2.26217900	0.59090200
H	1.87559400	-1.41282900	0.59279900
H	0.40554500	2.48487400	-0.62071200
N	2.56958400	1.15180800	-0.07664500
H	2.57878100	2.16882200	-0.06496600
C	3.82704900	0.57761600	-0.12425300
C	6.45699600	-0.43999000	-0.20322900
C	4.92407900	1.36801800	0.29684000
C	4.07198900	-0.72992700	-0.60837900
C	5.35566400	-1.22355400	-0.63885400
C	6.20862200	0.87234300	0.27300300
H	4.74554900	2.36474300	0.68867200
H	3.26871200	-1.32851900	-1.01794500
H	5.53606700	-2.21434000	-1.04424300
H	7.01526800	1.47841100	0.66384600
N	7.70252400	-1.01269100	-0.24672900
H	7.70145500	-2.02205300	-0.34961600
C	8.97353200	-0.44544700	-0.15952000
C	11.60619100	0.53787100	-0.01249700
C	9.25793700	0.88361900	-0.53289900
C	10.02835700	-1.27167400	0.27943200
C	11.32275300	-0.79086700	0.36141700
C	10.55261700	1.36568700	-0.44860800
H	8.48343900	1.52392100	-0.93602000
H	9.81692400	-2.28961100	0.59268500
H	12.09893800	-1.42970700	0.76410600
H	10.76364800	2.38437200	-0.75979100
N	12.88241500	1.09692200	0.07463100
H	12.89387600	2.10357000	0.20646800
C	14.11734600	0.51000800	0.00627700
C	16.73225100	-0.55816600	-0.11198000
C	15.23794900	1.26429000	0.45251400
C	14.33934400	-0.79303000	-0.51574000
C	15.61025100	-1.30960100	-0.56494500
C	16.50906800	0.74812200	0.40605800
H	15.07741900	2.25155000	0.87523000
H	13.51763200	-1.36785700	-0.92290200
H	15.77106600	-2.29449700	-0.99290500
H	17.33357400	1.32517400	0.80410400
N	17.96247400	-1.14073300	-0.17586500
H	17.95937300	-2.14017700	-0.35515700
C	19.24336500	-0.57684000	-0.00701000
C	21.83830800	0.41506700	0.31092500
C	19.54772000	0.73190300	-0.41724300
C	20.24917900	-1.39581300	0.53405300
C	21.53800000	-0.89671900	0.69193200
C	20.84147400	1.22004900	-0.24678600
H	18.79638500	1.34498100	-0.90157700
H	20.00980500	-2.41035500	0.84016000
H	22.30843600	-1.53256800	1.11713000
H	21.07351300	2.23009500	-0.57043600
H	22.84476200	0.80217600	0.43603400

OANI-^{5}ES	x	y	z
H	-20.13776700	1.87691100	-0.66995500
C	-20.28668300	0.86719100	-0.29848600
C	-20.64668100	-1.73659800	0.65034900
C	-19.19309500	0.14182400	0.20656800
C	-21.54636900	0.27955400	-0.33897200
C	-21.73076100	-1.02653600	0.12679000
C	-19.37989100	-1.16040400	0.70167500
H	-22.38531700	0.84131600	-0.73768000
H	-22.71543700	-1.48229700	0.09455500
H	-18.55807700	-1.69712600	1.16109600
H	-20.78894600	-2.73976900	1.04014000
N	-17.94446700	0.79088500	0.25236200
H	-17.99317500	1.79854100	0.37144700
C	-16.68523200	0.27962600	0.14839300
C	-14.01976600	-0.64001400	-0.05327100
C	-15.58978500	1.12150100	0.49471600
C	-16.40986800	-1.03708900	-0.31646500
C	-15.11421700	-1.47943400	-0.40627700
C	-14.29401100	0.67702400	0.40713300
H	-15.78826300	2.12088000	0.87004800
H	-17.21650100	-1.68063100	-0.64284700
H	-14.91476100	-2.47695000	-0.78594300
H	-13.48842400	1.32356400	0.73030400
N	-12.75940500	-1.15903600	-0.14941900
H	-12.71513200	-2.16584800	-0.26955300
C	-11.50984000	-0.51713100	-0.08362700
C	-8.95096500	0.62727600	0.01127800
C	-11.29841000	0.78138600	-0.57797100
