Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Comparing the Structures and Photophysical Properties of Two Charge Transfer Co-crystals

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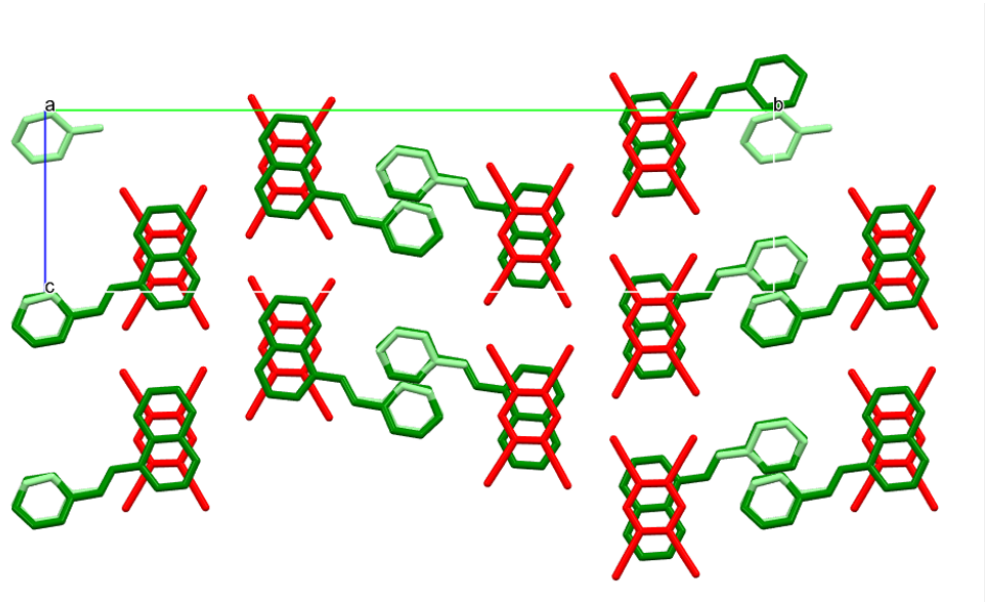
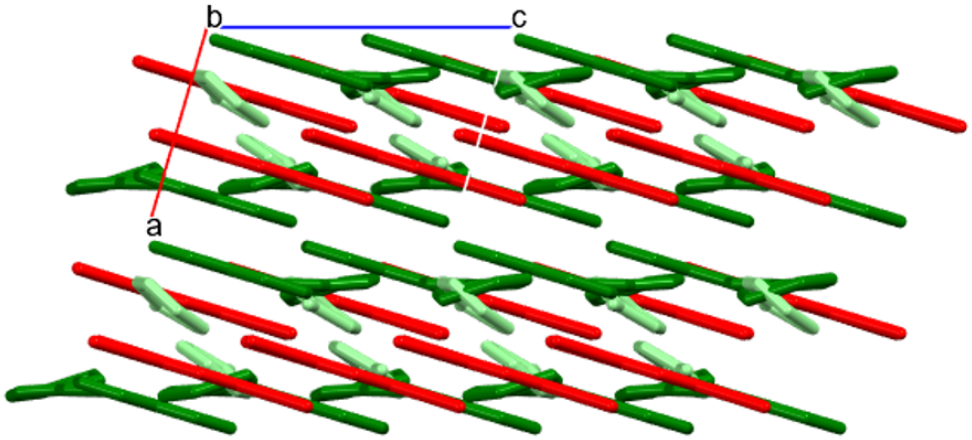


Figure S1: Expanded unit cell of Npe:TCNB (view along the crystallographic a-axis).



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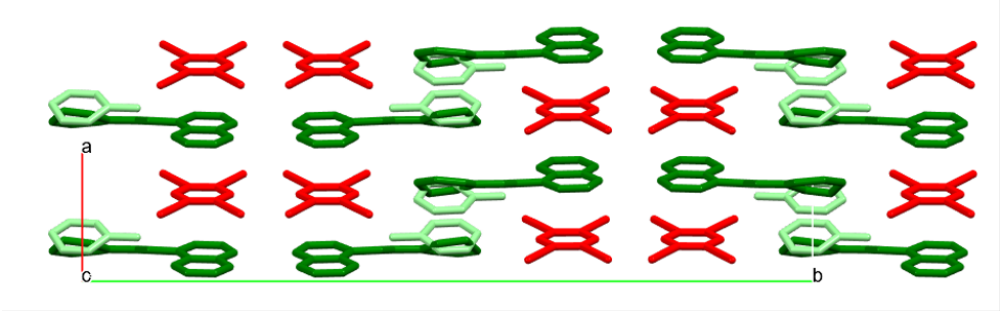

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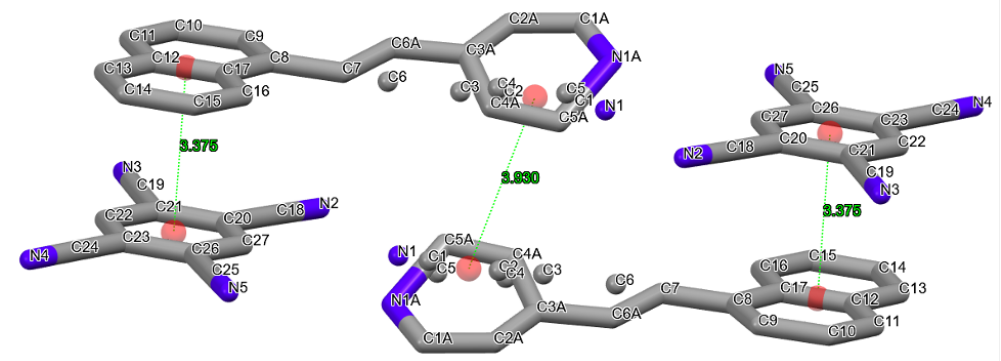

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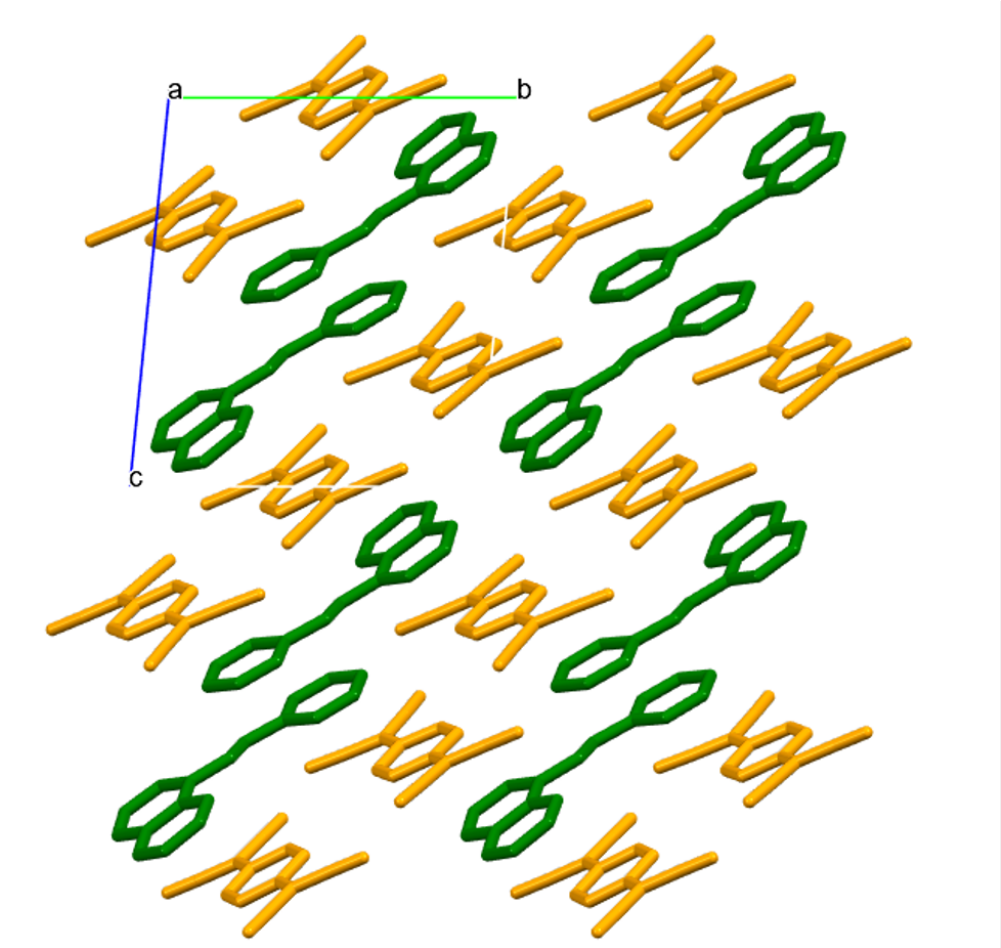

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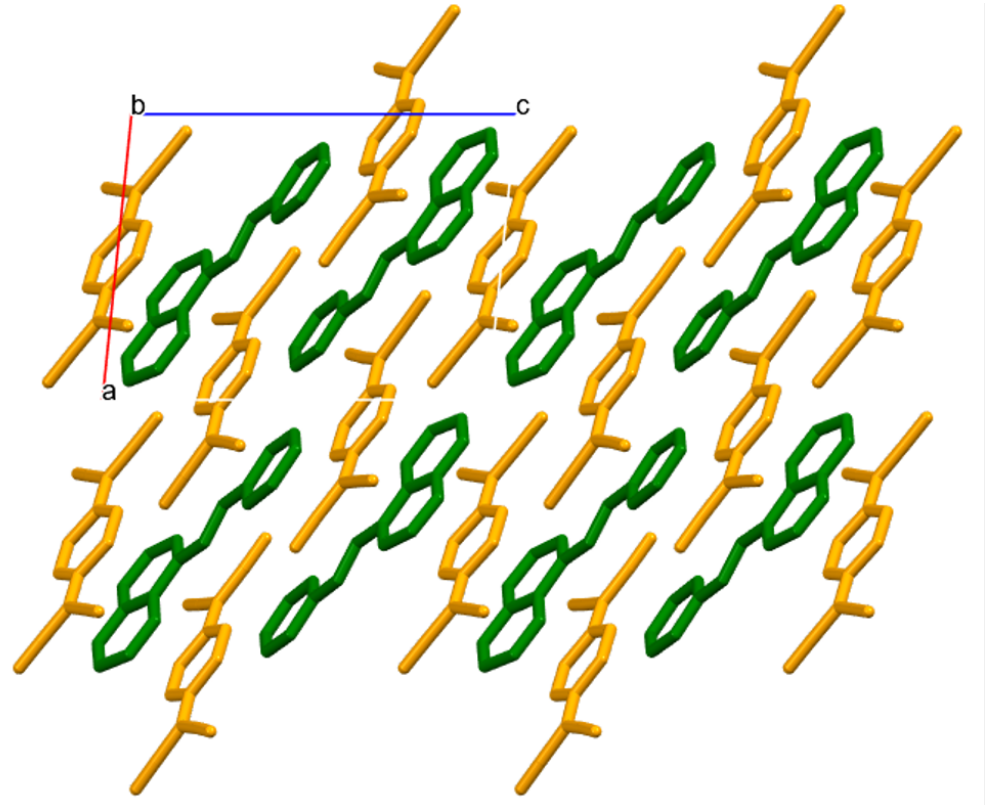


Figure S6: Expanded unit cell of Npe:TCNQ (view along the crystallographic b-axis).

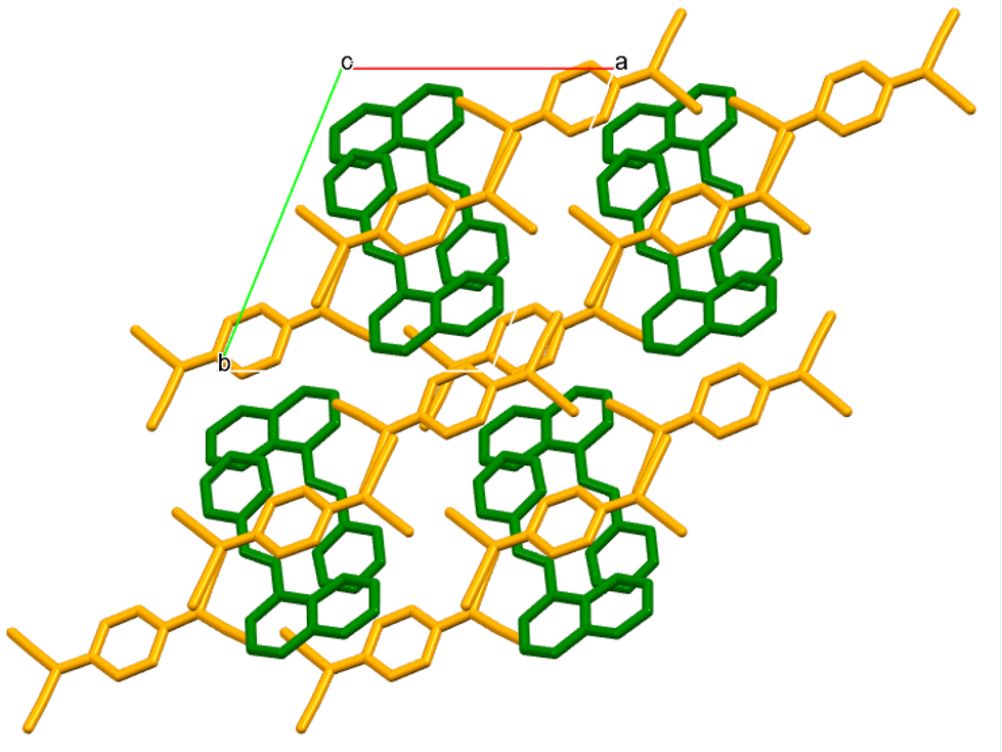
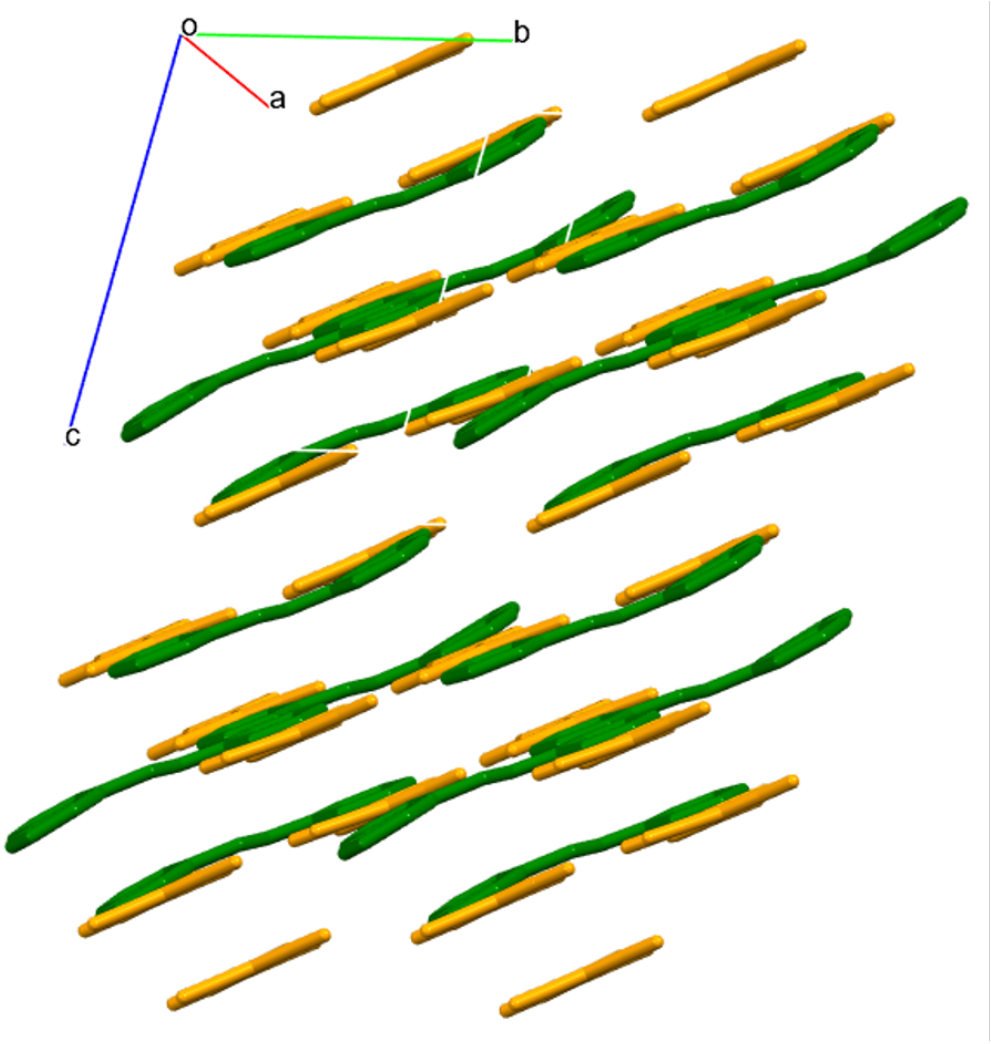


Figure S7: Expanded unit cell of Npe:TCNQ (view along the crystallographic c-axis).



