Charge Transfer In Molecular Co-Crystals: A Plane Wave Vs. Localized-Orbitals View. Structural Information From Calculated Raman And IR Phonons.

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Table S1. Experimental and optimized at PBE(D3BJ)/PAW level lattice parameters of Pery:F4TCNQ_1:1 and Pery-TCNQ_1:1.

Lattice parameters	Experimental	Optimized at PBE(D3BJ)/PAW level
Perylene-F4TCNQ_1:1		
a (Å)	7.03230	6.89434
b (Å)	7.30630	7.18129
c (Å)	11.29160	11.09266
α (°)	104.1040	103.7432
β (°)	101.8520	102.3057
γ (°)	90.4510	89.5734
Perylene-TCNQ_1:1		
a (Å)	7.20130	7.08654
b (Å)	10.83900	10.77898
c (Å)	14.47470	14.28034
α (°)	90	90
β (°)	90.3240	90.7128
γ (°)	90	90

Table S2. CT sensitive mode of pristine TCNQFn neutral and anion[1].

Species	CT sensitive mode neutral TCNQFn (cm^{-1})	CT sensitive mode anion $TCNQFn^{-}$ (cm^{-1})
TCNQF0	1543	1509
TCNQF4	1396	1353
-	1550	1501
-	1599	1540

Table S3. Summary of vibrational modes related to the Pery:F4TCNQ_1:1 molecular crystal; Ir intensity for all modes and Raman activity for low frequency modes and participation ratio are also reported; all data are being calculated at PBE(D3BJ)/PAW level.

Mode Number	Wavenumber (cm^{-1})	Symmetry	IR intensity (e^2 amu^{-1})	Raman Activity (Å^2 amu^{-1})	Participation ratio
1	-2.2E-05	Au	0	-	1
2	-9E-06	Au	0	-	1
3	0.000016	Au	0	-	1
4	10.48448	Au	14389.28	-	0.353
5	43.61846	Ag	0	117986616658.60	0.42795
6	57.03928	Ag	0	145332792588.52	0.37789
7	61.93832	Au	653.3099	-	0.81428
8	66.21773	Ag	0	279328049693.57	0.12488
9	75.27408	Ag	0	84808896818.13	0.52367
10	86.21304	Au	1843.767	-	0.90703

11	92.9138	Au	14978.35	-	0.44107
12	104.3672	Ag	0	1187490456188.02	0.13951
13	106.3875	Au	2378.176	-	0.83978
14	110.7717	Ag	0	17164370036.62	0.22171
15	114.8599	Au	332.6774	-	0.11803
16	130.6346	Ag	0	23823589830.05	0.54184
17	134.1103	Au	74.63634	-	0.1922
18	136.3912	Au	2967.579	-	0.37411
19	141.6625	Ag	0	420143182267.93	0.27847
20	152.8497	Ag	0	278976829733.99	0.30718
21	153.4247	Au	59.74291	-	0.3583
22	162.6706	Ag	0	146342151468.64	0.29799
23	166.3716	Au	4099.79	-	0.07234
24	180.4128	Ag	0	24542349991.13	0.05721
25	180.961	Au	3538.571	-	0.07904
26	190.3717	Au	703.1257	-	0.31574
27	233.7821	Ag	0	747279670258.74	0.54862
28	235.354	Ag	0	218958264265.72	0.18757
29	242.9386	Ag	0	278456048408.34	0.25085
30	249.8849	Au	5360.427	-	0.43731
31	255.3704	Au	39.36369	-	0.34135
32	256.5616	Au	1075.833	-	0.40393
33	276.612	Au	56.32393	-	0.25721
34	299.1414	Ag	0	1622847614698.18	0.35029
35	302.5352	Ag	0	2159238900359.67	0.40847
36	318.1119	Au	429.0718	-	0.06963
37	331.2515	Au	1194.536	-	0.16879
38	343.6296	Ag	0	2091748240528.73	0.18111
39	357.9979	Ag	0	202058516595.48	0.2553
40	367.7304	Ag	0	911246766023.18	0.2663
41	374.7582	Ag	0	612676444989.30	0.13664
42	414.6918	Ag	0	47253305945.78	0.16055
43	417.3006	Ag	0	2392903328462.59	0.32648
44	424.8839	Ag	0	-	0.24802
45	427.0234	Ag	0	-	0.21
46	429.6983	Au	1369.384	-	0.11114
47	441.1934	Ag	0	-	0.21822
48	444.8193	Ag	0	-	0.17134
49	455.8146	Au	66.06456	-	0.20638
50	462.1071	Au	58.23988	-	0.30677
51	464.0591	Ag	0	-	0.09698
52	479.0626	Au	1887.107	-	0.13737
53	492.0132	Ag	0	-	0.15276
54	497.3636	Au	41.45016	-	0.20861
55	521.3981	Au	899.728	-	0.25219
56	525.947	Au	6444.554	-	0.42566
57	527.2041	Au	7.892871	-	0.31755