C	-10.42749600	-1.23608900	0.45097000
C	-9.16242700	-0.67072700	0.50738000
C	-10.03338800	1.34835800	-0.51985200
H	-12.10479100	1.33222700	-1.04671000
H	-10.58700500	-2.23140500	0.85366100
H	-8.35587200	-1.22041400	0.97737000
H	-9.87471300	2.34446700	-0.92091400
N	-7.69689500	1.26098600	0.07413000
H	-7.73037400	2.26743700	0.20501100
C	-6.44524700	0.72397600	-0.01743700
C	-3.80026600	-0.25653500	-0.18618500
C	-5.33733100	1.53391400	0.36239200
C	-6.19357800	-0.59047100	-0.50011500
C	-4.90791600	-1.06340200	-0.57369500
C	-4.05103100	1.05991200	0.29038700
H	-5.51890900	2.53068300	0.75264100
H	-7.00878400	-1.20956400	-0.85182500
H	-4.72594800	-2.05893900	-0.96698700
H	-3.23634400	1.68028100	0.64089800
N	-2.55320300	-0.80684600	-0.26534900
H	-2.53479100	-1.81275000	-0.40214100
C	-1.28640000	-0.20538500	-0.16463500
C	1.30648000	0.84919000	-0.00454300
C	-1.02558300	1.09796200	-0.62167200
C	-0.23657200	-0.97483900	0.36525400
C	1.04491900	-0.45321000	0.45465200
C	0.25724400	1.61973200	-0.53218900
H	-1.80549600	1.68697400	-1.08885000
H	-0.43509500	-1.97442400	0.73925000
H	1.82716900	-1.04163300	0.91912000
H	0.45591500	2.61897300	-0.90672400
N	2.58207200	1.43458700	0.09474000
H	2.58634700	2.43467200	0.27050000
C	3.81143700	0.84905100	-0.01082400
C	6.41121000	-0.24087300	-0.20694100
C	4.94959700	1.58579800	0.42372600
C	4.00915200	-0.44843600	-0.55942700
C	5.27278100	-0.97498300	-0.64684700
C	6.21409400	1.05781000	0.33920700
H	4.80797400	2.56645900	0.86749800
H	3.17019600	-1.01102800	-0.94848800
H	5.41426500	-1.95551300	-1.09105400
H	7.05128200	1.61942100	0.73291500
N	7.63226600	-0.84265500	-0.30649300
H	7.60587400	-1.83944800	-0.49845200
C	8.92493700	-0.31238300	-0.15670600
C	11.56411400	0.59800800	0.10755800
C	9.25539200	1.00549900	-0.51706100
C	9.92935500	-1.16993200	0.32389700
C	11.23309200	-0.72010800	0.46601400
C	10.56088600	1.45422100	-0.37612600
H	8.51264200	1.66373400	-0.95130600
H	9.67688300	-2.18335900	0.62065800
H	11.97870400	-1.37938700	0.89390600
H	10.81410100	2.46675800	-0.67490500
N	12.86201900	1.11641800	0.26603700
H	12.90445900	2.10230200	0.50341800
C	14.06948900	0.48836500	0.14099500
C	16.63101200	-0.68431800	-0.09138300
C	15.22715000	1.15246500	0.63584700
C	14.22718900	-0.78001900	-0.48216400
C	15.47201600	-1.34818400	-0.58633600
C	16.47251600	0.58508700	0.53255700
H	15.11494900	2.10851800	1.13800800
H	13.37356000	-1.28729500	-0.91323400
H	15.58282400	-2.30590900	-1.08571300
H	17.32542500	1.08897600	0.96841200
N	17.83222600	-1.31666700	-0.21405700
H	17.77963800	-2.29943700	-0.46579600
C	19.13892400	-0.82917700	-0.02167100
C	21.77934300	0.01269700	0.33873500
C	19.49797700	0.49604800	-0.32256800
C	20.11245800	-1.73821300	0.42904100
C	21.42394700	-1.31289600	0.60987800
C	20.81462000	0.90792200	-0.13185500
H	18.77012400	1.18075900	-0.74219100
H	19.83044900	-2.76350300	0.65125700
H	22.16937900	-2.01686000	0.96649700
H	21.09021700	1.93020300	-0.37173600
H	22.80411400	0.34166700	0.48018200

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