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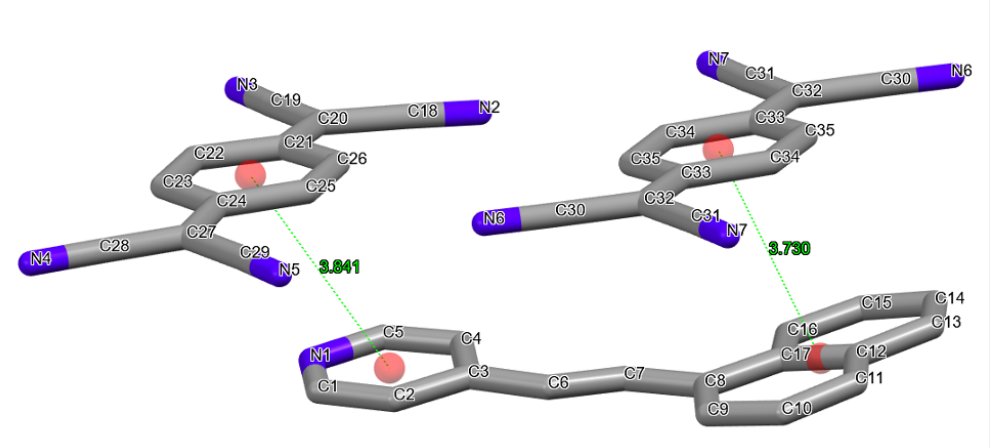
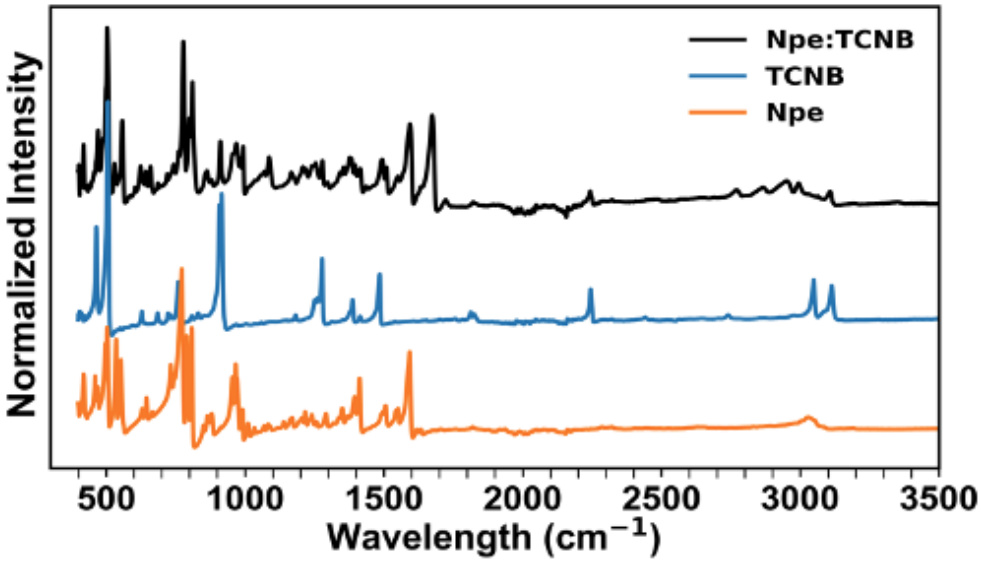


Figure S9: Expanded asymmetric unit of Npe:TCNQ (interatomic distances in Å).



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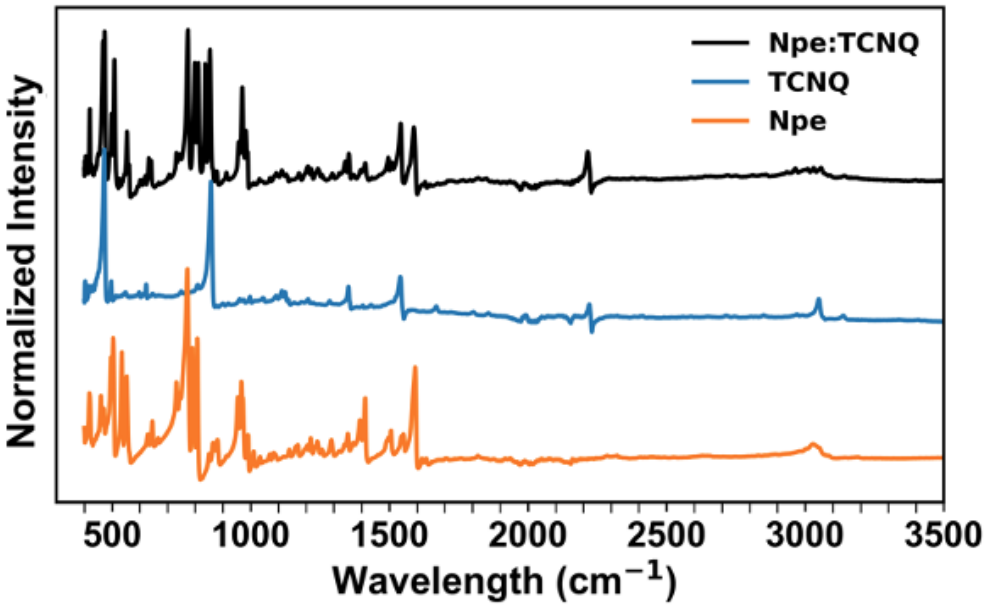

Figure S11: Infrared spectra of Npe, TCNQ, and Npe:TCNQ co-crystals.

1.2 Band Gap Analysis

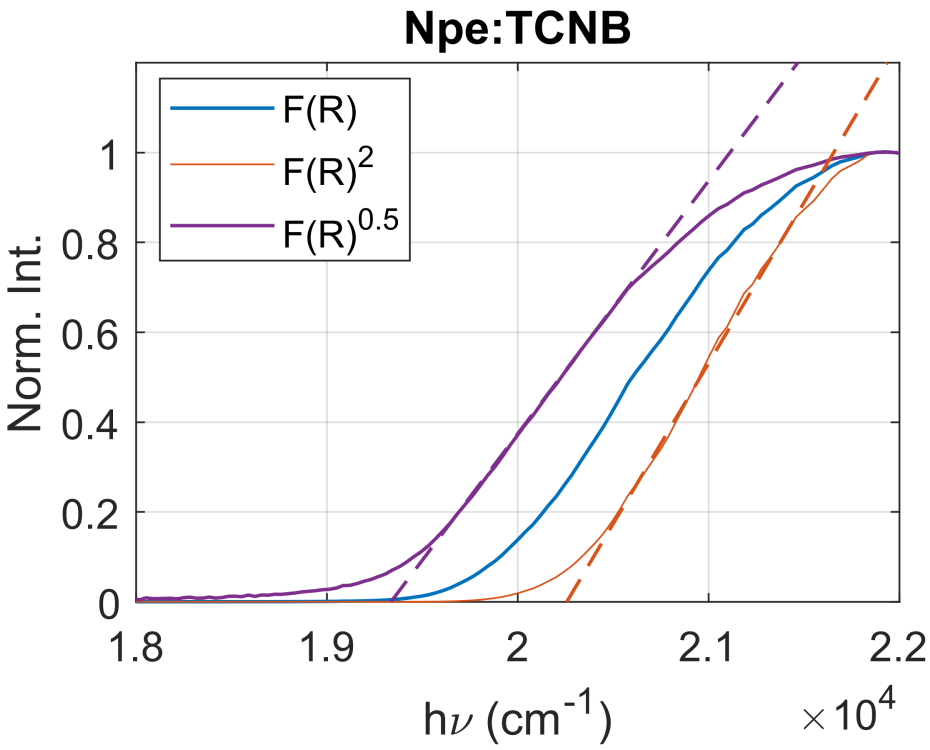

Figure S12: Plots of $F(R)1/\gamma$ vs. photon energy for Npe:TCNB.

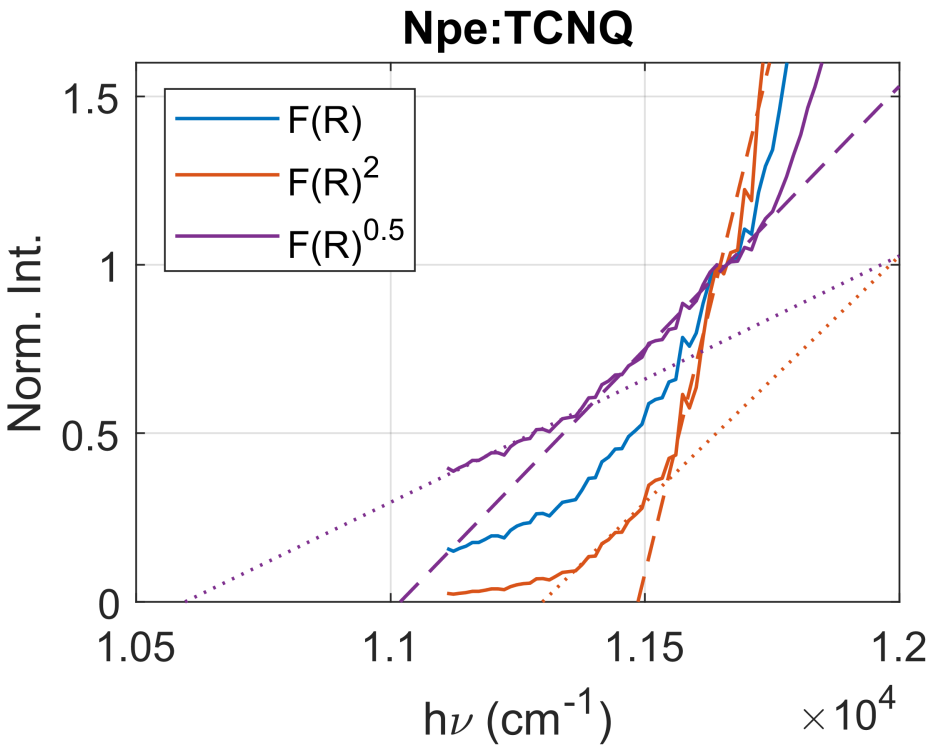

Figure S13: Plots of $F(R)1/\gamma$ vs. photon energy for Npe:TCNQ. Due to the vibronic structure observed in Npe:TCNQ, multiple linear fits were performed up to the lowest energy shoulder at 11600 cm^{-1}.

2 Computational Results

2.1 Further analysis of the Npe:TCNB theoretical dimer structures

The centroid-centroid distances between Npe and TCNB in the six isomers shown in Figure 2 agree with the experimentally observed distances, ranging between 3.3 and 3.5 Å. The values quantifying degree of CT are very consistent for all isomers in the S_0 and S_1 states, varying between 0.01e and 0.02e in S_0 and between 0.96e and 0.98e in S_1, as shown in Figure 2. In all isomers found, the S_1 state is a CT state characterized by the HOMO to LUMO transition. The computed oscillator strengths of these transitions, however, are quite different. Isomers a, d, and e exhibit S_1 oscillator strengths with values of 0.021, 0.016, and 0.023 a.u., respectively, higher than the other conformers where the S_1 state oscillator strength values range from 0.002 to 0.009 a.u. Of these, structure a (the lowest-energy isomer) is far closer geometrically to the experimental crystal structure than d or e, allowing structure a to emerge as the best model for Npe:TCNB, as predicted from energetic arguments alone in Section 3.1.

2.2 Further analysis of the Npe:TCNQ theoretical dimer structures

Between Npe and TCNQ, a centroid-centroid intermolecular distance of 3.4 Å is found in all structures except b, which exhibits a smaller distance of 3.2 Å. This shorter distance can be explained by the alignment between the TCNQ and Npe molecules, resulting in strong hydrogen bonding between the N atoms of the TCNQ and the H atoms of the Npe pyridine ring. In analysis of the degree of CT in the S_0 and S_1 states, we find that these quantities vary between conformers of Npe:TCNQ far more than in Npe:TCNB. In the S_0 state, CT values range from 0.01 to 0.07e, while in the S_1 state, CT values range from 0.92 to 0.97, exhibiting neutral character in the S_0 state and ionic character in the S_1 state, a trend also seen in Npe:TCNB. We turn to the S_1 oscillator strength to assess our choice of the lowest-energy conformer a as our model. Indeed, we find that conformer a emerges as the optimal candidate, as its S_1 oscillator strength is sufficiently large (0.030 a.u. compared to 0.002 a.u. in structurally similar isomer d).