58	531.5178	Ag	0	-	0.35234
59	547.9634	Au	2946.464	-	0.42199
60	554.0429	Ag	0	-	0.44974
61	579.296	Au	1.167619	-	0.3619
62	591.0223	Ag	0	-	0.15357
63	617.2262	Ag	0	-	0.32595
64	618.516	Au	35.18366	-	0.06966
65	619.3516	Ag	0	-	0.21708
66	626.9475	Ag	0	-	0.2805
67	627.331	Au	141.2111	-	0.09261
68	643.835	Ag	0	-	0.15458
69	650.3915	Au	14.82144	-	0.15973
70	666.9131	Au	2148.136	-	0.10848
71	719.9339	Ag	0	-	0.13555
72	758.6126	Au	7450.223	-	0.25474
73	763.6555	Au	447.9753	-	0.27581
74	764.2936	Ag	0	-	0.14015
75	766.37	Ag	0	-	0.25732
76	777.6179	Ag	0	-	0.19357
77	786.1997	Au	559.6706	-	0.18207
78	789.3389	Au	182.5359	-	0.2684
79	793.5201	Au	1.858598	-	0.21673
80	794.786	Ag	0	-	0.30043
81	819.0054	Au	3222.47	-	0.20886
82	822.4139	Au	4.412989	-	0.24605
83	854.1688	Ag	0	-	0.2624
84	884.044	Ag	0	-	0.20677
85	897.1974	Au	2.000598	-	0.11649
86	912.1805	Ag	0	-	0.14982
87	917.1885	Au	4608.431	-	0.12432
88	920.4315	Ag	0	-	0.17967
89	941.7413	Ag	0	-	0.23414
90	961.9076	Au	45468.83	-	0.13416
91	984.6625	Au	73.2422	-	0.07568
92	987.4619	Ag	0	-	0.07301
93	993.41	Ag	0	-	0.16159
94	998.8828	Au	4063.389	-	0.08576
95	999.6894	Ag	0	-	0.08511
96	1047.847	Au	5584.583	-	0.24624
97	1067.752	Ag	0	-	0.13922
98	1091.909	Au	358.4785	-	0.11926
99	1104.948	Ag	0	-	0.11815
100	1107.413	Ag	0	-	0.19372
101	1127.221	Au	1395.706	-	0.13742
102	1131.485	Au	23.24334	-	0.29127
103	1150.758	Ag	0	-	0.11414
104	1153.485	Au	46.24232	-	0.07274

105	1182.578	Ag	0	-	0.08306
106	1194.438	Au	24245.32	-	0.08897
107	1196.209	Ag	0	-	0.14131
108	1200.782	Au	12794.93	-	0.10433
109	1205.57	Ag	0	-	0.06149
110	1209.544	Au	326.0043	-	0.11667
111	1221.524	Au	6776.236	-	0.13235
112	1231.995	Ag	0	-	0.12784
113	1270.577	Ag	0	-	0.16431
114	1289.677	Ag	0	-	0.0562
115	1304.896	Au	23270.39	-	0.09559
116	1326.456	Au	2.861844	-	0.10146
117	1348.008	Au	915.4931	-	0.20558
118	1363.535	Ag	0	-	0.16885
119	1372.609	Ag	0	-	0.0838
120	1372.673	Au	6.800088	-	0.36158
121	1373.102	Au	166.4115	-	0.11811
122	1378.475	Ag	0	-	0.2435
123	1380.763	Au	369.8808	-	0.10843
124	1427.527	Ag	0	-	0.15853
125	1437.736	Au	323.3936	-	0.15693
126	1443.642	Ag	0	-	0.14772
127	1453.286	Ag	0	-	0.16736
128	1459.322	Ag	0	-	0.12268
129	1463.504	Au	13992.91	-	0.11495
130	1494.058	Au	10144.69	-	0.09795
131	1498.232	Au	16.50364	-	0.12842
132	1529.082	Ag	0	-	0.2248
133	1533.979	Au	35156.83	-	0.07429
134	1558.95	Ag	0	-	0.10416
135	1564.404	Au	25.77551	-	0.42363
136	1566.433	Ag	0	-	0.30216
137	1576.918	Au	754.7912	-	0.23921
138	1591.555	Au	290.7829	-	0.29087
139	1600.87	Ag	0	-	0.3465
140	1630.942	Ag	0	-	0.0909
141	2205.909	Au	22284.81	-	0.09604
142	2208.695	Ag	0	-	0.09489
143	2233.255	Ag	0	-	0.09132
144	2233.697	Au	3.44757	-	0.09008
145	3118.048	Ag	0	-	0.10408
146	3118.239	Au	114.997	-	0.09794
147	3127.609	Ag	0	-	0.04229
148	3127.777	Au	158.6584	-	0.04243
149	3130.634	Ag	0	-	0.08647
150	3130.886	Au	656.4042	-	0.0815
151	3140.544	Au	728.2658	-	0.08064

