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

Electronic supplementary information for "Interaction in the indole…imidazole heterodimer: Structure, Franck-Condon analysis and energy decomposition".

J. Grant Hill[1]

School of Chemistry, Joseph Black Building, University of Glasgow, Glasgow, G12 8QQ, UK.

Aloke Das

Department of Chemistry, Indian Institute of Science Education and Research (IISER), Dr. Homi Bhabha Road, Pune 411008, Maharashtra, India.

[1] Electronic mail: Grant.Hill@sheffield.ac.uk
Present address: *Department of Chemistry, University of Sheffield, Sheffield S3 7HF, UK.*

Table SI. SAPT2+3/aug-cc-pVDZ contributions (kcal mol^{-1}) to the total interaction energy for four proposed structures of the indole…imidazole heterodimer. All ground electronic state geometries optimized at the M05-2X/6-31+G(d) level.

Structure	$E_{\text{electrostatic}}$	E_{exchange}	$E_{\text{induction}}$	$E_{\text{dispersion}}$
HB	–13.07	14.32	–4.69	–6.36
T1	–6.31	8.79	–2.43	–8.15
T2	–6.23	9.08	–2.67	–7.97
Syn-PD	–8.17	11.37	–1.95	–9.37

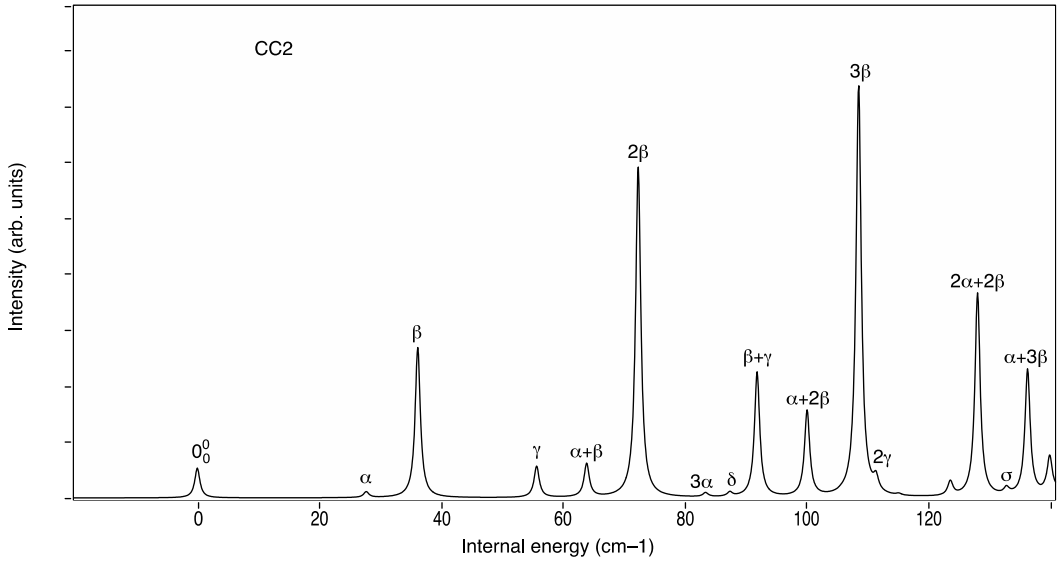

Fig. S1. Franck-Condon simulated electronic spectrum for the HB indole…imidazole structure obtained from calculations at the CC2/def2-TZVPP level of theory.