2.3 Figures

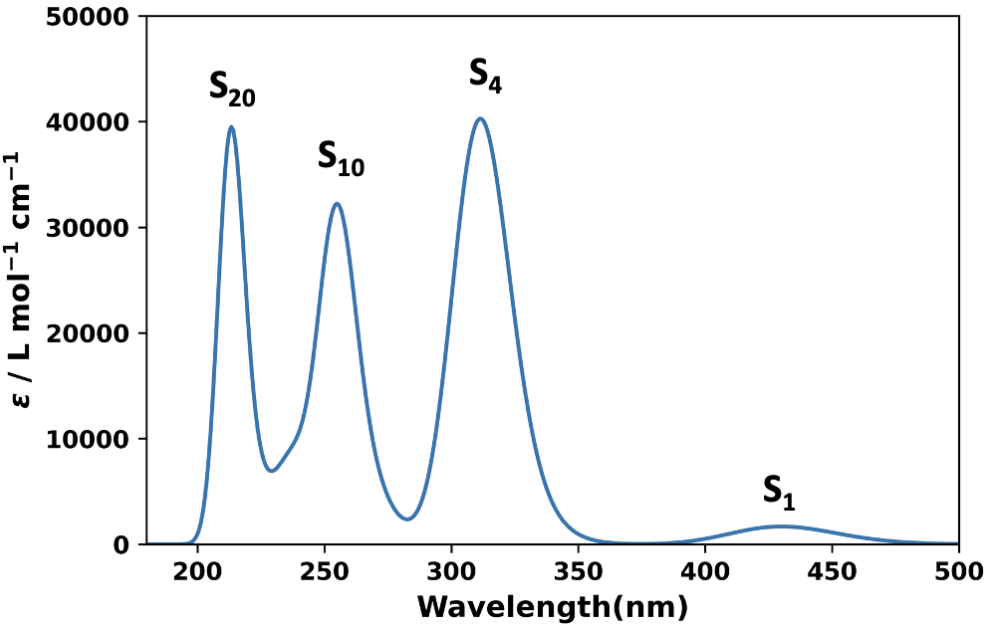

Figure S14: Simulated UV-Vis absorption spectra of Npe:TCNB conformer a, computed with CAM-B3LYP-D3/6-31+G(d,p).

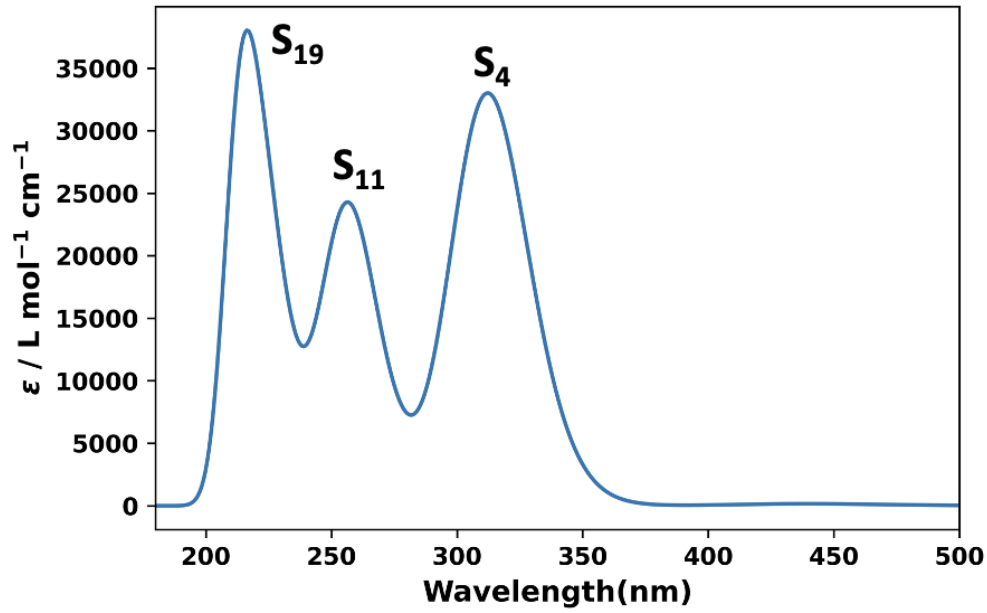

Figure S15: Simulated UV-Vis absorption spectra of Npe:TCNB conformer b, computed with CAM-B3LYP-D3/6-31+G(d,p).

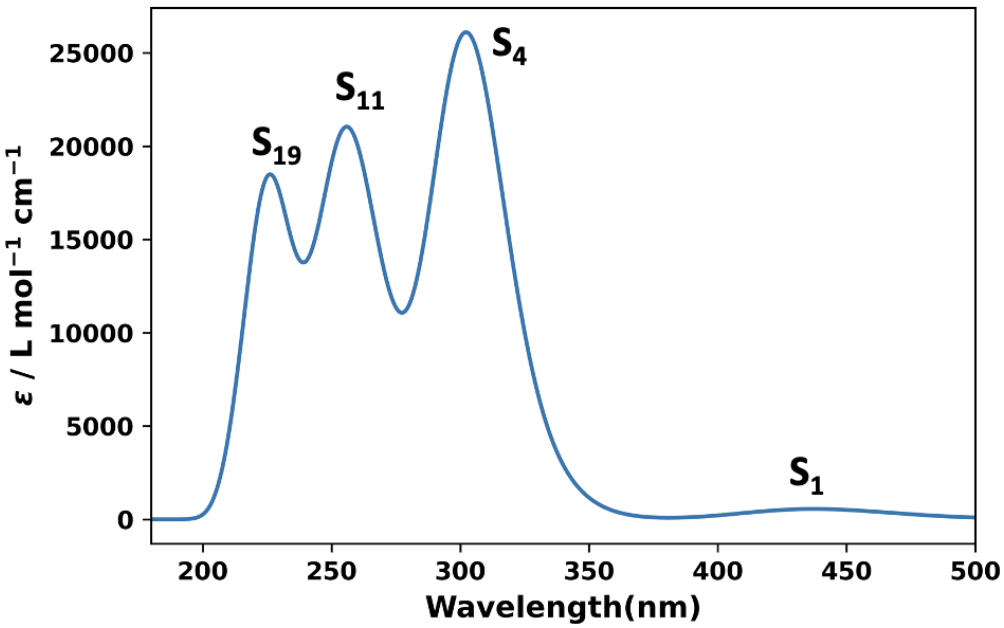

Figure S16: Simulated UV-Vis absorption spectra of Npe:TCNB conformer c, computed with CAM-B3LYP-D3/6-31+G(d,p).

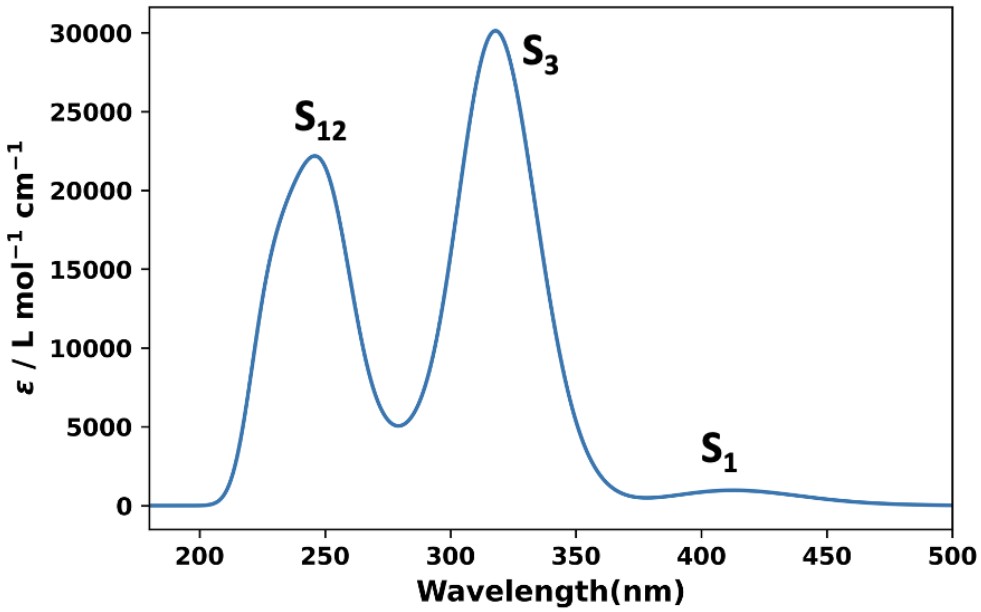

Figure S17: Simulated UV-Vis absorption spectra of Npe:TCNB conformer d, computed with CAM-B3LYP-D3/6-31+G(d,p).

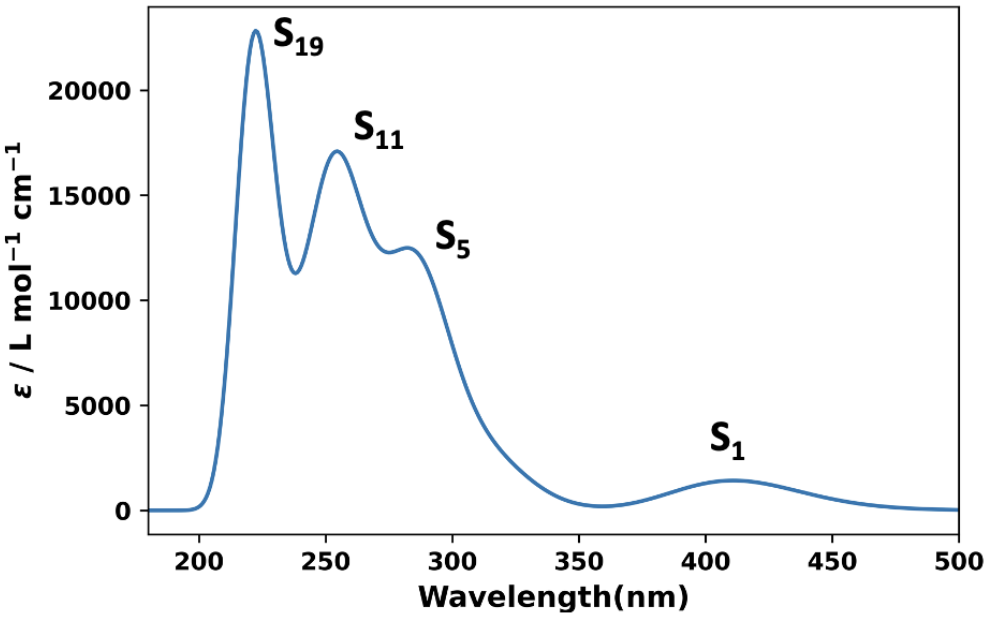

Figure S18: Simulated UV-Vis absorption spectra of Npe:TCNB conformer e, computed with CAM-B3LYP-D3/6-31+G(d,p).

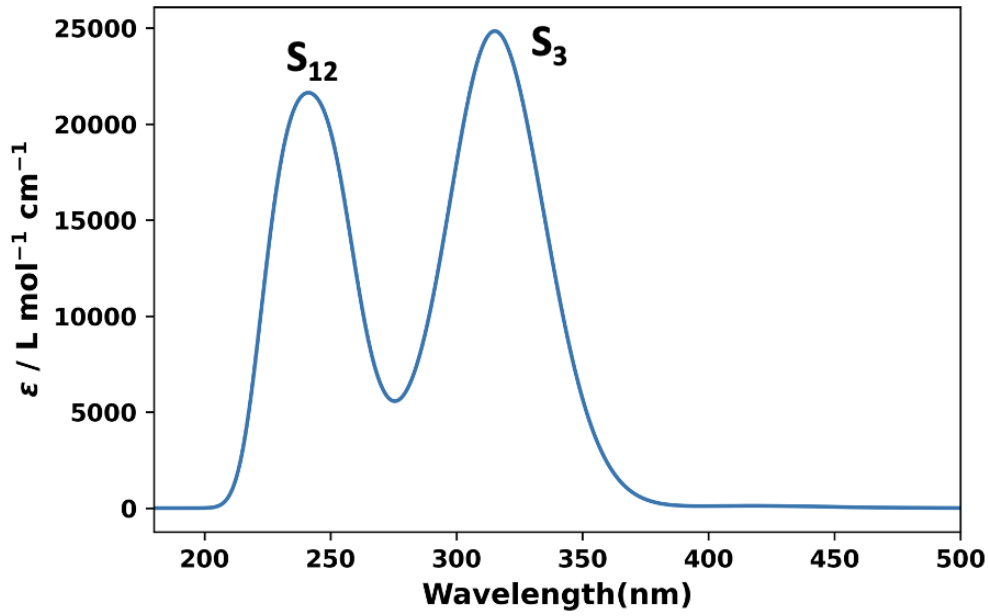

Figure S19: Simulated UV-Vis absorption spectra of Npe:TCNB conformer f, computed with CAM-B3LYP-D3/6-31+G(d,p).

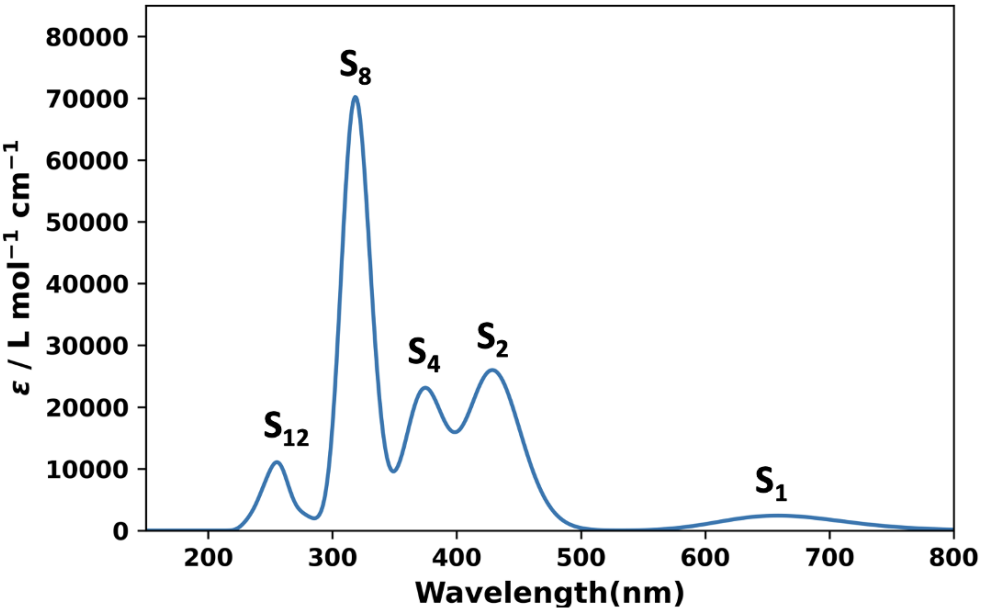

Figure S20: Simulated UV-Vis absorption spectra of Npe:TCNQ conformer a, computed with CAM-B3LYP-D3/6-31+G(d,p).