152	3140.738	Ag	0	-	0.09386
153	3141.196	Ag	0	-	0.0505
154	3141.606	Au	309.5508	-	0.04718
155	3166.668	Au	314.8112	-	0.05948
156	3167.904	Ag	0	-	0.07035

Table S4. Summary of vibrational modes related to the Pery:TCNQ_1:1 molecular crystal; Ir intensity for all modes and Raman activity for low frequency modes and participation ratio are also reported; all data are being calculated at PBE(D3BJ)/PAW level.

Mode Number	Wavenumber (cm^{-1})	Symmetry	IR intensity (e^2 amu^{-1})	Raman Activity ($Å^2$ amu^{-1})	Participation ratio
1	0.000011	Au	0	-	1
2	0.000011	Bu	0	-	1
3	0.00002	Bu	0	-	1
4	30.566124	Ag	0	236119809.01	0.40839
5	31.457028	Bu	1.679069	-	0.92555
6	41.294614	Au	0.07956	-	0.41195
7	47.147254	Bg	0	9789250.13	0.34576
8	51.403462	Au	0.00013	-	0.63926
9	59.520943	Bu	14.657417	-	0.47135
10	61.766338	Au	0.022216	-	0.42307
11	62.29172	Ag	0	4601270561.58	0.59446
12	63.902498	Bg	0	3773332.07	0.50178
13	67.882726	Bu	341.094826	-	0.58761
14	74.950622	Bg	0	461985834.26	0.31065
15	75.984217	Au	0.211251	-	0.40339
16	81.471515	Au	0.274514	-	0.47838
17	82.840032	Ag	0	1485937859.06	0.24873
18	83.917721	Bg	0	714609811.66	0.30401
19	88.469757	Bu	278.055391	-	0.33983
20	88.995255	Au	0.085537	-	0.43555
21	93.21897	Ag	0	26431648237.01	0.28397
22	96.290284	Bu	1827.795685	-	0.48942
23	105.571263	Bu	16.544536	-	0.09447
24	108.567216	Au	0.03953	-	0.38948
25	109.862251	Bg	0	32358068.69	0.44971
26	118.935569	Ag	0	9324943897.85	0.36669
27	119.079401	Au	0.10026	-	0.34532
28	121.230716	Bu	331.046754	-	0.14716
29	123.144135	Ag	0	16036343446.05	0.4171
30	123.736031	Bg	0	12854289.27	0.23993
31	124.31077	Au	0.454876	-	0.48105
32	130.975828	Bu	64.639153	-	0.31041
33	131.662968	Ag	0	709922221.90	0.16063
34	135.108379	Bg	0	63653274.13	0.24333
35	137.790957	Au	0.203739	-	0.36587

