crystals

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Supplementary Information

Adenine as a Halogen Bond Acceptor: a Combined Experimental and DFT Study

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Content

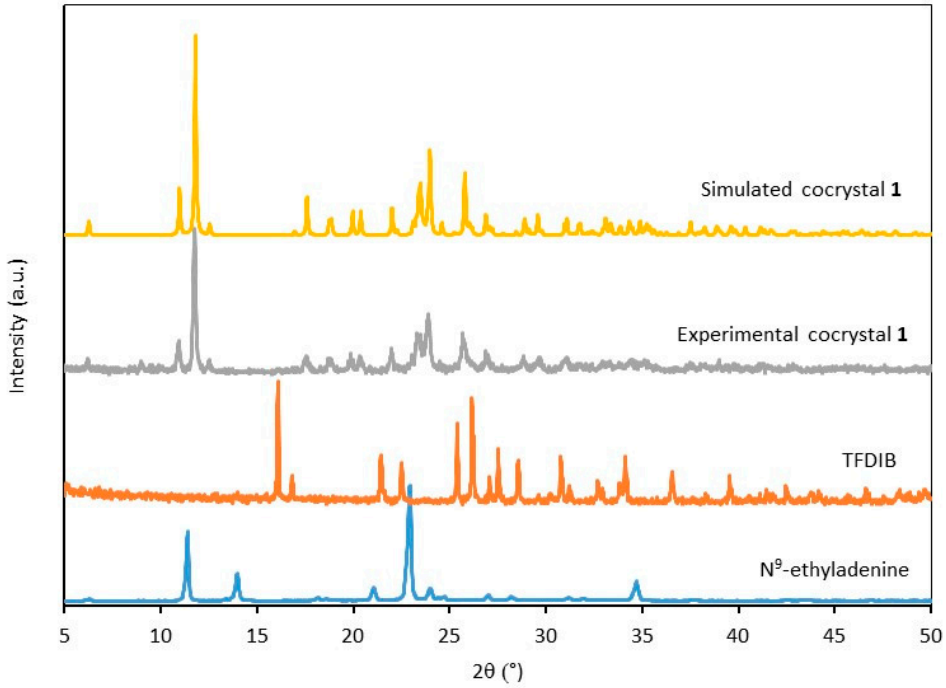

Figure S1. PXRD patterns of N^9-ethyladenine, 1,2,4,5-tetrafluoro-3,6-diiodobenzene (TFDIB) and experimental and simulated cocrystal **1**.

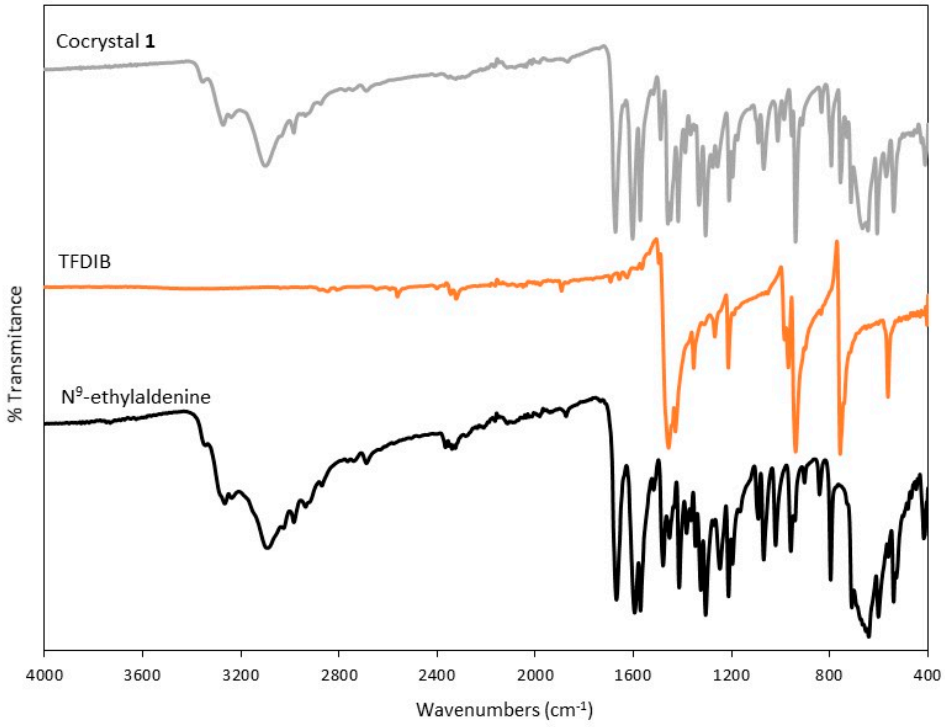

Figure S2. ATR-FT-IR spectra of N^9-ethyladenine, 1,2,4,5-tetrafluoro-3,6-diiodobenzene (TFDIB) and cocrystal **1**.