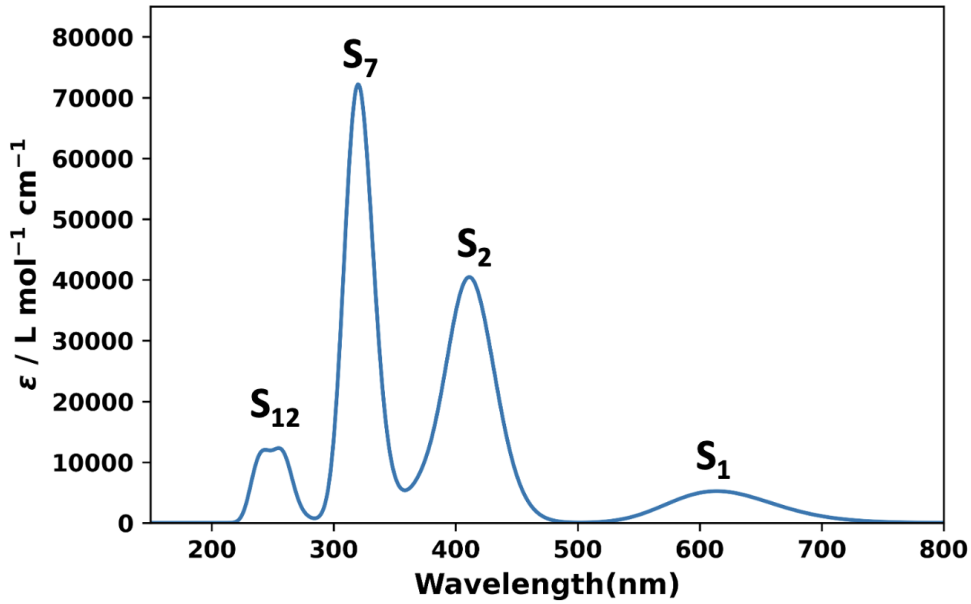

Figure S21: Simulated UV-Vis absorption spectra of Npe:TCNQ conformer b, computed with CAM-B3LYP-D3/6-31+G(d,p).

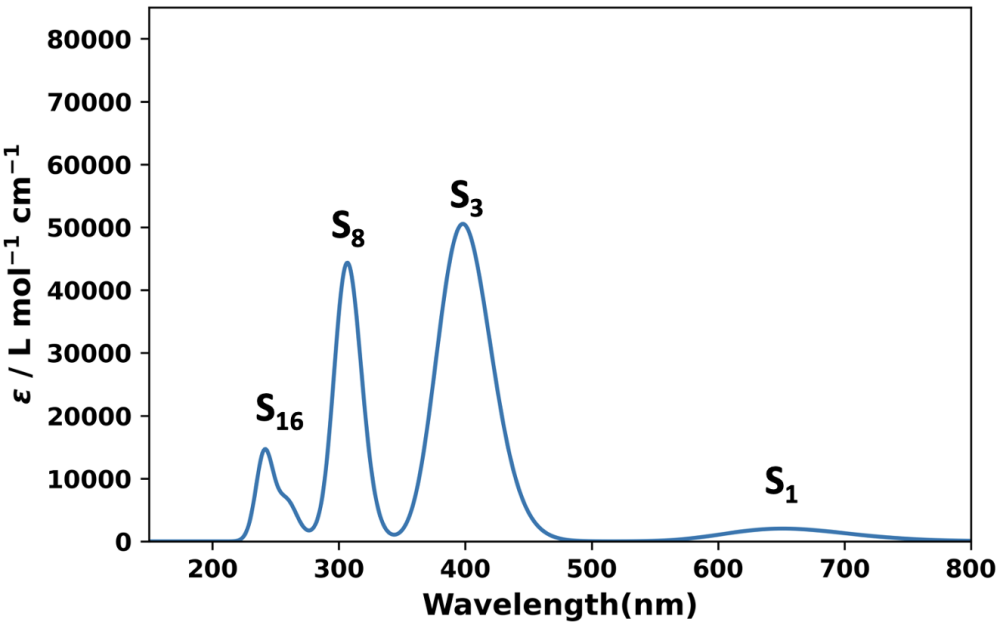

Figure S22: Simulated UV-Vis absorption spectra of Npe:TCNQ conformer c, computed with CAM-B3LYP-D3/6-31+G(d,p).

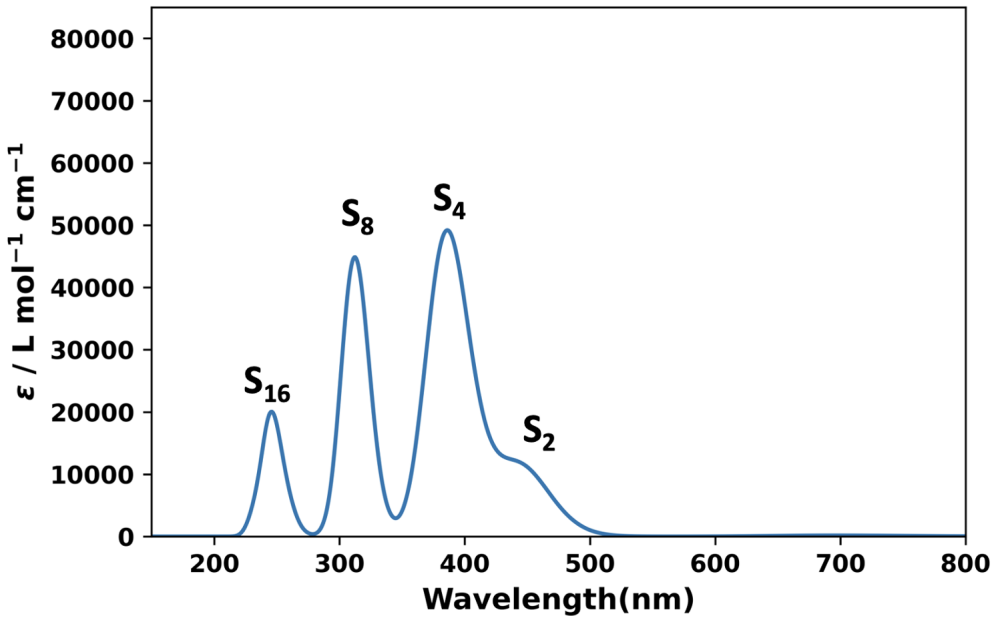

Figure S23: Simulated UV-Vis absorption spectra of Npe:TCNQ conformer d, computed with CAM-B3LYP-D3/6-31+G(d,p).

2.4 Energetics

Table S1: Relative energies of Npe:TCNQ conformers optimized with different functionals and basis sets. All relative energies are zero-point energy corrected.

Model Chemistry / Conformer	a	b	c	d
B3LYP/6-31G(d,p)	0.000	0.096	0.014	0.014
B3LYP/6-31+G(d,p)	0.016	0.000	0.029	0.027
B3LYP/6-311+G(d,p)	0.017	0.000	N/A	0.024
B3LYP-D3/6-31G(d,p)	0.016	0.000	0.077	0.106
B3LYP-D3/6-31+G(d,p)	0.008	0.000	0.074	0.102
B3LYP-D3/6-311+G(d,p)	0.007	0.000	0.077	0.104
CAM-B3LYP/6-31G(d,p)	0.000	0.080	0.068	0.019
CAM-B3LYP/6-31+G(d,p)	0.006	0.059	0.000	0.000
CAM-B3LYP/6-311+G(d,p)	0.004	0.056	0.000	0.000
CAM-B3LYP-D3/6-31G(d,p)	0.000	0.003	0.024	0.028
CAM-B3LYP-D3/6-31+G(d,p)	0.000	0.010	0.026	0.029
CAM-B3LYP-D3/6-311+G(d,p)	0.000	0.010	0.031	0.034
ωB97X-D/6-31G(d,p)	0.003	0.000	0.006	0.018
ωB97X-D/6-31+G(d,p)	0.000	0.006	0.017	0.032
ωB97X-D/6-311+G(d,p)	0.000	0.011	0.024	0.035
M062x/6-31G(d,p)	0.012	0.000	0.040	0.055
M062x/6-31+G(d,p)	0.013	0.000	0.042	0.054
M062x/6-311+G(d,p)	0.010	0.000	0.048	0.062

Table S2: Relative energies of Npe:TCNB conformers optimized with different functionals and basis sets. All relative energies are zero-point energy corrected.

Model Chemistry / Conformer	a	b	c	d	e	f
B3LYP/6-31G(d,p)	0.000	0.005	0.073	0.023	0.235	0.083
B3LYP/6-31+G(d,p)	0.000	0.002	0.075	N/A	0.215	0.078
B3LYP/6-311+G(d,p)	0.000	0.002	0.073	N/A	0.208	0.024
B3LYP-D3/6-31G(d,p)	0.000	0.015	0.059	0.113	0.129	0.182
B3LYP-D3/6-31+G(d,p)	0.000	0.009	0.063	0.121	0.110	0.190
B3LYP-D3/6-311+G(d,p)	0.000	0.013	0.066	0.129	0.106	0.203
CAM-B3LYP/6-31G(d,p)	0.000	0.004	0.069	0.040	0.208	0.119
CAM-B3LYP/6-31+G(d,p)	0.000	0.000	0.071	0.011	0.183	0.103
CAM-B3LYP/6-311+G(d,p)	0.000	0.000	0.070	0.037	0.178	0.108
CAM-B3LYP-D3/6-31G(d,p)	0.000	0.016	0.060	0.103	0.133	0.171
CAM-B3LYP-D3/6-31+G(d,p)	0.000	0.009	0.062	0.107	0.111	0.179
CAM-B3LYP-D3/6-311+G(d,p)	0.000	0.014	0.064	0.115	0.106	0.190
ωB97X-D/6-31G(d,p)	0.000	0.017	0.055	0.114	0.113	0.182
ωB97X-D/6-31+G(d,p)	0.000	0.012	0.054	0.120	0.083	0.181
ωB97X-D/6-311+G(d,p)	0.000	0.018	0.061	0.130	0.082	0.200
M062x/6-31G(d,p)	0.000	0.015	0.053	0.129	0.132	0.191
M062x/6-31+G(d,p)	0.000	0.012	0.054	0.136	0.108	0.204
M062x/6-311+G(d,p)	0.000	0.015	0.055	0.153	0.099	0.221

2.5 Excited State Properties

2.5.1 Npe:TCNQ

Table S3: Excitation energies and oscillator strengths of Npe:TCNQ conformer a at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.030	1.884	658.24
S2	0.310	2.884	429.93
S3	0.015	3.035	408.45
S4	0.280	3.315	374.00
S5	0.001	3.629	341.65
S6	0.008	3.783	327.71
S7	0.000	3.810	325.42
S8	0.860	3.894	318.40
S9	0.011	4.435	279.54
S10	0.014	4.479	276.78
S11	0.003	4.653	266.48
S12	0.076	4.789	258.89
S13	0.036	4.863	254.95
S14	0.015	4.942	250.88
S15	0.010	4.993	248.30
S16	0.017	5.073	244.40
S17	0.028	5.086	243.77
S18	0.000	5.221	237.46
S19	0.017	5.311	233.44
S20	0.000	5.351	231.68

Table S4: Excitation energies and oscillator strengths of Npe:TCNQ conformer b at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.065	2.020	613.83
S2	0.489	3.010	411.95
S3	0.002	3.121	397.30
S4	0.071	3.299	375.79
S5	0.033	3.648	339.88
S6	0.002	3.748	330.83
S7	0.879	3.876	319.88
S8	0.002	3.945	314.25
S9	0.004	4.441	279.19
S10	0.003	4.493	275.97
S11	0.003	4.671	265.42
S12	0.091	4.772	259.80
S13	0.032	4.848	255.72
S14	0.006	4.901	252.98
S15	0.046	5.011	247.44
S16	0.043	5.122	242.06
S17	0.025	5.156	240.45
S18	0.038	5.244	236.43
S19	0.000	5.250	236.16
S20	0.022	5.308	233.57

Table S5: Excitation energies and oscillator strengths of Npe:TCNQ conformer c at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.025	1.905	651.01
S2	0.066	2.947	420.74
S3	0.418	3.080	402.50
S4	0.243	3.219	385.20
S5	0.001	3.713	333.89
S6	0.003	3.743	331.28
S7	0.001	3.885	319.13
S8	0.547	4.042	306.76
S9	0.011	4.389	282.48
S10	0.000	4.502	275.38
S11	0.003	4.755	260.73
S12	0.070	4.777	259.57
S13	0.002	4.867	254.74
S14	0.011	5.063	244.90
S15	0.036	5.090	243.59
S16	0.125	5.143	241.09
S17	0.001	5.227	237.19
S18	0.008	5.237	236.74
S19	0.004	5.332	232.54
S20	0.005	5.367	231.01

Table S6: Excitation energies and oscillator strengths of Npe:TCNQ conformer d at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.002	1.782	695.55
S2	0.135	2.788	444.76
S3	0.051	3.084	402.07
S4	0.573	3.220	385.09
S5	0.003	3.624	342.13
S6	0.000	3.715	333.78
S7	0.003	3.873	320.12
S8	0.552	3.971	312.25
S9	0.000	4.450	278.64
S10	0.001	4.476	277.02
S11	0.003	4.706	263.44
S12	0.027	4.800	258.32
S13	0.043	4.863	254.94
S14	0.029	5.006	247.66
S15	0.034	5.052	245.43
S16	0.145	5.061	244.99
S17	0.002	5.193	238.75
S18	0.022	5.207	238.10
S19	0.013	5.307	233.62
S20	0.026	5.346	231.94

2.5.2 Npe:TCNB

Table S7: Excitation energies and oscillator strengths of Npe:TCNB conformer a at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.021	2.883	430.05
S2	0.020	3.738	331.66
S3	0.017	3.884	319.25
S4	0.478	3.985	311.14
S5	0.006	4.202	295.09
S6	0.001	4.503	275.34
S7	0.040	4.577	270.91
S8	0.003	4.701	263.76
S9	0.013	4.795	258.58
S10	0.356	4.859	255.16
S11	0.004	4.882	253.95
S12	0.005	4.931	251.44
S13	0.024	5.042	245.90
S14	0.010	5.056	245.21
S15	0.000	5.108	242.71
S16	0.082	5.246	236.35
S17	0.002	5.366	231.06
S18	0.000	5.474	226.51
S19	0.049	5.542	223.71
S20	0.480	5.814	213.23

Table S8: Excitation energies and oscillator strengths of Npe:TCNB conformer b at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.003	2.823	439.18
S2	0.026	3.778	328.21
S3	0.066	3.881	319.46
S4	0.463	3.986	311.07
S5	0.012	4.154	298.50
S6	0.003	4.498	275.61
S7	0.063	4.575	271.01
S8	0.003	4.684	264.68
S9	0.019	4.770	259.92
S10	0.033	4.795	258.55
S11	0.209	4.821	257.20
S12	0.090	4.899	253.09
S13	0.004	4.988	248.56
S14	0.021	5.018	247.09
S15	0.020	5.069	244.61
S16	0.030	5.220	237.53
S17	0.019	5.385	230.23
S18	0.001	5.486	226.00
S19	0.257	5.495	225.65
S20	0.526	5.786	214.28

Table S9: Excitation energies and oscillator strengths of Npe:TCNB conformer c at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.009	2.835	437.33
S2	0.022	3.771	328.82
S3	0.025	3.908	317.25
S4	0.358	4.106	301.99
S5	0.050	4.131	300.10
S6	0.001	4.507	275.11
S7	0.084	4.581	270.65
S8	0.018	4.730	262.14
S9	0.010	4.754	260.80
S10	0.013	4.783	259.24
S11	0.131	4.829	256.75
S12	0.109	4.893	253.39
S13	0.018	4.932	251.40
S14	0.018	5.062	244.94
S15	0.030	5.104	242.92
S16	0.054	5.275	235.06
S17	0.017	5.349	231.77
S18	0.011	5.495	225.63
S19	0.216	5.498	225.52
S20	0.074	5.744	215.86