36	145.678039	Bg	0	18609997.41	0.12584
37	146.414299	Ag	0	38907946410.85	0.15446
38	153.087501	Bu	173.375751	-	0.36221
39	153.088244	Au	0.036049	-	0.23649
40	154.102497	Bu	3.676373	-	0.30258
41	158.846706	Ag	0	7516512248.32	0.08747
42	161.60262	Bg	0	147220789.81	0.16978
43	169.192519	Ag	0	26090188816.30	0.44056
44	171.679347	Bg	0	783912141.41	0.46313
45	184.923496	Ag	0	1235443661.86	0.36978
46	192.444577	Bg	0	452977973.09	0.32265
47	196.901552	Bu	20.83836	-	0.26248
48	203.796306	Au	0.004655	-	0.25402
49	222.003498	Ag	0	6827865410.67	0.3556
50	233.776651	Bg	0	1356316440.41	0.36159
51	236.436375	Au	0.420484	-	0.33663
52	236.512399	Bu	734.57584	-	0.27569
53	246.589288	Bu	48.284446	-	0.19486
54	248.176986	Au	0.005231	-	0.22804
55	256.290231	Bu	7.238614	-	0.23215
56	257.478168	Au	0.007257	-	0.2278
57	282.715011	Au	0.024586	-	0.24851
58	285.731992	Bu	46.55793	-	0.22691
59	299.70127	Ag	0	279582630.87	0.27519
60	299.781023	Bg	0	1363351044.63	0.27391
61	330.093701	Ag	0	902728616.74	0.25269
62	330.749873	Bg	0	786374426.31	0.2567
63	333.199591	Ag	0	271351299930.60	0.1312
64	333.531529	Bg	0	451550099.09	0.1614
65	352.165309	Ag	0	46748357254.05	0.31751
66	354.618463	Bg	0	79618880.69	0.31502
67	364.98898	Ag	0	4305635718.39	0.37781
68	365.338614	Bg	0	74082185.48	0.24087
69	366.61863	Bg	0	141644916.77	0.40789
70	366.892144	Ag	0	783094429.16	0.14588
71	397.74761	Bu	2.802426	-	0.1183
72	397.765775	Au	0.000209	-	0.11766
73	411.851544	Ag	0	-	0.31085
74	413.216972	Bg	0	-	0.30546
75	425.624999	Bg	0	-	0.29291
76	425.970433	Ag	0	-	0.29125
77	446.033335	Ag	0	-	0.11929
78	446.090146	Bg	0	-	0.11959
79	456.83819	Bg	0	-	0.22526
80	456.878691	Au	0.007875	-	0.1977
81	457.219766	Bu	3.812514	-	0.18952
82	457.567485	Ag	0	-	0.22181

83	458.530801	Au	0.002118	-	0.20822
84	459.099501	Bu	0.114699	-	0.20395
85	465.400497	Bu	107.148953	-	0.31554
86	466.400448	Au	0.028824	-	0.30828
87	473.75547	Bu	191.142334	-	0.15628
88	474.443868	Au	0.071089	-	0.16357
89	508.895012	Au	0.004117	-	0.09082
90	510.164051	Bu	0.200384	-	0.10501
91	515.91367	Au	0.001393	-	0.21237
92	517.006275	Bu	110.447123	-	0.21567
93	523.94942	Au	0.147972	-	0.19176
94	526.353966	Bu	210.20284	-	0.28305
95	528.674678	Ag	0	-	0.46161
96	528.765895	Bg	0	-	0.45464
97	530.140886	Bg	0	-	0.17089
98	531.425651	Ag	0	-	0.17836
99	532.913038	Bu	41.983122	-	0.13273
100	533.238626	Au	0.032426	-	0.13838
101	552.47536	Ag	0	-	0.32358
102	553.363329	Bg	0	-	0.32132
103	554.759228	Au	0.004558	-	0.18062
104	555.308262	Bu	3.93763	-	0.17461
105	577.980854	Au	0.010422	-	0.2407
106	578.772608	Bu	0.169414	-	0.24802
107	584.979018	Bg	0	-	0.17494
108	585.103039	Ag	0	-	0.17421
109	602.599442	Ag	0	-	0.0902
110	602.674578	Bg	0	-	0.08596
111	605.64195	Au	0.01018	-	0.11355
112	606.02961	Bu	2.194902	-	0.11279
113	610.89634	Bu	44.385476	-	0.14769
114	610.904144	Au	0.028846	-	0.14778
115	613.630738	Ag	0	-	0.10699
116	614.123894	Bg	0	-	0.10632
117	617.823979	Bg	0	-	0.21332
118	617.855243	Ag	0	-	0.29828
119	624.650631	Bg	0	-	0.24478
120	628.039871	Ag	0	-	0.29956
121	646.749593	Ag	0	-	0.13906
122	646.894091	Bg	0	-	0.14044
123	656.369875	Au	0.000054	-	0.15441
124	656.567912	Bu	129.31478	-	0.15362
125	724.892416	Bg	0	-	0.14849
126	726.019228	Ag	0	-	0.16469
127	737.553434	Bg	0	-	0.14093
128	737.641865	Ag	0	-	0.13655
129	759.312377	Bg	0	-	0.1985