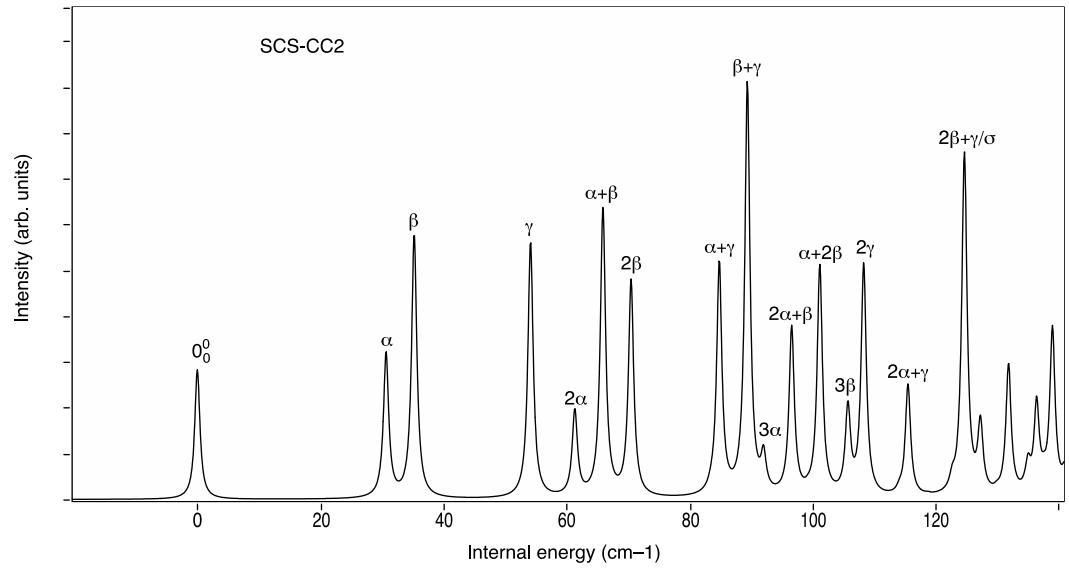

Fig. S2. Franck-Condon simulated electronic spectrum for the HB indole…imidazole structure obtained from calculations at the SCS-CC2/def2-TZVPP level of theory.

OPTIMIZED GEOMETRIES

HB structure

25
S0 structure for HB indole…imidazole M05-2X/6-31+G*

C	-1.250493	0.135229	-0.320761
C	-2.499175	0.567452	0.192973
C	-3.512097	-0.383648	0.402822
C	-3.259699	-1.711840	0.105660
C	-2.009438	-2.119312	-0.405869
C	-0.991575	-1.206660	-0.627727
C	-1.132555	2.344621	-0.005185
C	-2.396311	1.986818	0.383518
H	-4.476959	-0.079661	0.791524
H	-4.033484	-2.453425	0.262562
H	-1.846011	-3.165258	-0.635761
H	-0.034865	-1.512176	-1.034307
H	0.537729	1.208940	-0.706140
H	-0.662801	3.315437	-0.012370
H	-3.159148	2.651357	0.756642
N	-0.441232	1.238957	-0.435886
C	4.420947	-0.460629	0.066574
C	3.730038	0.297395	-0.839805
C	2.324107	-0.208641	0.697834
N	3.506252	-0.776378	1.043757
H	3.678471	-1.328418	1.867350
H	5.443793	-0.792854	0.104012
H	4.092394	0.740052	-1.752732
H	1.427351	-0.303581	1.291079
N	2.425269	0.447612	-0.436254

25
S1 structure for HB indole…imidazole TD-M05-2X/6-31+G*

C	-1.267185	0.090100	-0.249883
C	-2.518336	0.588171	0.151494
C	-3.604554	-0.301415	0.395751
C	-3.350037	-1.687115	0.175984
C	-2.113725	-2.150736	-0.221680
C	-0.984875	-1.265686	-0.435582
C	-1.042415	2.334175	-0.137899
C	-2.390481	1.997284	0.212826
H	-4.571536	0.058506	0.716016
H	-4.153431	-2.397739	0.327535
H	-1.971972	-3.212578	-0.381785
H	-0.047300	-1.620390	-0.838727
H	0.593756	1.100210	-0.610278
H	-0.551086	3.291190	-0.185053
H	-3.156147	2.712288	0.472295
N	-0.409865	1.192647	-0.408253
C	4.486992	-0.273641	0.039224
C	3.711589	0.575084	-0.702888
C	2.365930	-0.459777	0.613015
N	3.610590	-0.926655	0.873870
H	3.844899	-1.630227	1.554264
H	5.545531	-0.466514	0.047475
H	4.022013	1.261276	-1.473144
H	1.479022	-0.817858	1.115332
N	2.392852	0.449950	-0.337229