Table S10: Excitation energies and oscillator strengths of Npe:TCNB conformer d at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.016	3.005	412.63
S2	0.187	3.865	320.75
S3	0.305	3.912	316.91
S4	0.006	4.148	298.87
S5	0.014	4.299	288.42
S6	0.033	4.305	288.01
S7	0.001	4.499	275.56
S8	0.002	4.514	274.68
S9	0.035	4.616	268.59
S10	0.003	4.763	260.30
S11	0.004	4.795	258.57
S12	0.230	4.910	252.54
S13	0.017	4.989	248.54
S14	0.012	5.064	244.84
S15	0.019	5.179	239.41
S16	0.084	5.187	239.04
S17	0.085	5.196	238.59
S18	0.004	5.308	233.60
S19	0.169	5.471	226.64
S20	0.001	5.504	225.27

Table S11: Excitation energies and oscillator strengths of Npe:TCNB conformer e at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.023	3.018	410.88
S2	0.007	3.898	318.04
S3	0.027	3.927	315.71
S4	0.004	4.133	299.95
S5	0.165	4.315	287.33
S6	0.003	4.556	272.12
S7	0.058	4.583	270.52
S8	0.006	4.776	259.60
S9	0.100	4.799	258.36
S10	0.012	4.803	258.16
S11	0.113	4.928	251.62
S12	0.014	4.955	250.22
S13	0.023	5.069	244.60
S14	0.007	5.094	243.38
S15	0.011	5.126	241.89
S16	0.035	5.198	238.52
S17	0.026	5.434	228.15
S18	0.004	5.471	226.63
S19	0.270	5.566	222.74
S20	0.088	5.675	218.49

Table S12: Excitation energies and oscillator strengths of Npe:TCNB conformer f at the CAM-B3LYP-D3/6-31+G(d,p) level of theory

Excited State	Oscillator Strength	E (eV)	E (nm)
S1	0.002	2.967	417.84
S2	0.191	3.793	326.89
S3	0.260	3.994	310.46
S4	0.003	4.117	301.16
S5	0.068	4.260	291.08
S6	0.000	4.281	289.61
S7	0.002	4.463	277.77
S8	0.002	4.480	276.77
S9	0.035	4.604	269.30
S10	0.004	4.754	260.80
S11	0.005	4.814	257.56
S12	0.180	4.919	252.03
S13	0.051	4.997	248.12
S14	0.003	5.042	245.91
S15	0.004	5.176	239.55
S16	0.047	5.203	238.29
S17	0.157	5.234	236.89
S18	0.009	5.326	232.80
S19	0.000	5.438	227.98
S20	0.142	5.478	226.35

2.6 Geometries

2.6.1 Monomer Optimized Geometries

Npe

E=-709.793714 E_h

0 1

H	-0.77115	-0.799086	0.879519
H	-0.87117	1.741053	-0.814270
H	-5.38473	-1.529269	1.558058
H	-5.34332	1.108336	-1.594221
N	-5.48399	-0.210198	-0.019065
H	-2.91635	-1.467138	1.760004
C	-4.79778	-0.908312	0.886069
H	-2.88553	1.277052	-1.555187
C	-4.77316	0.552246	-0.854454
C	-3.41319	-0.874530	0.998251
C	-3.38982	0.654042	-0.825180
C	-2.66965	-0.067860	0.132785
C	-1.20767	-0.021327	0.258901
C	-0.41240	0.915132	-0.274255
H	4.46426	-3.093441	-0.164285
H	2.07143	-3.461807	-0.755678
H	0.49422	-1.600252	-0.754509
C	3.77175	-2.258173	-0.161917
C	2.41284	-2.467786	-0.485571
H	0.89869	3.135538	0.072813
C	1.52429	-1.423750	-0.475151
C	4.21212	-0.995547	0.129999
H	4.85043	1.564254	0.592439
H	3.30679	3.495529	0.509980
H	5.25925	-0.815125	0.354509
C	1.57026	2.282074	0.081861
C	1.04788	1.019981	-0.115663
C	1.93826	-0.106187	-0.141090
C	3.32075	0.108878	0.132821
C	3.79480	1.421207	0.382219
C	2.93989	2.489203	0.337756

TCNB

E=-600.830452 E_h

0 1

N	3.41977	2.049057	-0.000007
C	2.43855	1.438636	0.000008
N	3.41977	-2.049060	0.000033
C	2.43855	-1.438636	-0.000029
N	-3.41979	2.049011	0.000000
C	-2.43855	1.438627	0.000010
N	-3.41978	-2.049018	0.000024
C	-2.43855	-1.438624	-0.000028
H	0.00001	2.479386	0.000011
H	0.00000	-2.479384	-0.000015
C	1.20749	-0.703056	-0.000010
C	1.20749	0.703057	0.000001
C	0.00000	1.396228	0.000005
C	-1.20747	0.703065	0.000002
C	-1.20747	-0.703061	-0.000011
C	0.00000	-1.396225	-0.000006

TCNQ

E=-678.139475 E_h

0 1

C	3.55427	-0.101710	-1.200959
C	3.12639	-2.070474	0.155950
C	2.63650	-0.857155	-0.412279
C	1.33424	-0.433766	-0.208625
H	1.53135	1.388635	-1.393966
C	0.85381	0.795466	-0.790202
H	-0.76546	2.135349	-1.034813
C	-0.41817	1.208998	-0.591304
N	4.28461	0.525477	-1.844522
N	3.50560	-3.058588	0.625799
C	-3.55427	0.101710	1.200959
C	-3.12639	2.070474	-0.155950
C	-2.63650	0.857155	0.412279
C	-1.33424	0.433766	0.208625
H	-1.53135	-1.388635	1.393966
C	-0.85381	-0.795466	0.790202
H	0.76546	-2.135349	1.034813
C	0.41817	-1.208998	0.591304
N	-4.28461	-0.525477	1.844522
N	-3.50560	3.058588	-0.625799

2.6.2 Npe:TCNQ Optimized Geometries

Npe:TCNQ conformer a

SCF=-1388.27454303 E_h

0 1

H	-4.55633	-1.783357	-2.256453
N	6.29838	-0.505046	-1.267842
H	6.85494	0.169781	0.595166
C	6.03539	-0.240235	0.010943
H	5.52737	-1.217057	-3.039312
C	5.29845	-1.006754	-1.997921
C	-4.33553	1.507465	-1.564542
C	-4.66333	0.920872	0.773552
C	-3.76942	1.326246	-0.264985
C	-2.43434	1.519733	-0.024928
H	-1.93964	2.062737	-2.084482
C	-1.53331	1.917818	-1.090197
H	0.44265	2.391798	-1.662886
C	-0.22138	2.098107	-0.857984
N	-4.77895	1.660445	-2.622516
N	-5.36873	0.587048	1.628205
C	2.25375	1.824747	1.978003
C	2.58277	2.413411	-0.359626
C	1.68242	2.048065	0.688143
C	0.33891	1.891972	0.462449
H	-0.15724	1.343921	2.520663
C	-0.56308	1.502009	1.528429
H	-2.53757	1.028620	2.102798
C	-1.87686	1.329702	1.298824
N	2.70191	1.618195	3.025184
N	3.29010	2.709813	-1.226283
H	-0.30949	-1.291692	-2.181225
C	-1.22848	-1.505645	-1.650085
H	-2.40487	-1.320037	-3.416938
C	-2.40797	-1.516157	-2.349903
C	-3.63040	-1.774879	-1.691677
H	-4.57375	-2.175445	0.183164
C	-3.63992	-1.994574	-0.339906
C	-1.19499	-1.755995	-0.251409
C	-2.43677	-1.976713	0.412582
H	-3.41487	-2.318564	2.308613
C	-2.45932	-2.166539	1.816370
H	-1.30579	-2.333295	3.605171
C	-1.29073	-2.170762	2.532632
H	0.85379	-2.058846	2.459461
C	-0.05866	-1.994626	1.877320
C	0.01998	-1.778221	0.513552
H	1.36422	-1.819476	-1.203254
C	1.32159	-1.597396	-0.142686
H	2.40538	-0.930071	1.524332
C	2.43947	-1.179968	0.467267
H	4.64731	-0.215224	1.651203
C	4.79714	-0.458181	0.604020
C	3.75083	-0.981157	-0.159817
H	3.27498	-1.673730	-2.162734
C	4.02880	-1.261220	-1.501839

Npe:TCNQ conformer b

SCF=-1388.26917485 E_h

0 1

H	4.62585	3.389692	-1.826617
N	-5.75810	0.986529	0.641421
H	-6.06930	0.085057	2.465172
C	-5.31518	0.492087	1.797268
H	-5.21563	1.883435	-1.132519
C	-4.84289	1.484443	-0.193042
C	3.96126	-1.339672	-1.040709
C	3.33787	-2.726725	0.854202
C	2.92248	-1.918669	-0.249337
C	1.59572	-1.726564	-0.537189
H	1.94589	-0.408492	-2.246386
C	1.18254	-0.904516	-1.657838
H	-0.41054	-0.133139	-2.805826
C	-0.11818	-0.748576	-1.962477
N	4.79778	-0.875301	-1.692091
N	3.65458	-3.385330	1.751741
C	-3.51024	-1.887661	-0.742907
C	-2.89597	-0.432566	-2.599359
C	-2.48204	-1.243342	-1.497863
C	-1.15614	-1.392463	-1.179516
H	-1.50881	-2.676963	0.553185
C	-0.74348	-2.198846	-0.047286
H	0.85197	-2.960579	1.106191
C	0.55740	-2.353731	0.257790
N	-4.31847	-2.431550	-0.118330
N	-3.20021	0.241862	-3.489559
H	0.48228	2.803311	-0.947693
C	1.51819	2.587000	-0.719241
H	2.21927	3.815694	-2.309945
C	2.49639	3.167541	-1.485021
C	3.86129	2.934836	-1.206340
H	5.25641	1.947413	0.073097
C	4.21178	2.136533	-0.151903
C	1.84443	1.732759	0.367830
C	3.22292	1.525243	0.661099
H	4.64582	0.550387	1.962864
C	3.59132	0.701189	1.753023
H	2.91927	-0.540081	3.354805
C	2.63283	0.100602	2.528026
H	0.53509	-0.253754	2.817912
C	1.27188	0.276349	2.224957
C	0.85420	1.072597	1.173205
H	-0.79517	1.518496	-0.166051
C	-0.56751	1.199261	0.844279
H	-1.40418	0.626125	2.686653
C	-1.59679	0.928853	1.660503
H	-3.68121	0.051234	3.119150
C	-3.97513	0.474046	2.163693
C	-3.01354	0.985110	1.288822
H	-2.80861	1.946176	-0.650528
C	-3.48166	1.508636	0.077710

Npe:TCNQ conformer c

SCF=-1388.27262371 E_h

0 1

C	-1.71706	-2.872065	1.930820
C	-3.81413	-1.682959	1.590617
C	-2.39322	-1.628375	1.733655
C	-1.70780	-0.444456	1.659809
H	0.26185	-1.333927	1.990844
C	-0.26397	-0.408786	1.787192
H	1.50220	0.740190	1.691564
C	0.42047	0.735636	1.622589
N	-1.14656	-3.866894	2.086551
N	-4.96510	-1.706228	1.471926
C	-0.22852	4.328498	0.659245
C	1.86416	3.128415	0.971888
C	0.43617	3.116077	1.018018
C	-0.26514	1.973900	1.308505
H	-2.24077	2.882685	1.073678
C	-1.71542	1.955701	1.269606
H	-3.48016	0.803118	1.366108
C	-2.39858	0.809573	1.430730
N	-0.78883	5.294060	0.352984
N	3.01994	3.111285	0.908024
H	0.30338	1.498617	-1.850985
C	-0.74234	1.220720	-1.894723
H	-1.36662	3.234764	-2.210458
C	-1.68084	2.202552	-2.094110
C	-3.05444	1.880757	-2.143481
H	-4.50601	0.315648	-2.032009
C	-3.45299	0.578468	-1.996637
C	-1.11744	-0.139652	-1.744384
C	-2.50500	-0.459331	-1.800044
H	-3.98156	-2.035056	-1.695380
C	-2.92142	-1.806189	-1.653244
H	-2.31555	-3.831212	-1.356759
C	-1.99814	-2.799088	-1.460052
H	0.08689	-3.295233	-1.259001
C	-0.62508	-2.488911	-1.394688
C	-0.16716	-1.193189	-1.515724
H	1.64303	-0.037187	-1.948587
C	1.26550	-0.887019	-1.388438
H	1.75758	-2.432295	-0.058565
C	2.11953	-1.571218	-0.617228
H	4.06842	-3.261062	0.190320
C	4.42373	-2.252964	0.000956
C	3.54287	-1.259083	-0.433733
H	3.45306	0.853209	-0.925170
C	4.07823	0.016040	-0.637268
H	5.85789	1.215255	-0.561100
C	5.43366	0.224995	-0.421044
H	-3.78734	2.665473	-2.298167
H	6.46416	-2.709469	0.508022
C	5.76629	-1.943532	0.179780
N	6.27888	-0.729453	-0.024632

Npe:TCNQ conformer d

SCF=-1388.27712288 E_h

0 1

C	1.96437	2.939945	-1.168401
C	0.17804	4.286118	-0.218664
C	0.57747	3.070416	-0.854071
C	-0.31842	2.063033	-1.105012
H	1.15143	0.675985	-1.946602
C	0.10562	0.807260	-1.694921
H	-0.43855	-1.130881	-2.326495
C	-0.77115	-0.189572	-1.904325
N	3.08807	2.811289	-1.414769
N	-0.16193	5.257314	0.311373
C	-4.45706	-0.907976	-1.472802
C	-2.65959	-2.314896	-2.307078
C	-3.06789	-1.050912	-1.778920
C	-2.17432	-0.035615	-1.568325
H	-3.64551	1.352716	-0.740485
C	-2.60056	1.227727	-0.999144
H	-2.04928	3.151568	-0.331509
C	-1.72153	2.218652	-0.774226
N	-5.58079	-0.777173	-1.229822
N	-2.31551	-3.335215	-2.730962
H	-0.24142	-2.692188	0.741179
C	-1.10901	-2.169480	1.125063
H	-2.41143	-3.793258	0.673716
C	-2.33169	-2.790475	1.080042
C	-3.48908	-2.127005	1.543040
H	-4.27821	-0.329417	2.382424
C	-3.39178	-0.852534	2.036297
C	-0.96860	-0.857248	1.648350
C	-2.14085	-0.187074	2.103293
H	-2.94271	1.634385	2.948982
C	-2.04199	1.136587	2.602598
H	-0.75434	2.782160	3.038376
C	-0.83053	1.771876	2.650095
H	1.29345	1.607460	2.313795
C	0.33603	1.106216	2.218046
C	0.29574	-0.179438	1.720274
H	1.55467	-1.935676	1.421827
C	1.52656	-0.858383	1.291690
H	2.55909	0.820235	0.571424
C	2.59312	-0.249917	0.756677
H	4.54121	0.804155	-0.776433
C	4.74612	-0.214609	-0.463648
C	3.83934	-0.907570	0.342644
H	3.54868	-2.805430	1.355719
C	4.18461	-2.213399	0.707120
H	5.65878	-3.765164	0.521818
C	5.37691	-2.752263	0.246120
H	-4.45310	-2.621660	1.494186
H	6.62749	-0.319980	-1.501202
C	5.91560	-0.846719	-0.871128
N	6.23974	-2.094998	-0.533651