130	761.523274	Bu	323.872535	-	0.24409
131	763.901581	Au	0.231454	-	0.15525
132	764.66423	Bu	719.002856	-	0.20212
133	765.844514	Ag	0	-	0.12729
134	768.827169	Bg	0	-	0.21086
135	769.24238	Au	0.000012	-	0.13845
136	773.446266	Ag	0	-	0.15357
137	781.258554	Bu	102.357518	-	0.17316
138	781.427273	Bg	0	-	0.07665
139	781.700091	Au	0.079971	-	0.13867
140	782.068082	Ag	0	-	0.09563
141	784.40086	Bu	7.67148	-	0.27343
142	785.193032	Au	0.00657	-	0.17899
143	790.895316	Bg	0	-	0.3366
144	791.492212	Ag	0	-	0.29481
145	815.514326	Bu	455.497109	-	0.1974
146	820.06494	Au	0.104818	-	0.19617
147	821.747232	Bu	14.674056	-	0.31315
148	823.511267	Au	0.038896	-	0.18495
149	826.143012	Au	0.005955	-	0.08411
150	826.209172	Bu	7.997594	-	0.08516
151	852.852648	Ag	0	-	0.22199
152	853.544969	Bg	0	-	0.22203
153	902.851282	Au	0.000583	-	0.14579
154	904.164163	Bu	1.685368	-	0.13781
155	904.230548	Ag	0	-	0.13105
156	918.515894	Bg	0	-	0.10724
157	919.035336	Au	0.108267	-	0.14091
158	924.447289	Ag	0	-	0.12834
159	927.105559	Bg	0	-	0.11066
160	935.688794	Bu	305.048064	-	0.13339
161	941.266895	Bg	0	-	0.2101
162	941.834542	Ag	0	-	0.21547
163	958.032382	Au	0.020639	-	0.07061
164	958.20943	Bu	4.150211	-	0.07069
165	959.82891	Ag	0	-	0.07761
166	959.983918	Bg	0	-	0.07787
167	972.162173	Au	0.003236	-	0.12451
168	973.682998	Bu	125.526811	-	0.12192
169	974.630646	Ag	0	-	0.17396
170	975.367146	Bg	0	-	0.21789
171	975.476163	Ag	0	-	0.09892
172	977.545338	Bg	0	-	0.10812
173	978.163232	Au	0.001182	-	0.1556
174	978.556278	Bu	17.697342	-	0.08688
175	981.684072	Bg	0	-	0.08937
176	983.291567	Bu	284.80454	-	0.12072

177	987.978989	Ag	0	-	0.14071
178	988.419319	Bg	0	-	0.13017
179	989.895374	Ag	0	-	0.09704
180	991.6165	Au	0.095246	-	0.12581
181	998.514629	Bu	0.498388	-	0.10334
182	998.782588	Au	0.006914	-	0.10143
183	1043.999542	Bu	943.933763	-	0.26652
184	1045.258806	Au	0.678158	-	0.22563
185	1070.155191	Ag	0	-	0.12429
186	1071.130352	Bg	0	-	0.12726
187	1093.32602	Au	0.000976	-	0.08823
188	1096.164443	Bu	21.591781	-	0.08941
189	1106.479371	Bg	0	-	0.11847
190	1106.630724	Ag	0	-	0.13555
191	1115.606161	Au	0.005165	-	0.05976
192	1116.705189	Bu	2.640148	-	0.06014
193	1124.170443	Au	0.190965	-	0.14012
194	1125.340792	Bu	34.81855	-	0.13917
195	1144.175432	Bg	0	-	0.0788
196	1144.552853	Ag	0	-	0.07892
197	1144.68112	Bu	5.23753	-	0.06871
198	1146.303593	Au	0.033	-	0.06682
199	1178.790641	Bg	0	-	0.06058
200	1179.031166	Ag	0	-	0.05797
201	1187.418691	Bg	0	-	0.06634
202	1188.314186	Ag	0	-	0.06454
203	1191.674988	Bg	0	-	0.08588
204	1191.924994	Ag	0	-	0.09118
205	1194.167447	Bu	950.843501	-	0.10092
206	1194.913637	Au	0.47352	-	0.10079
207	1205.516217	Ag	0	-	0.08157
208	1206.07482	Bg	0	-	0.07456
209	1211.011781	Bu	65.787693	-	0.0929
210	1211.606639	Au	0.05901	-	0.10596
211	1211.917985	Bu	12.657754	-	0.15119
212	1212.785766	Au	0.005349	-	0.15285
213	1225.521631	Bu	73.053925	-	0.09653
214	1225.813103	Au	0.134171	-	0.10236
215	1232.146115	Ag	0	-	0.09766
216	1232.33259	Bg	0	-	0.09544
217	1295.556103	Ag	0	-	0.07123
218	1296.895825	Bg	0	-	0.07194
219	1300.321554	Bg	0	-	0.05499
220	1300.674949	Ag	0	-	0.05419
221	1307.74361	Au	1.674364	-	0.11109
222	1308.022241	Bu	3537.979037	-	0.11252
223	1349.197376	Au	1.04316	-	0.09227