25
Fitted S1 structure for HB indole…imidazole
C -1.25475 0.110198 -0.242225
C -2.50874 0.574995 0.193060
C -3.60276 -0.328284 0.340665
C -3.35300 -1.68718 -0.011485
C -2.11374 -2.11778 -0.435364
C -0.97717 -1.22424 -0.543397
C -1.02025 2.33076 0.090096
C -2.37322 1.97074 0.397205
H -4.57317 0.006467 0.679030
H -4.16548 -2.40103 0.056740
H -1.97753 -3.15830 -0.698634
H -0.028661 -1.54915 -0.946877
H 0.609976 1.14135 -0.506418
H -0.523559 3.28556 0.133992
H -3.13546 2.66330 0.719689
N -0.393525 1.21733 -0.286617
C 4.47861 -0.347251 -0.017466
C 3.70998 0.534629 -0.729859
C 2.37032 -0.465891 0.630336
N 3.60898 -0.978956 0.844239
H 3.83757 -1.69989 1.51194
H 5.53089 -0.576895 -0.049346
H 4.02115 1.22000 -1.50781
H 1.48767 -0.800177 1.16371
N 2.39972 0.452004 -0.315660

T1 structure

25
S0 structure for T1 indole…imidazole M05-2X/6-31+G*
C -1.415724 -0.191099 0.745852
C -1.675443 -0.168843 -0.647508
C -1.665384 1.066061 -1.319636
C -1.402666 2.220439 -0.598850
C -1.153022 2.172070 0.790352
C -1.156245 0.971350 1.479665
C -1.745226 -2.303196 0.064712
C -1.884195 -1.530502 -1.055186
H -1.858438 1.112230 -2.384567
H -1.394598 3.178087 -1.104230
H -0.951646 3.091687 1.325164
H -0.951749 0.934239 2.542494
H -1.278226 -1.832717 2.080079
H -1.826192 -3.371964 0.181260
H -2.110313 -1.885865 -2.047533
N -1.467027 -1.503215 1.149345
C 1.805970 -0.924898 -0.399447
C 3.104928 -1.156894 -0.023753
C 2.872795 0.964422 -0.040412
N 1.675495 0.440936 -0.409330
H 0.830422 0.954760 -0.615064
H 0.988253 -1.577796 -0.655969
H 3.602576 -2.105651 0.095729
H 3.040206 2.026972 0.036667
N 3.762244 0.028361 0.198731

S1 structure for T1 indole…imidazole M05-2X/6-31+G*

C	-0.946005	0.016517	0.801286
C	-1.316537	0.709061	-0.396188
C	-0.561796	1.858496	-0.811213
C	0.467156	2.276044	0.059223
C	0.808212	1.575199	1.229703
C	0.072497	0.451592	1.682112
C	-2.733590	-1.034792	-0.096764
c	-2.441127	0.025574	-0.933700
H	-0.894845	2.478209	-1.633264
H	1.025341	3.175496	-0.179446
H	1.615311	1.956313	1.843912
H	0.324748	-0.080035	2.588193
H	-1.862749	-1.641756	1.740695
H	-3.508158	-1.781583	-0.157327
H	-2.982964	0.282002	-1.830951
N	-1.817240	-1.044081	0.933461
C	0.624374	-1.288414	-0.904854
C	1.414473	-1.856062	0.134451
C	2.433495	-0.120380	-0.531362
N	1.355273	-0.241524	-1.366490
H	0.900045	0.572166	-1.799851
H	-0.288857	-1.626279	-1.368822
H	1.190281	-2.744467	0.702858
H	3.170752	0.654631	-0.651048
N	2.516850	-1.131781	0.340012

T2 structure

25

S0 structure for T2 indole…imidazole M05-2X/6-31+G*

C	1.341749	0.342454	0.761821
C	1.573426	0.516533	-0.623831
C	2.024548	-0.579412	-1.380992
C	2.229357	-1.790841	-0.745619
C	1.993832	-1.938883	0.638312
C	1.547501	-0.880819	1.409739
C	0.832747	2.465455	0.237373
C	1.240432	1.881822	-0.933701
H	2.206122	-0.474276	-2.443702
H	2.575271	-2.643692	-1.315833
H	2.160089	-2.902211	1.103652
H	1.354772	-0.998750	2.468894
H	0.599308	1.709954	2.203942
H	0.508438	3.475566	0.430045
H	1.315353	2.369768	-1.892476
N	0.895693	1.546244	1.257278
C	-3.034857	0.746219	-0.271477
C	-3.739019	-0.362938	0.122200
C	-1.737682	-1.030234	-0.210671
N	-1.753008	0.300862	-0.481428
H	-0.957544	0.855186	-0.767248
H	-3.320507	1.773398	-0.421318
H	-4.784021	-0.429113	0.378604
H	-0.839563	-1.622189	-0.295295
N	-2.921247	-1.465645	0.157265