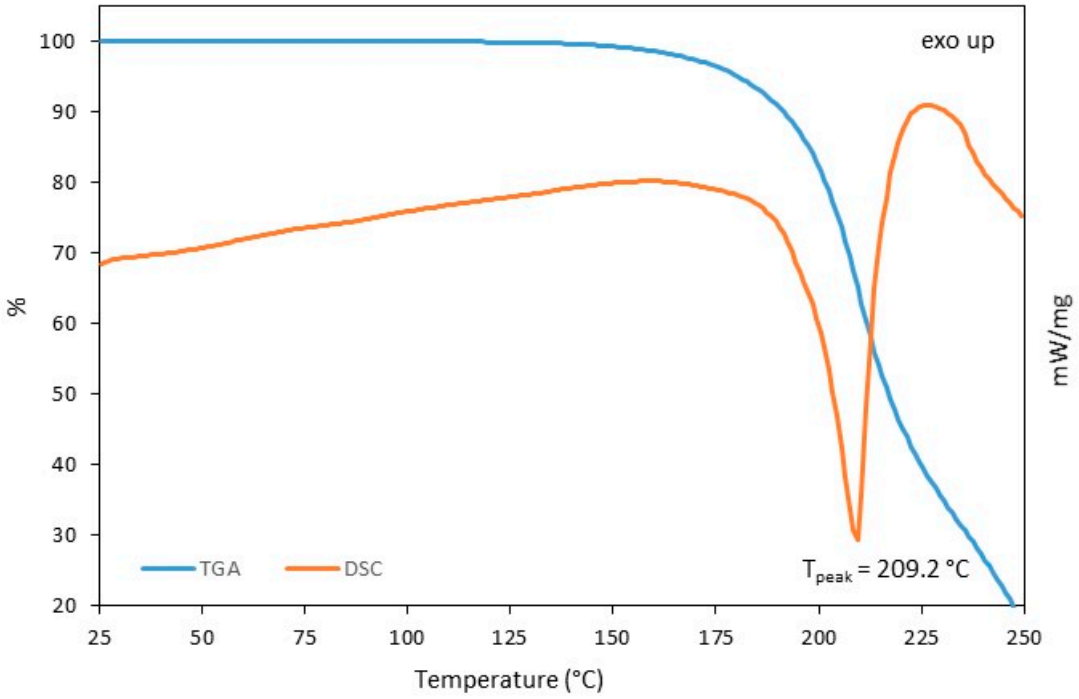

Figure S3. TGA-DSC trace of cocrystal **1**.

Table S1. Cartesian coordinates of optimized complexes.

Dimer Figure 5a

7	0.132552	-1.740075	-0.760544
7	0.291371	-4.029912	-1.515790
7	-0.026850	-1.130514	1.485885
1	-0.059856	-0.131063	1.234254
1	-0.066464	-1.412693	2.455519
7	0.092401	-4.142976	2.069102
7	0.270974	-5.604072	0.354786
6	0.235434	-2.708571	-1.690332
1	0.277223	-2.359724	-2.720298
6	0.233117	-4.349926	-0.210434
6	0.125764	-3.464770	0.865608
6	0.075220	-2.086511	0.548870
6	0.177581	-5.406856	1.717026
1	0.184954	-6.248167	2.399534
6	0.328311	-6.870268	-0.369291
1	0.609717	-7.643298	0.353880
1	1.126280	-6.788998	-1.114906
6	-1.004158	-7.198277	-1.047142
1	-1.807400	-7.278826	-0.304618
1	-0.925396	-8.151429	-1.584782
1	-1.260371	-6.410707	-1.763608
7	-0.132552	1.740075	0.760544
7	-0.291371	4.029912	1.515790
7	0.026850	1.130514	-1.485885
1	0.059856	0.131063	-1.234254
1	0.066464	1.412693	-2.455519
7	-0.092401	4.142976	-2.069102

7	-0.270974	5.604072	-0.354786
6	-0.235434	2.708571	1.690332
1	-0.277223	2.359724	2.720298
6	-0.233117	4.349926	0.210434
6	-0.125764	3.464770	-0.865608
6	-0.075220	2.086511	-0.548870
6	-0.177581	5.406856	-1.717026
1	-0.184954	6.248167	-2.399534
6	-0.328311	6.870268	0.369291
1	-0.609717	7.643298	-0.353880
1	-1.126280	6.788998	1.114906
6	1.004158	7.198277	1.047142
1	1.807400	7.278826	0.304618
1	0.925396	8.151429	1.584782
1	1.260371	6.410707	1.763608