224	1349.417848	Bu	3230.154127	-	0.09411
225	1354.669858	Au	0.058502	-	0.16884
226	1355.218579	Bu	46.385409	-	0.18087
227	1364.191922	Ag	0	-	0.16402
228	1364.613633	Au	0.060201	-	0.06527
229	1365.234734	Bu	14.291056	-	0.06328
230	1365.251693	Bg	0	-	0.16052
231	1377.035274	Bu	19.664748	-	0.18085
232	1377.430347	Au	0.207882	-	0.18555
233	1380.114833	Ag	0	-	0.16762
234	1380.556641	Bg	0	-	0.17407
235	1380.578886	Bu	14.998433	-	0.15296
236	1381.127848	Au	0.143018	-	0.14291
237	1384.920311	Ag	0	-	0.14453
238	1385.058358	Bg	0	-	0.21255
239	1404.093639	Ag	0	-	0.1172
240	1404.571265	Bg	0	-	0.11858
241	1434.525954	Au	0.09781	-	0.14035
242	1435.41792	Bu	1.705424	-	0.14387
243	1446.958445	Bg	0	-	0.12734
244	1447.223173	Ag	0	-	0.12986
245	1449.56112	Ag	0	-	0.18174
246	1449.690266	Bg	0	-	0.12152
247	1460.676215	Ag	0	-	0.07892
248	1461.018638	Bg	0	-	0.07975
249	1468.412843	Bu	1679.794613	-	0.10157
250	1468.542735	Au	0.666394	-	0.10063
251	1493.48541	Bu	1287.280028	-	0.12607
252	1494.405605	Au	0.342733	-	0.12501
253	1504.447118	Bu	333.413564	-	0.08073
254	1505.268721	Au	0.322742	-	0.08674
255	1510.604627	Au	1.35747	-	0.10938
256	1510.654405	Bu	2105.485373	-	0.10803
257	1527.995454	Bg	0	-	0.28991
258	1528.036382	Ag	0	-	0.29109
259	1559.467593	Bg	0	-	0.22954
260	1560.590916	Ag	0	-	0.18371
261	1569.208587	Au	0.196378	-	0.19049
262	1569.652828	Bu	2.826156	-	0.18806
263	1570.612211	Bg	0	-	0.17001
264	1570.768409	Ag	0	-	0.18877
265	1576.507443	Au	0.024451	-	0.32489
266	1576.961001	Bu	18.22354	-	0.32062
267	1590.705213	Au	0.412442	-	0.15295
268	1591.305814	Bu	1130.803076	-	0.15245
269	1598.183384	Ag	0	-	0.31154
270	1598.522225	Bg	0	-	0.30235