2.6.3 Npe:TCNB Optimized Geometries

Npe:TCNB conformer a

E=1310.652160 E_h

0 1

N	-4.19737	-2.835595	-1.486689
C	-3.42182	-1.978913	-1.493854
N	-0.18609	-3.555226	-1.909517
C	-0.60947	-2.483960	-1.816092
N	1.07715	3.136304	-1.612539
C	0.28239	2.297536	-1.590540
N	-2.94264	3.874952	-1.063350
C	-2.52576	2.805567	-1.198513
H	-3.98887	0.593542	-1.201778
H	0.84996	-0.272665	-1.844503
C	-0.66588	1.222636	-1.564000
C	-2.03544	1.469537	-1.372963
C	-2.93321	0.405584	-1.351785
C	-2.47898	-0.898904	-1.513803
C	-1.10609	-1.144895	-1.689107
C	-0.20862	-0.082634	-1.719885
H	2.36241	1.572161	0.224087
H	1.83000	-1.028540	1.738304
H	6.59010	0.756996	-1.638932
H	6.15930	-2.390665	0.969763
N	6.47895	-0.858957	-0.368842
H	4.34539	1.649277	-1.074932
C	5.96505	0.243938	-0.912714
H	3.91639	-1.646458	1.663491
C	5.72414	-1.497169	0.529912
C	4.70701	0.743985	-0.596979
C	4.45806	-1.080182	0.914299
C	3.91417	0.071970	0.336814
C	2.57874	0.595022	0.648710
C	1.62943	-0.032120	1.356994
H	-4.04906	-2.551977	1.947560
H	-1.82827	-3.579436	1.490948
H	0.16965	-2.198775	1.346538
C	-3.16556	-1.924947	1.899139
C	-1.90478	-2.507995	1.642203
H	1.01239	2.542203	1.760826
C	-0.78049	-1.726486	1.564829
C	-3.26662	-0.569699	2.069488
H	-3.21033	2.106556	2.317810
H	-1.21000	3.544825	2.145077
H	-4.23111	-0.109906	2.264897
C	0.14262	1.896226	1.803145
C	0.30328	0.534395	1.643536
C	-0.84649	-0.318394	1.742979
C	-2.12167	0.265921	1.992918
C	-2.23249	1.671929	2.133728
C	-1.12280	2.469138	2.037773

Npe:TCNB conformer b

E=1310.651819 E_h

0 1

H	-2.87818	-2.205387	0.953701
H	-1.77413	0.588261	0.426267
N	1.82302	4.367473	-0.216614
C	1.83731	3.263360	-0.557493
N	-1.50894	2.532258	-1.748295
C	-0.48962	1.993062	-1.669064
N	5.28237	-1.497471	-0.767701
C	4.30735	-0.914794	-0.981021
N	2.03043	-3.243939	-2.579756
C	2.01986	-2.145744	-2.220159
H	3.91682	1.628642	-0.361884
H	-0.06893	-0.521395	-2.382534
C	0.74809	1.280220	-1.546743
C	1.87897	1.894332	-0.981257
C	3.05080	1.164425	-0.815398
C	3.10457	-0.169566	-1.211167
C	1.98168	-0.776924	-1.795614
C	0.80617	-0.048315	-1.955009
H	-7.49605	-1.413898	0.409416
H	-5.80916	1.973431	-1.198964
N	-6.76130	0.322467	-0.416799
H	-5.27970	-2.327062	1.038062
C	-6.59190	-0.851331	0.191298
H	-3.53102	1.223753	-0.670030
C	-5.65782	1.022563	-0.695176
C	-5.34868	-1.363552	0.542779
C	-4.37207	0.600806	-0.387302
C	-4.19584	-0.626899	0.260748
C	-2.88305	-1.163106	0.642191
C	-1.73789	-0.469154	0.667489
H	3.41129	1.979236	3.194207
H	1.14813	2.940654	2.802745
H	-0.62894	1.577393	1.844424
C	2.63224	1.363496	2.756936
C	1.34800	1.908488	2.536240
H	-0.84705	-2.946701	0.168168
C	0.35300	1.141755	1.984859
C	2.88381	0.055741	2.432421
H	3.12361	-2.522550	1.713067
H	1.36709	-3.911830	0.668397
H	3.86292	-0.379275	2.610980
C	-0.10880	-2.335305	0.676059
C	-0.41923	-1.028852	0.997315
C	0.58570	-0.208822	1.611629
C	1.87507	-0.762023	1.860287
C	2.13609	-2.114062	1.522104
C	1.16020	-2.884599	0.947736

Npe:TCNB conformer c

E=1310.649880 E_h

0 1

H	2.43359	2.055117	0.490868
H	2.12211	-0.911518	1.152582
N	-5.54502	-0.304294	0.650060
C	-4.52013	-0.608984	0.211457
N	-4.26690	0.987685	-3.037543
C	-3.61261	0.322062	-2.356088
N	0.37379	-3.632404	1.506409
C	-0.30327	-2.971002	0.843206
N	1.70868	-2.207356	-2.027817
C	0.63846	-1.967668	-1.663239
H	-2.76471	-2.165420	1.437096
H	-1.15312	-0.473747	-2.937129
C	-2.78297	-0.514771	-1.539428
C	-3.23388	-0.987144	-0.296101
C	-2.41737	-1.807910	0.476717
C	-1.14514	-2.145121	0.027869
C	-0.68581	-1.659188	-1.208670
C	-1.50828	-0.851389	-1.986750
H	7.11737	2.093539	-0.305781
H	6.06918	-1.817132	-1.022037
N	6.70641	0.111893	-0.684349
H	4.81267	2.677518	0.397193
C	6.33921	1.334601	-0.298914
H	3.72157	-1.414039	-0.383574
C	5.75987	-0.830044	-0.689107
C	5.04751	1.661970	0.093921
C	4.44202	-0.607547	-0.312700
C	4.06302	0.670786	0.106897
C	2.69757	1.001237	0.535513
C	1.80899	0.121684	1.013099
H	-3.03535	3.549681	-1.129261
H	-0.81076	3.063991	-2.137196
H	0.79345	1.636561	-0.973567
C	-2.32588	2.925806	-0.596869
C	-1.06276	2.650610	-1.165955
H	0.68684	-0.840205	3.165308
C	-0.15918	1.854630	-0.509135
C	-2.65890	2.378077	0.613140
H	-3.10631	1.147790	2.948756
H	-1.55048	-0.384045	4.117309
H	-3.63567	2.561663	1.050336
C	0.01391	-0.167392	2.643105
C	0.44241	0.428914	1.473885
C	-0.46002	1.287471	0.759271
C	-1.74921	1.543601	1.314428
C	-2.12274	0.937053	2.539874
C	-1.26131	0.088255	3.184203

Npe:TCNB conformer d

E=1310.648214 E_h

0 1

N	0.22911	3.953242	0.125114
C	-0.36723	3.047025	-0.273663
N	-3.83041	3.676900	0.513116
C	-3.21829	2.844039	-0.003771
N	-3.67218	-2.482557	-2.487241
C	-3.10091	-1.543445	-2.130705
N	0.38564	-2.250698	-2.727678
C	-0.24421	-1.370444	-2.322601
H	0.73070	0.923290	-1.416397
H	-4.20396	0.584523	-0.988557
C	-2.40700	-0.372813	-1.678422
C	-1.00944	-0.280740	-1.791490
C	-0.34812	0.857536	-1.340505
C	-1.07047	1.896811	-0.763103
C	-2.46788	1.798413	-0.635460
C	-3.13016	0.667638	-1.101173
H	0.18853	-2.564153	0.675098
H	0.84800	0.160683	1.886372
H	-4.49379	-2.624939	0.991475
H	-3.53772	0.892717	2.898044
N	-4.13282	-0.836611	1.948601
H	-2.11194	-3.160699	0.590783
C	-3.71810	-1.947087	1.337565
H	-1.12487	0.517423	2.605748
C	-3.18595	-0.001108	2.389341
C	-2.37954	-2.248919	1.115623
C	-1.82606	-0.213132	2.218183
C	-1.38894	-1.359751	1.542305
C	0.01209	-1.629900	1.203043
C	1.03860	-0.792233	1.402112
H	5.50593	2.938627	-0.820779
H	3.20983	3.429081	0.034363
H	1.80149	1.646764	0.869916
C	4.88180	2.131537	-0.452132
C	3.58326	2.410284	0.029208
H	2.32914	-3.140956	1.318614
C	2.78607	1.397014	0.496120
C	5.34755	0.843591	-0.447367
H	6.02528	-1.754454	-0.344781
H	4.60658	-3.602599	0.478629
H	6.34478	0.617734	-0.813150
C	2.93254	-2.320355	0.945657
C	2.41698	-1.041548	0.962419
C	3.23336	0.048935	0.510727
C	4.54437	-0.225267	0.028194
C	5.02241	-1.559789	0.022801
C	4.23440	-2.583787	0.475633

Npe:TCNB conformer e

E=1310.648088 E_h

0 1

H	-3.41825	2.604684	-0.410592
H	-1.28625	2.855747	0.470619
N	4.73265	-1.688165	1.720057
C	4.12367	-0.999329	1.019765
N	3.77916	-2.789370	-2.110603
C	3.42383	-1.788672	-1.654638
N	1.27785	4.158862	0.889016
C	1.64821	3.158575	0.443904
N	0.13539	2.950663	-2.831288
C	0.85186	2.317476	-2.182080
H	3.18801	1.387190	1.683792
H	1.87532	-0.023502	-2.885214
C	2.98109	-0.535162	-1.117469
C	3.34419	-0.137435	0.180546
C	2.91368	1.086778	0.681016
C	2.10574	1.911624	-0.095480
C	1.72701	1.506948	-1.386665
C	2.17267	0.290094	-1.892928
H	-6.20904	-0.988816	-1.849055
H	-4.56756	-2.349302	1.665748
N	-5.44771	-1.769799	-0.102855
H	-4.81465	1.061644	-1.812009
C	-5.50204	-0.822983	-1.040264
H	-3.09750	-0.372640	1.861232
C	-4.59155	-1.575779	0.902658
C	-4.72018	0.325644	-1.019647
C	-3.76178	-0.467879	1.011132
C	-3.80625	0.515029	0.019436
C	-2.96278	1.722729	0.033641
C	-1.71802	1.857588	0.507534
H	0.52147	-3.729570	-1.316862
H	-0.90290	-2.064826	-2.505060
H	-1.53089	0.033215	-1.412690
C	0.24168	-2.806110	-0.821623
C	-0.56279	-1.859661	-1.495233
H	-0.56776	2.003895	2.864960
C	-0.91924	-0.685831	-0.882883
C	0.67996	-2.545948	0.449748
H	1.43804	-1.788426	2.911530
H	0.87414	0.351136	4.018244
H	1.31099	-3.259521	0.971377
C	-0.32399	1.069992	2.367950
C	-0.84724	0.823681	1.116227
C	-0.49701	-0.390915	0.440231
C	0.33028	-1.338790	1.109877
C	0.81082	-1.055290	2.413389
C	0.49906	0.130918	3.024137

Npe:TCNB conformer f

E=1310.645596 E_h

0 1

H	0.79238	-0.458958	2.112141
H	0.59751	2.175850	0.572725
N	-3.78440	3.093156	-1.733286
C	-3.23200	2.082264	-1.641701
N	0.19163	2.777832	-2.538019
C	-0.43414	1.858024	-2.224647
N	-3.93412	-3.514447	0.068938
C	-3.33957	-2.620755	-0.359174
N	0.04417	-3.825343	-0.785247
C	-0.54485	-2.847599	-0.966511
H	-4.31311	-0.190936	-0.798734
H	0.52134	-0.588452	-1.855436
C	-1.18783	0.712814	-1.805460
C	-2.55694	0.824231	-1.509200
C	-3.26431	-0.283952	-1.051602
C	-2.61125	-1.499489	-0.876856
C	-1.24207	-1.612306	-1.177145
C	-0.53787	-0.506915	-1.643899
H	-3.78782	-1.332522	2.823376
H	-3.79785	2.610254	1.648439
N	-3.91393	0.637105	2.231966
H	-1.32919	-1.491983	2.579974
C	-3.21524	-0.468628	2.496256
H	-1.35597	2.637017	1.352174
C	-3.21940	1.711035	1.842821
C	-1.83536	-0.557465	2.357492
C	-1.84278	1.721319	1.668792
C	-1.11134	0.551986	1.909360
C	0.33283	0.423399	1.677802
C	1.07435	1.276895	0.958776
H	5.20371	-3.302330	-0.468673
H	2.72638	-3.385255	-0.150007
H	1.48748	-1.371272	0.379659
C	4.65534	-2.393880	-0.243255
C	3.25706	-2.443855	-0.053087
H	2.67688	3.304517	0.777552
C	2.55698	-1.303223	0.244851
C	5.30757	-1.193313	-0.159007
H	6.35620	1.263598	-0.020422
H	5.11464	3.367678	0.371822
H	6.37946	-1.136309	-0.323707
C	3.21020	2.374547	0.605100
C	2.50925	1.186037	0.646739
C	3.20015	-0.041706	0.363253
C	4.60549	0.006572	0.126733
C	5.28477	1.250315	0.154761
C	4.59841	2.413812	0.373584

3 Crystal data and structure

Table S13: Crystal data and structure refinement for CY_D1 (Npe:TCNB).