25

S1 structure for T2 indole…imidazole M05-2X/6-31+G*

C	0.900715	0.926177	0.444038

C	0.787538	0.534261	-0.903647
C	1.629251	-0.497954	-1.415810
C	2.623955	-1.006736	-0.528080
C	2.735391	-0.566555	0.778877
C	1.864584	0.428251	1.331860
C	-0.865866	2.062584	-0.411680
C	-0.320946	1.238791	-1.443233
H	1.610760	-0.771115	-2.462383
H	3.317261	-1.756808	-0.889576
H	3.512162	-0.982642	1.409309
H	1.953620	0.768780	2.353691
H	-0.316629	2.257458	1.588837
H	-1.693790	2.750289	-0.427482
H	-0.682476	1.209506	-2.459533
N	-0.122779	1.856101	0.684844
C	-1.920270	-1.115850	-0.880476
C	-2.725858	-0.384510	-0.011324
C	-1.133593	-1.171213	1.159439
N	-0.941937	-1.653026	-0.102696
H	-0.041725	-1.968143	-0.465760
H	-1.994328	-1.314057	-1.936233
H	-3.636971	0.142872	-0.243814
H	-0.448315	-1.388212	1.962344
N	-2.225137	-0.436132	1.253685

Syn-PD structure

25
S0 structure for Syn-PD indole…imidazole M05-2X/6-31+G*

C	0.950318	0.018452	-0.709022
C	1.607119	0.946978	0.134938
C	2.773528	0.545046	0.808458
C	3.234915	-0.748845	0.638349
C	2.558370	-1.659283	-0.200458
C	1.412418	-1.290512	-0.885133
C	-0.208643	1.934572	-0.759852
C	0.846280	2.166257	0.080551
H	3.302097	1.239194	1.451101
H	4.132149	-1.070543	1.152427
H	2.945798	-2.664145	-0.314823
H	0.892856	-1.986105	-1.533563
H	-0.884655	0.191241	-1.753905
H	-1.012728	2.588293	-1.057156
H	1.065208	3.094142	0.584563
N	-0.142825	0.652580	-1.251009
C	-1.747946	-1.348760	0.520307
C	-3.377287	-0.184950	-0.227727
C	-2.826683	0.550207	0.789671
N	-1.788088	-0.212528	1.262341
H	-1.103807	0.068636	1.946149
H	-1.004588	-2.113315	0.678325
H	-4.228966	0.061554	-0.840865
H	-3.069629	1.512819	1.205434
N	-2.693097	-1.368157	-0.391071

25
S1 structure for Syn-PD indole…imidazole M05-2X/6-31+G*

C	0.892201	0.369685	-0.905393
C	1.031225	1.015622	0.335923
C	1.997047	0.548408	1.276480
C	2.815546	-0.539728	0.858892
C	2.673510	-1.138893	-0.378988
C	1.672841	-0.712907	-1.323720
C	-0.813326	1.867232	-0.760605
C	-0.031504	1.956051	0.430392
H	2.153136	1.047085	2.222644
H	3.580542	-0.907439	1.532528
H	3.326998	-1.959456	-0.648601
H	1.563279	-1.176524	-2.294140
H	-0.592173	0.633435	-2.425935
H	-1.667689	2.435573	-1.085513
H	-0.232958	2.633100	1.246584
N	-0.241693	0.923490	-1.526051
C	-1.588924	-1.550001	-0.373069
C	-2.798988	-0.115070	0.630641
C	-1.640370	-0.255100	1.392758
N	-0.903847	-1.194807	0.745724
H	0.062531	-1.424686	0.950571
H	-1.198765	-2.264624	-1.079326
H	-3.644830	0.522475	0.830828
H	-1.316842	0.194859	2.315224
N	-2.752858	-0.929480	-0.457491