271	1606.151178	Ag	0	-	0.12104
272	1607.928416	Bg	0	-	0.12061
273	2204.594163	Bu	1186.71256	-	0.08318
274	2205.521031	Au	0.728111	-	0.08157
275	2205.791563	Ag	0	-	0.08428
276	2206.468677	Bg	0	-	0.08361
277	2227.322881	Au	0.946777	-	0.08145
278	2227.520736	Bg	0	-	0.08385
279	2227.630633	Ag	0	-	0.08459
280	2227.698734	Bu	2.819532	-	0.08298
281	3098.187874	Bu	11.130176	-	0.02668
282	3098.211062	Ag	0	-	0.02681
283	3098.23895	Bg	0	-	0.02668
284	3098.279615	Au	0.031507	-	0.02668
285	3105.898484	Au	0.304534	-	0.05426
286	3105.9303	Bu	14.78283	-	0.05413
287	3106.349298	Ag	0	-	0.05152
288	3106.367019	Bg	0	-	0.05137
289	3115.492497	Bu	2.193735	-	0.08387
290	3115.709882	Au	0.018985	-	0.07332
291	3115.829703	Bg	0	-	0.0661
292	3116.018419	Ag	0	-	0.05907
293	3116.41296	Bu	23.548536	-	0.07249
294	3116.420541	Au	0.014028	-	0.08221
295	3117.057732	Ag	0	-	0.04335
296	3117.139802	Bg	0	-	0.04661
297	3121.859967	Bu	13.515721	-	0.02889
298	3121.866759	Au	0.00217	-	0.02869
299	3122.675169	Bg	0	-	0.02785
300	3122.676794	Ag	0	-	0.02795
301	3130.321278	Au	0.000167	-	0.05241
302	3130.369421	Ag	0	-	0.05228
303	3130.7261	Bu	0.232385	-	0.05341
304	3130.778717	Bg	0	-	0.0541
305	3133.878664	Bu	14.418815	-	0.02861
306	3133.8983	Au	0.000047	-	0.02852
307	3134.741496	Ag	0	-	0.02849
308	3134.840857	Bg	0	-	0.02863
309	3143.34424	Bu	222.740247	-	0.04357
310	3143.535966	Au	0.033731	-	0.04492
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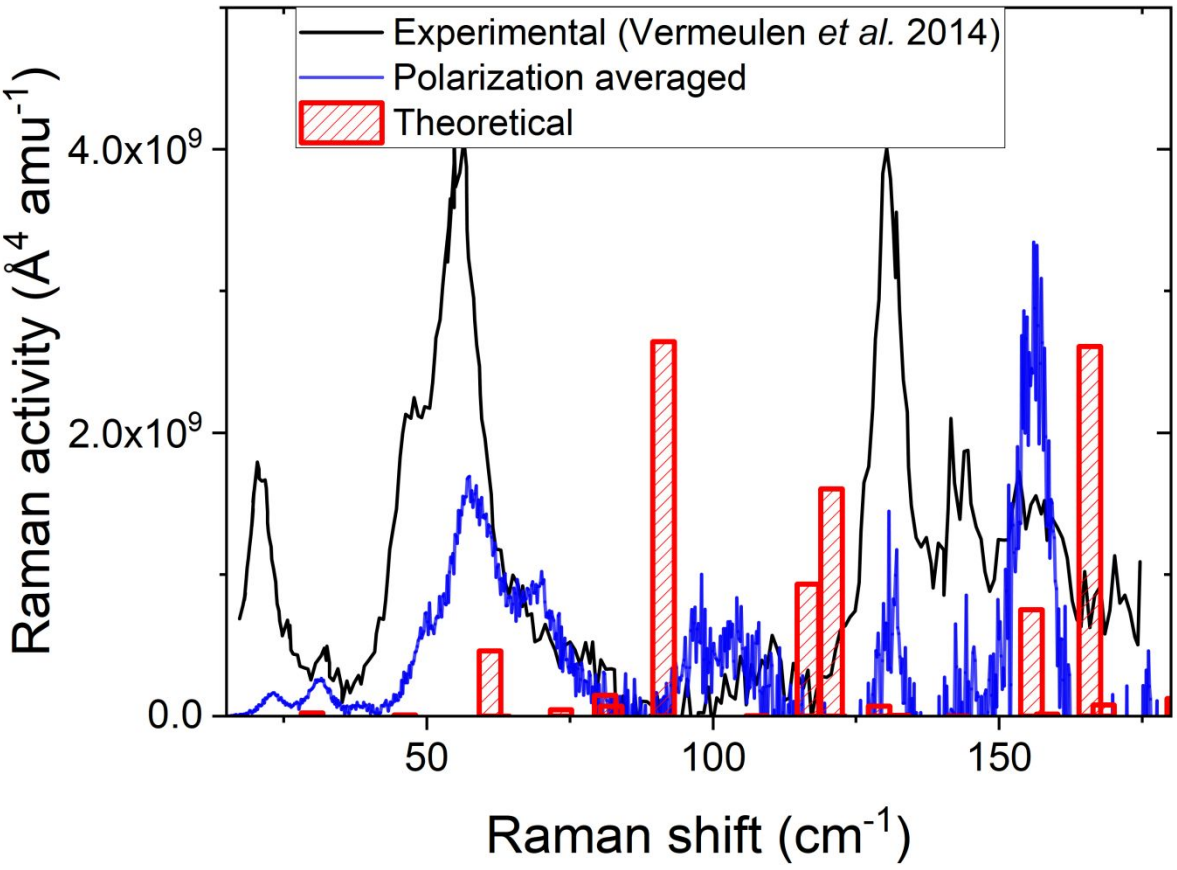

Figure S1. Comparison between Vermeulen *et al.*[2], polarization averaged (this work) and theoretical Raman spectra of Perylene:TCNQ at stoichiometry 1:1.