Identification code	CY_D1
Empirical formula	C27H15N5
Formula weight	409.44
Temperature/K	99.95(10)
Crystal system	monoclinic
Space group	P21/c
a/Å	6.7312(3)
b/Å	36.6599(13)
c/Å	9.5150(4)
α/°	90
β/°	106.283(4)
γ/°	90
Volume/Å^3	2253.79(17)
Z	4
ρ_{calc}g/cm^3	1.207
μ/mm^{-1}	0.586
F(000)	848.0
Crystal size/mm^3	0.17 × 0.077 × 0.037
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	9.65 to 144.258
Index ranges	$-8 \leq h \leq 6, -44 \leq k \leq 39, -11 \leq l \leq 11$
Reflections collected	8966
Independent reflections	4325 [R_{int} = 0.0264, R_{sigma} = 0.0314]
Data/restraints/parameters	4325/102/353
Goodness-of-fit on F^2	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.1237, wR_2 = 0.3330
Final R indexes [all data]	R_1 = 0.1331, wR_2 = 0.3397
Largest diff. peak/hole / e Å^{-3}	0.94/-0.34

Table S14: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for CY_D1. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	x	U (eq)
N2	-1655(7)	3894.2(11)	6917(4)	41.4(10)
N3	-1692(5)	2800.7(10)	6873(4)	29.1(8)
N4	-4799(5)	2831.7(10)	-677(4)	27.7(8)
N5	-4820(8)	3928.5(11)	-541(4)	46.0(11)
C18	-2127(7)	3733.5(11)	5830(5)	30.2(9)
C19	-2154(6)	2957.0(10)	5783(4)	21.2(8)
C20	-2705(6)	3538.1(11)	4466(4)	23.6(8)
C21	-2719(5)	3158.1(10)	4430(4)	19.3(8)
C22	-3270(5)	2974.0(10)	3104(4)	19.4(8)
C23	-3793(5)	3169.1(11)	1802(4)	20.7(8)
C24	-4354(6)	2981.1(11)	428(4)	21.3(8)
C25	-4372(7)	3759.5(12)	508(4)	31.4(10)
C26	-3787(6)	3552.2(11)	1842(4)	23.3(8)
C27	-3236(7)	3738.6(11)	3164(4)	27.5(9)
C7	2421(9)	4079.6(14)	4804(5)	44.1(12)
C8	2322(6)	3689.5(12)	4587(4)	28.1(9)
C9	2838(6)	3459.6(14)	5803(5)	33.5(10)
C10	2779(6)	3081.6(13)	5647(5)	31.3(10)
C11	2208(6)	2925.3(12)	4300(5)	28.5(9)
C12	1697(6)	3144.5(11)	3034(4)	24.1(8)
C13	1117(6)	2979.4(13)	1631(5)	31.5(10)
C14	613(7)	3184.4(15)	394(5)	37.1(11)
C15	658(7)	3563.2(15)	497(5)	37.2(11)
C16	1207(7)	3737.8(13)	1836(4)	31.6(10)
C17	1750(6)	3532.3(12)	3153(4)	24.7(9)
N1	3690(20)	5411(3)	6736(13)	73(3)
C1	4550(30)	5176(3)	7748(14)	90(4)
C2	4460(30)	4801(3)	7532(13)	89(4)
C3	3468(19)	4644(3)	6169(11)	47(2)
C4	2350(40)	4911(8)	5190(40)	69(4)
C5	2430(30)	5265(5)	5560(20)	68(4)
C6	3409(19)	4254(3)	5976(12)	50(2)
N1A	2350(30)	5407(4)	6920(20)	74(4)
C1A	2170(40)	5150(4)	7880(20)	90(4)
C2A	2360(40)	4779(5)	7630(20)	88(4)
C3A	2480(30)	4644(4)	6358(17)	44(3)
C4A	2930(60)	4887(14)	5160(60)	69(5)
C5A	3180(50)	5252(9)	5380(40)	72(5)
C6A	2460(30)	4249(5)	6080(19)	43(3)

Table S15: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for CY_D1. The Anisotropic displacement factor exponent takes the form: $-2\pi 2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	57(3)	35(2)	28(2)	-6.8(16)	4.1(18)	4.2(18)
N3	31.9(19)	30.1(19)	22.3(17)	0.9(14)	2.8(14)	0.5(14)
N4	28.5(17)	34.1(19)	20.6(17)	-1.4(14)	7.0(13)	-0.6(14)
N5	69(3)	38(2)	28(2)	9.2(17)	7.5(19)	8(2)
C18	39(2)	24(2)	24(2)	1.9(17)	4.8(17)	3.0(17)
C19	21.7(18)	22.1(18)	20.7(19)	-0.2(15)	7.5(14)	-0.9(15)
C20	26(2)	27(2)	17.0(18)	-1.5(15)	4.4(15)	0.6(15)
C21	14.0(16)	26.0(19)	18.0(18)	0.0(14)	4.6(13)	-0.1(14)
C22	18.6(17)	19.9(18)	20.4(18)	-0.8(14)	6.6(14)	-1.2(14)
C23	16.1(17)	27(2)	18.5(18)	-1.4(15)	4.1(14)	0.8(14)
C24	16.9(17)	28.2(19)	18.6(18)	1.0(15)	4.9(14)	-0.1(14)
C25	46(3)	26(2)	21(2)	0.2(17)	8.3(18)	3.2(18)
C26	26(2)	27(2)	16.3(18)	1.5(15)	4.3(15)	2.9(15)
C27	39(2)	21.9(19)	20.5(19)	2.4(15)	6.3(17)	2.2(17)
C7	61(3)	35(3)	34(2)	3(2)	9(2)	1(2)
C8	25(2)	33(2)	26(2)	-3.9(17)	6.2(16)	-1.4(16)
C9	23(2)	57(3)	19.0(19)	-4.5(18)	4.2(16)	-1.6(19)
C10	21(2)	45(3)	27(2)	10.3(18)	5.3(16)	-0.3(18)
C11	19.4(19)	32(2)	36(2)	6.9(17)	10.4(16)	3.7(16)
C12	15.5(17)	32(2)	26(2)	1.9(16)	7.5(15)	-1.8(15)
C13	19.6(19)	39(2)	37(2)	-11.4(19)	10.3(17)	-5.8(17)
C14	23(2)	64(3)	24(2)	-11(2)	6.9(17)	-8(2)
C15	29(2)	64(3)	19(2)	5(2)	6.7(17)	2(2)
C16	37(2)	36(2)	22(2)	4.4(17)	8.3(17)	1.6(18)
C17	22.6(19)	33(2)	16.9(18)	-1.1(15)	2.6(15)	1.0(16)
N1	98(8)	34(4)	83(6)	-3(4)	17(6)	-2(6)
C1	162(10)	41(5)	59(5)	1(4)	16(6)	-7(6)
C2	163(10)	37(4)	57(5)	-5(4)	11(6)	-9(6)
C3	65(6)	41(4)	38(4)	-1(3)	18(4)	9(5)
C4	86(13)	39(5)	78(5)	3(4)	17(8)	12(8)
C5	87(12)	42(4)	76(6)	-2(4)	23(7)	16(7)
C6	65(6)	41(4)	40(4)	1(3)	11(5)	4(5)
N1A	89(10)	39(6)	80(8)	5(6)	-1(9)	-8(8)
C1A	162(11)	33(6)	57(7)	-6(5)	4(8)	1(7)
C2A	160(11)	36(6)	52(6)	-12(5)	3(8)	5(7)
C3A	58(7)	38(5)	40(5)	3(4)	22(5)	5(6)
C4A	91(14)	38(6)	78(6)	-1(5)	20(9)	14(9)
C5A	91(14)	41(6)	80(7)	-3(6)	17(9)	12(9)
C6A	59(7)	38(5)	34(5)	-1(4)	17(6)	5(6)

Table S16: Bond Lengths for CY_D1.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N2	C18	1.155(6)	C11	C12	1.408(6)
N3	C19	1.149(5)	C12	C13	1.417(6)
N4	C24	1.148(5)	C12	C17	1.426(6)
N5	C25	1.141(6)	C13	C14	1.357(7)
C18	C20	1.437(5)	C14	C15	1.392(7)
C19	C21	1.439(5)	C15	C16	1.381(6)
C20	C21	1.393(5)	C16	C17	1.419(5)
C20	C27	1.398(5)	N1	C1	1.300(16)
C21	C22	1.387(5)	N1	C5	1.31(2)
C22	C23	1.388(5)	C1	C2	1.390(15)
C23	C24	1.432(5)	C2	C3	1.404(15)
C23	C26	1.405(5)	C3	C4	1.41(3)
C25	C26	1.437(5)	C3	C6	1.440(14)
C26	C27	1.388(5)	C4	C5	1.34(3)
C7	C8	1.444(6)	N1A	C1A	1.34(3)
C7	C6	1.296(12)	N1A	C5A	1.80(4)
C7	C6A	1.358(17)	C1A	C2A	1.40(2)
C8	C9	1.394(6)	C2A	C3A	1.33(2)
C8	C17	1.431(5)	C3A	C4A	1.55(6)
C9	C10	1.393(7)	C3A	C6A	1.47(2)
C10	C11	1.358(6)	C4A	C5A	1.36(4)

Table S17: Bond Angles for CY_D1.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	C18	C20	179.1(5)	C11	C12	C17	120.4(4)
N3	C19	C21	179.0(4)	C13	C12	C17	119.7(4)
C21	C20	C18	121.2(3)	C14	C13	C12	121.1(4)
C21	C20	C27	120.4(3)	C13	C14	C15	119.8(4)
C27	C20	C18	118.4(4)	C16	C15	C14	121.5(4)
C20	C21	C19	119.5(3)	C15	C16	C17	120.3(4)
C22	C21	C19	120.0(3)	C12	C17	C8	118.1(4)
C22	C21	C20	120.5(3)	C16	C17	C8	124.2(4)
C21	C22	C23	119.8(3)	C16	C17	C12	117.7(4)
C22	C23	C24	120.2(3)	C1	N1	C5	113.9(12)
C22	C23	C26	119.6(3)	N1	C1	C2	123.7(12)
C26	C23	C24	120.2(3)	C1	C2	C3	122.1(11)
N4	C24	C23	179.7(5)	C2	C3	C4	110.6(17)
N5	C25	C26	179.0(5)	C2	C3	C6	120.8(9)
C23	C26	C25	120.5(3)	C4	C3	C6	127.8(17)
C27	C26	C23	121.0(3)	C5	C4	C3	121(2)
C27	C26	C25	118.5(4)	N1	C5	C4	125.9(16)
C26	C27	C20	118.8(4)	C7	C6	C3	126.1(9)
C6	C7	C8	127.2(7)	C1A	N1A	C5A	116.3(18)
C6A	C7	C8	124.8(9)	N1A	C1A	C2A	122(2)
C9	C8	C7	119.3(4)	C3A	C2A	C1A	123.8(19)
C9	C8	C17	119.0(4)	C2A	C3A	C4A	122(2)
C17	C8	C7	121.6(4)	C2A	C3A	C6A	122.2(15)
C10	C9	C8	121.4(4)	C6A	C3A	C4A	115(2)
C11	C10	C9	120.8(4)	C5A	C4A	C3A	120(4)
C10	C11	C12	120.2(4)	C4A	C5A	N1A	113(3)
C11	C12	C13	119.9(4)	C7	C6A	C3A	127.6(14)

Table S18: Torsion Angles for CY_D1.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C18	C20	C21	C19	0.3(6)	C13	C12	C17	C16	0.0(6)
C18	C20	C21	C22	-179.6(4)	C13	C14	C15	C16	0.0(7)
C18	C20	C27	C26	179.7(4)	C14	C15	C16	C17	0.2(7)
C19	C21	C22	C23	-179.3(3)	C15	C16	C17	C8	-179.5(4)
C20	C21	C22	C23	0.6(5)	C15	C16	C17	C12	-0.2(6)
C21	C20	C27	C26	0.4(6)	C17	C8	C9	C10	-0.9(6)
C21	C22	C23	C24	179.7(3)	C17	C12	C13	C14	0.1(6)
C21	C22	C23	C26	-0.9(5)	N1	C1	C2	C3	2(3)
C22	C23	C26	C25	-178.5(4)	C1	N1	C5	C4	-17(2)
C22	C23	C26	C27	0.9(6)	C1	C2	C3	C4	-9(2)
C23	C26	C27	C20	-0.7(6)	C1	C2	C3	C6	179.7(15)
C24	C23	C26	C25	1.0(6)	C2	C3	C4	C5	4(3)
C24	C23	C26	C27	-179.6(4)	C2	C3	C6	C7	174.8(13)
C25	C26	C27	C20	178.7(4)	C3	C4	C5	N1	9(3)
C27	C20	C21	C19	179.6(4)	C4	C3	C6	C7	6(2)
C27	C20	C21	C22	-0.3(6)	C5	N1	C1	C2	11(3)
C7	C8	C9	C10	-179.6(4)	C6	C7	C8	C9	18.3(10)
C7	C8	C17	C12	179.8(4)	C6	C7	C8	C17	-160.2(8)
C7	C8	C17	C16	-1.0(7)	C6	C3	C4	C5	174.4(14)
C8	C7	C6	C3	-179.4(9)	N1A	C1A	C2A	C3A	-9(4)
C8	C7	C6A	C3A	-177.4(13)	C1A	N1A	C5A	C4A	18(3)
C8	C9	C10	C11	-0.2(6)	C1A	C2A	C3A	C4A	15(4)
C9	C8	C17	C12	1.2(6)	C1A	C2A	C3A	C6A	-173(2)
C9	C8	C17	C16	-179.6(4)	C2A	C3A	C4A	C5A	-1(4)
C9	C10	C11	C12	1.0(6)	C2A	C3A	C6A	C7	175(2)
C10	C11	C12	C13	179.6(4)	C3A	C4A	C5A	N1A	-14(3)
C10	C11	C12	C17	-0.8(6)	C4A	C3A	C6A	C7	-13(3)
C11	C12	C13	C14	179.8(4)	C5A	N1A	C1A	C2A	-7(3)
C11	C12	C17	C8	-0.4(6)	C6A	C7	C8	C9	-17.9(12)
C11	C12	C17	C16	-179.6(4)	C6A	C7	C8	C17	163.5(10)
C12	C13	C14	C15	-0.2(6)	C6A	C3A	C4A	C5A	-173(2)
C13	C12	C17	C8	179.3(4)					

Table S19: Crystal data and structure refinement for CY_B8b (2Npe:3TCNQ).