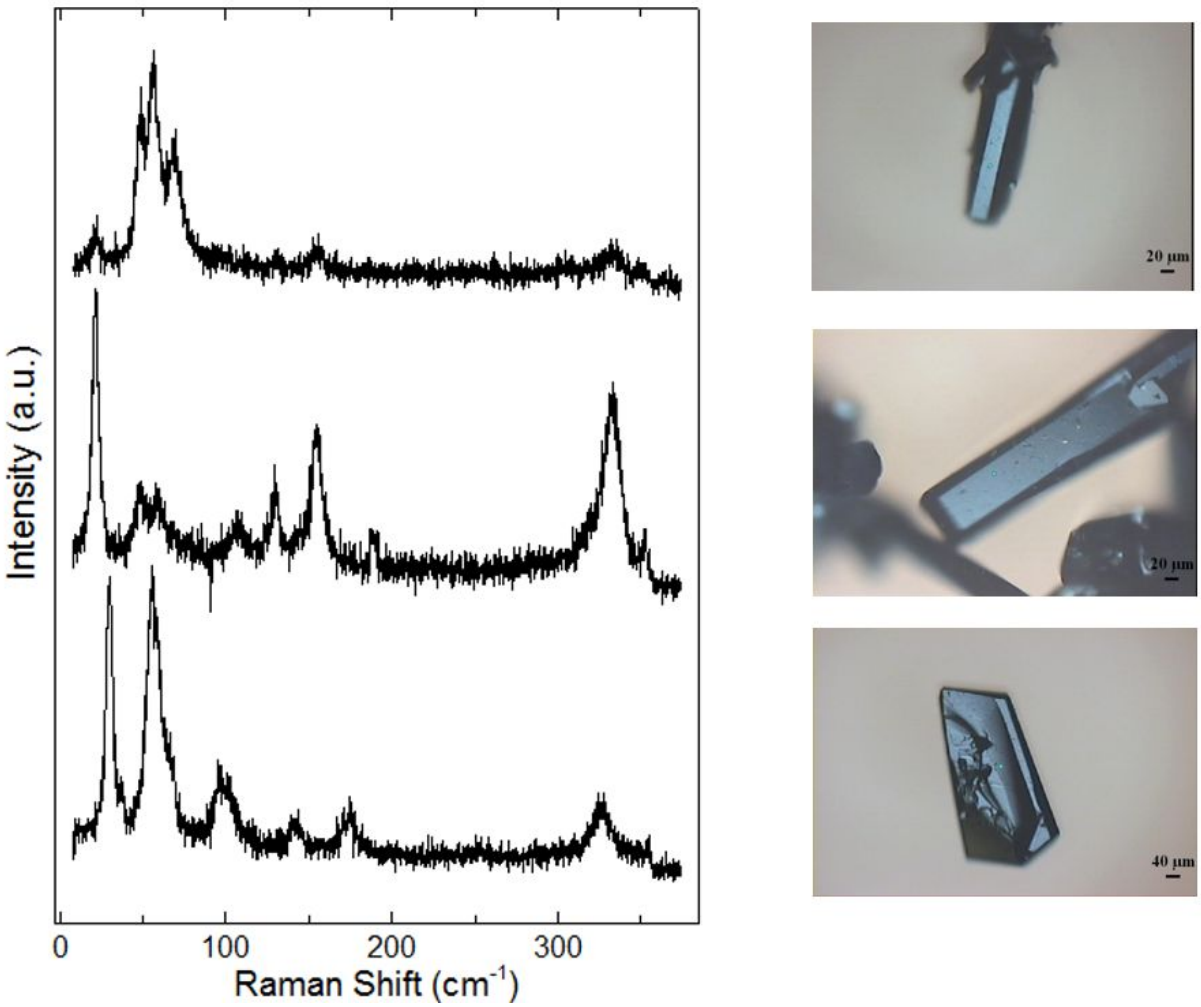

Figure S2. Raman spectra of Perylene:TCNQ at stochiometry 1:1 taken at different crystal orientations. On the right the pictures of the CT crystals in the different orientations.

References

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(2) Vermeulen, D.; Zhu, L. Y.; Goetz, K. P.; Hu, P.; Jiang, H.; Day, C. S.; Jurchescu, O. D.; Coropceanu, V.; Kloc, C.; McNeil, L. E. Charge Transport Properties of Perylene–TCNQ Crystals: The Effect of Stoichiometry. *J. Phys. Chem. C* **2014**, *118* (42), 24688–24696. https://doi.org/10.1021/jp508520x.