Identification code	**CY_B8b**
Empirical formula	C35H19N6
Formula weight	537.57
Temperature/K	102(3)
Crystal system	triclinic
Space group	P-1
a/Å	9.8862(4)
b/Å	11.8127(5)
c/Å	12.3102(5)
α/°	93.827(3)
β/°	93.940(3)
γ/°	111.868(4)
Volume/Å^3	1324.40(9)
Z	2
ρ_{calc}g/cm^3	1.348
μ/mm^{-1}	0.660
F(000)	556.0
Crystal size/mm^3	0.421 × 0.186 × 0.044
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/Å	7.234 to 146
Index ranges	$-9 \leq h \leq 12, -14 \leq k \leq 14, -15 \leq l \leq 15$
Reflections collected	14402
Independent reflections	5154 [R_{int} = 0.0235, R_{sigma} = 0.0209]
Data/restraints/parameters	5154/0/379
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0372, wR_2 = 0.1021
Final R indexes [all data]	R_1 = 0.0431, wR_2 = 0.1073
Largest diff. peak/hole / eÅ^{-3}	0.27/-0.20

Table S20: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for CY_B8b. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	1754.8(11)	2813.2(9)	5140.8(8)	24.2(2)
C1	1194.4(13)	3679.2(11)	5065.0(10)	25.7(3)
C2	1780.3(13)	4703.0(11)	4502.8(10)	24.8(2)
C3	3050.3(12)	4888.3(10)	3985.9(9)	21.4(2)
C4	3636.5(12)	3981.6(10)	4055.1(9)	23.3(2)
C5	2962.3(12)	2987.9(10)	4627.5(9)	23.0(2)
C6	3680.7(12)	5984.6(10)	3414.4(9)	23.3(2)
C7	4986.0(12)	6354.3(10)	3015.3(9)	20.9(2)
C8	5605.1(12)	7426.0(10)	2399.7(9)	20.1(2)
C9	4924.5(13)	8255.1(10)	2302.6(9)	23.5(2)
C10	5399.9(13)	9208.0(10)	1622.9(10)	24.9(2)
C11	6557.8(13)	9338.1(10)	1026.7(9)	23.8(2)
C12	7325.6(12)	8546.7(10)	1121.9(9)	20.7(2)
C13	8543.0(13)	8690.5(10)	522.8(9)	24.5(2)
C14	9327.7(13)	7955.6(11)	630.6(10)	26.5(3)
C15	8917.3(13)	7039.1(10)	1358.3(9)	24.1(2)
C16	7728.9(12)	6856.3(10)	1935.0(9)	21.3(2)
C17	6877.6(12)	7591.7(9)	1833.5(9)	19.1(2)
N2	3622.3(12)	1340.6(10)	1897.2(9)	30.2(2)
N3	1605.0(11)	-1815.1(9)	3678.5(8)	26.7(2)
N4	-5149.5(12)	1092.3(10)	4599.2(9)	33.0(3)
N5	-2828.5(12)	4011.3(9)	2777.1(9)	30.5(2)
C18	2644.7(13)	781.7(11)	2346.1(9)	22.6(2)
C19	1483.1(12)	-967.5(10)	3351.9(9)	21.2(2)
C20	1417.4(12)	110.7(10)	2917.2(9)	20.0(2)
C21	300.0(12)	524.4(10)	3037.1(8)	19.0(2)
C22	-920.0(12)	-97.3(10)	3649.2(9)	18.9(2)
C23	-1954.6(12)	371.2(10)	3802.3(8)	19.0(2)
C24	-1880.4(12)	1493.5(10)	3351.5(8)	18.6(2)
C25	-691.2(12)	2083.7(10)	2705.4(9)	20.0(2)
C26	336.5(12)	1618.9(10)	2554.8(9)	20.3(2)
C27	-2902.5(12)	2000.7(10)	3524.0(9)	20.0(2)
C28	-4128.5(13)	1468.2(10)	4135.1(9)	23.2(2)
C29	-2839.5(12)	3119.6(10)	3092.3(9)	22.3(2)
N6	621.3(11)	4687.9(10)	1454.5(9)	31.0(2)
N7	2584.4(12)	7746.7(9)	-449.0(9)	30.1(2)
C30	1571.4(13)	5193.4(10)	960.2(9)	23.0(2)
C31	2662.4(12)	6888.3(10)	-115.6(9)	21.8(2)
C32	2743.4(12)	5821.9(10)	329.2(9)	20.1(2)
C33	3863.1(12)	5422.4(9)	170.7(8)	18.6(2)
C34	5001.9(12)	6044.2(10)	-506.9(9)	19.9(2)
C35	3924.9(12)	4367.0(9)	671.2(9)	19.8(2)

Table S21: Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for CY_B8b. The anisotropic displacement factor exponent takes the form: $-2\pi 2[h^2 a^* 2U_{11} + 2hka^* b^* U_{12} + \ldots].$]

Atom	$\mathbf{U_{11}}$	$\mathbf{U_{22}}$	$\mathbf{U_{33}}$	$\mathbf{U_{23}}$	$\mathbf{U_{13}}$	$\mathbf{U_{12}}$
N1	24.8(5)	24.2(5)	24.2(5)	4.3(4)	1.9(4)	9.9(4)
C1	24.8(6)	26.7(6)	27.9(6)	4.9(5)	7.3(5)	11.4(5)
C2	24.5(6)	24.2(6)	29.6(6)	4.8(5)	6.1(5)	12.6(5)
C3	19.6(5)	22.5(5)	21.8(5)	1.7(4)	0.6(4)	7.9(4)
C4	20.3(6)	23.7(6)	26.6(6)	2.4(4)	2.7(4)	9.2(5)
C5	22.1(6)	22.0(6)	26.1(5)	2.2(4)	0.1(4)	10.0(5)
C6	23.5(6)	22.9(6)	25.3(5)	3.8(4)	2.3(4)	10.7(5)
C7	22.0(6)	20.0(5)	21.4(5)	1.8(4)	0.8(4)	9.0(4)
C8	20.6(5)	17.8(5)	21.5(5)	0.2(4)	-0.7(4)	7.5(4)
C9	21.7(6)	21.1(5)	28.2(6)	1.0(4)	2.0(4)	9.1(4)
C10	26.5(6)	19.1(5)	31.7(6)	1.0(4)	-1.7(5)	12.7(5)
C11	27.8(6)	16.9(5)	25.6(5)	3.5(4)	-1.8(4)	7.8(4)
C12	21.5(5)	16.6(5)	21.9(5)	0.9(4)	-1.1(4)	5.4(4)
C13	24.2(6)	21.4(5)	24.6(5)	3.6(4)	1.8(4)	4.6(4)
C14	21.9(6)	28.0(6)	28.0(6)	-0.4(5)	4.4(5)	7.8(5)
C15	23.2(6)	23.4(6)	27.5(6)	-0.2(4)	0.3(4)	11.6(5)
C16	22.8(6)	18.3(5)	23.1(5)	1.6(4)	-0.4(4)	8.7(4)
C17	20.4(5)	15.8(5)	19.7(5)	0.5(4)	-0.5(4)	5.8(4)
N2	27.9(5)	34.9(6)	34.3(6)	12.1(4)	10.4(4)	16.8(5)
N3	23.7(5)	27.0(5)	34.0(5)	7.8(4)	6.1(4)	13.5(4)
N4	30.8(6)	35.3(6)	44.7(6)	19.4(5)	16.1(5)	21.4(5)
N5	36.0(6)	25.3(5)	35.4(6)	8.2(4)	5.2(5)	16.6(4)
C18	23.1(6)	26.7(6)	22.9(5)	4.8(4)	3.3(4)	14.4(5)
C19	16.6(5)	26.1(6)	22.8(5)	2.1(4)	4.0(4)	9.9(4)
C20	19.6(5)	21.5(5)	19.8(5)	2.2(4)	1.3(4)	8.9(4)
C21	18.5(5)	20.2(5)	17.6(5)	0.9(4)	0.0(4)	7.1(4)
C22	19.6(5)	17.4(5)	19.8(5)	3.7(4)	0.7(4)	7.2(4)
C23	18.7(5)	19.1(5)	18.8(5)	3.6(4)	1.9(4)	6.6(4)
C24	18.6(5)	19.4(5)	17.8(5)	1.8(4)	-0.8(4)	7.8(4)
C25	20.0(5)	20.1(5)	20.6(5)	5.3(4)	2.2(4)	7.7(4)
C26	18.9(5)	21.3(5)	21.0(5)	6.0(4)	3.7(4)	7.2(4)
C27	20.2(5)	20.7(5)	20.7(5)	4.2(4)	2.7(4)	9.1(4)
C28	24.7(6)	23.9(6)	27.9(6)	8.3(5)	4.6(5)	15.7(5)
C29	21.4(6)	23.6(6)	24.8(5)	3.3(4)	3.8(4)	11.6(5)
N6	26.3(5)	31.5(6)	39.5(6)	12.3(5)	8.2(5)	13.4(5)
N7	30.0(5)	24.2(5)	39.2(6)	6.8(4)	-0.2(4)	13.9(4)
C30	21.9(6)	21.8(5)	27.8(6)	4.0(4)	0.1(5)	11.2(5)
C31	18.3(5)	21.5(6)	26.2(5)	2.0(4)	0.0(4)	8.7(4)
C32	20.2(5)	17.7(5)	22.6(5)	2.5(4)	0.0(4)	7.8(4)
C33	19.2(5)	16.1(5)	19.6(5)	0.6(4)	-1.6(4)	6.3(4)
C34	21.5(6)	16.5(5)	21.0(5)	3.7(4)	-0.3(4)	6.7(4)
C35	19.7(5)	17.5(5)	21.2(5)	3.8(4)	0.9(4)	6.0(4)

Table S22: Bond Lengths for CY_B8b.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C1	1.3380(15)	N4	C28	1.1496(15)
N1	C5	1.3433(15)	N5	C29	1.1431(15)
C1	C2	1.3865(16)	C18	C20	1.4388(15)
C2	C3	1.3974(15)	C19	C20	1.4354(15)
C3	C4	1.3994(15)	C20	C21	1.3769(15)
C3	C6	1.4632(16)	C21	C22	1.4494(15)
C4	C5	1.3823(16)	C21	C26	1.4477(14)
C6	C7	1.3391(16)	C22	C23	1.3499(15)
C7	C8	1.4719(15)	C23	C24	1.4499(14)
C8	C9	1.3862(15)	C24	C25	1.4467(14)
C8	C17	1.4360(15)	C24	C27	1.3743(15)
C9	C10	1.4049(16)	C25	C26	1.3402(15)
C10	C11	1.3683(16)	C27	C28	1.4322(15)
C11	C12	1.4123(15)	C27	C29	1.4389(15)
C12	C13	1.4170(16)	N6	C30	1.1482(16)
C12	C17	1.4315(15)	N7	C31	1.1454(15)
C13	C14	1.3697(17)	C30	C32	1.4342(15)
C14	C15	1.4111(17)	C31	C32	1.4333(15)
C15	C16	1.3701(16)	C32	C33	1.3758(15)
C16	C17	1.4224(15)	C33	C34	1.4483(15)
N2	C18	1.1498(16)	C33	C35	1.4463(14)
N3	C19	1.1470(15)	C34	C35[1]	1.3428(15)

[1] 1-X,1-Y,-Z.

Table S23: Bond Angles for CY_B8b.

Atom	Atom	Atom	Angle/Å	Atom	Atom	Atom	Angle/Å
C1	N1	C5	115.57(10)	C19	C20	C18	115.22(9)
N1	C1	C2	124.17(11)	C21	C20	C18	120.38(10)
C1	C2	C3	119.91(11)	C21	C20	C19	124.38(10)
C2	C3	C4	116.21(10)	C20	C21	C22	121.88(10)
C2	C3	C6	119.62(10)	C20	C21	C26	119.81(10)
C4	C3	C6	124.17(10)	C26	C21	C22	118.30(9)
C5	C4	C3	119.46(10)	C23	C22	C21	120.33(10)
N1	C5	C4	124.66(10)	C22	C23	C24	120.99(10)
C7	C6	C3	125.51(10)	C25	C24	C23	118.39(9)
C6	C7	C8	125.99(10)	C27	C24	C23	121.76(10)
C9	C8	C7	120.72(10)	C27	C24	C25	119.85(9)
C9	C8	C17	118.71(10)	C26	C25	C24	120.56(10)
C17	C8	C7	120.47(9)	C25	C26	C21	121.33(10)
C8	C9	C10	121.78(10)	C24	C27	C28	123.63(10)
C11	C10	C9	120.35(10)	C24	C27	C29	122.57(10)
C10	C11	C12	120.35(10)	C28	C27	C29	113.80(9)
C11	C12	C13	120.67(10)	N4	C28	C27	175.58(11)
C11	C12	C17	119.88(11)	N5	C29	C27	177.29(12)
C13	C12	C17	119.45(10)	N6	C30	C32	179.17(12)
C14	C13	C12	121.45(11)	N7	C31	C32	178.37(12)
C13	C14	C15	119.20(11)	C31	C32	C30	115.29(9)
C16	C15	C14	121.02(11)	C33	C32	C30	121.85(10)
C15	C16	C17	121.32(10)	C33	C32	C31	122.86(10)
C12	C17	C8	118.74(10)	C32	C33	C34	120.77(10)
C16	C17	C8	123.75(10)	C32	C33	C35	120.76(10)
C16	C17	C12	117.51(10)	C35	C33	C34	118.47(10)
N2	C18	C20	178.55(12)	C35[1]	C34	C33	120.24(10)
N3	C19	C20	176.44(11)	C34[1]	C35	C33	121.29(10)

[1] 1-X,1-Y,-Z.

Table S24: Torsion angles for CY_B8b.

A	B	C	D	Angle/Å	A	B	C	D	Angle/Å
N1	C1	C2	C3	-1.12(19)	C15	C16	C17	C8	178.69(10)
C1	N1	C5	C4	0.54(17)	C15	C16	C17	C12	-1.19(16)
C1	C2	C3	C4	1.48(17)	C17	C8	C9	C10	3.39(16)
C1	C2	C3	C6	-178.66(11)	C17	C12	C13	C14	-1.76(17)
C2	C3	C4	C5	-0.91(16)	C18	C20	C21	C22	-177.19(10)
C2	C3	C6	C7	170.55(11)	C18	C20	C21	C26	2.03(16)
C3	C4	C5	N1	-0.10(18)	C19	C20	C21	C22	1.39(17)
C3	C6	C7	C8	177.30(10)	C19	C20	C21	C26	-179.39(10)
C4	C3	C6	C7	-9.60(19)	C20	C21	C22	C23	176.29(10)
C5	N1	C1	C2	0.08(17)	C20	C21	C26	C25	-176.35(10)
C6	C3	C4	C5	179.23(11)	C21	C22	C23	C24	0.66(16)
C6	C7	C8	C9	8.48(18)	C22	C21	C26	C25	2.89(16)
C6	C7	C8	C17	-167.77(11)	C22	C23	C24	C25	1.73(15)
C7	C8	C9	C10	-172.92(10)	C22	C23	C24	C27	-178.23(10)
C7	C8	C17	C12	171.41(10)	C23	C24	C25	C26	-1.80(15)
C7	C8	C17	C16	-8.47(16)	C23	C24	C27	C28	-1.21(17)
C8	C9	C10	C11	0.39(18)	C23	C24	C27	C29	179.40(10)
C9	C8	C17	C12	-4.92(15)	C24	C25	C26	C21	-0.53(16)
C9	C8	C17	C16	175.21(10)	C25	C24	C27	C28	178.83(10)
C9	C10	C11	C12	-2.59(17)	C25	C24	C27	C29	-0.57(17)
C10	C11	C12	C13	-178.80(11)	C26	C21	C22	C23	-2.94(15)
C10	C11	C12	C17	0.92(17)	C27	C24	C25	C26	178.17(11)
C11	C12	C13	C14	177.97(11)	C30	C32	C33	C34	177.46(10)
C11	C12	C17	C8	2.84(16)	C30	C32	C33	C35	-2.14(16)
C11	C12	C17	C16	-177.28(10)	C31	C32	C33	C34	-2.74(17)
C12	C13	C14	C15	-0.28(17)	C31	C32	C33	C35	177.65(10)
C13	C12	C17	C8	-177.44(9)	C32	C33	C34	C35[1]	-178.83(10)
C13	C12	C17	C16	2.45(16)	C32	C33	C35	C34[1]	178.82(10)
C13	C14	C15	C16	1.61(17)	C34	C33	C35	C34[1]	-0.79(17)
C14	C15	C16	C17	-0.84(17)	C35	C33	C34	C35[1]	0.78(17)

[1] 1-X,1-Y,-Z.