Dimer Figure 5b

7	2.989081	0.169778	2.808869
7	4.830603	-0.119997	1.271690
7	0.759539	0.220322	2.167792
1	0.546809	0.349067	3.147515
1	-0.007333	0.182439	1.489579
7	1.846732	-0.189847	-0.716791
7	4.071221	-0.362055	-1.032393
6	4.285349	0.055552	2.481606
1	4.982701	0.115197	3.314471
6	3.885590	-0.180912	0.321655
6	2.501132	-0.079367	0.498684
6	2.056968	0.105680	1.831048
6	2.817238	-0.352149	-1.591392
1	2.682957	-0.476891	-2.659148
6	5.359242	-0.471431	-1.711770
1	5.165143	-0.878839	-2.709870
1	5.963274	-1.194920	-1.154543
6	6.077381	0.877794	-1.787344
1	5.474557	1.608320	-2.340551
1	7.041305	0.759240	-2.297621
1	6.259041	1.258629	-0.776883
7	-2.989081	-0.169778	-2.808869
7	-4.830603	0.119997	-1.271690
7	-0.759539	-0.220322	-2.167792
1	-0.546809	-0.349067	-3.147515
1	0.007333	-0.182439	-1.489579
7	-1.846732	0.189847	0.716791
7	-4.071221	0.362055	1.032393
6	-4.285349	-0.055552	-2.481606
1	-4.982701	-0.115197	-3.314471
6	-3.885590	0.180912	-0.321655
6	-2.501132	0.079367	-0.498684
6	-2.056968	-0.105680	-1.831048
6	-2.817238	0.352149	1.591392
1	-2.682957	0.476891	2.659148
6	-5.359242	0.471431	1.711770
1	-5.165143	0.878839	2.709870

1	-5.963274	1.194920	1.154543
6	-6.077381	-0.877794	1.787344
1	-5.474557	-1.608320	2.340551
1	-7.041305	-0.759240	2.297621
1	-6.259041	-1.258629	0.776883
Trimer Fig 5c			
7	0.803107	-3.120473	-0.336933
7	2.885260	-4.343297	-0.280882
7	0.667974	-0.797869	-0.356528
1	-0.356728	-0.864114	-0.394103
1	1.084952	0.130640	-0.240410
7	3.763911	-0.865130	-0.263498
7	4.818546	-2.854570	-0.233427
6	1.554936	-4.233838	-0.319239
1	0.998871	-5.169847	-0.335117
6	3.468803	-3.131646	-0.262398
6	2.832625	-1.889403	-0.280912
6	1.412021	-1.903588	-0.323708
6	4.924896	-1.485463	-0.230092
1	5.894131	-1.001616	-0.207501
6	5.892025	-3.839887	-0.150359
1	6.819963	-3.331568	-0.433570
1	5.681831	-4.616368	-0.892913
6	5.993868	-4.451983	1.247728
1	6.206653	-3.678751	1.995765
1	6.800174	-5.194214	1.270930
1	5.052305	-4.948006	1.505652
7	-2.296313	-0.883155	-0.347662
7	-4.376209	0.342153	-0.354956
7	-2.114537	-3.125525	0.270872
1	-1.112075	-3.137256	0.025879
1	-2.574689	-3.980799	0.547543
7	-5.150739	-2.993018	0.734429
7	-6.248599	-1.049523	0.376501
6	-3.062497	0.204287	-0.538407
1	-2.532856	1.085564	-0.896156
6	-4.927783	-0.807759	0.074545
6	-4.268948	-2.018944	0.307841
6	-2.872706	-2.034169	0.076782
6	-6.311508	-2.374555	0.756434
1	-7.254273	-2.821972	1.047380
6	-7.351252	-0.102637	0.227099
1	-8.196925	-0.499180	0.799140
1	-7.040202	0.843280	0.683828
6	-7.720639	0.109846	-1.243644
1	-8.028170	-0.835972	-1.704301
1	-8.548350	0.826414	-1.323213
1	-6.858656	0.506273	-1.790705
7	3.968167	4.440732	-0.191073
7	1.882878	5.552267	0.331203
7	4.180581	2.137655	-0.432280
1	5.165007	2.302509	-0.597575
1	3.836268	1.174955	-0.371478

7	1.142149	2.050628	0.154595
7	0.037131	3.969521	0.566125
6	3.194006	5.509616	0.060415
1	3.706818	6.468785	0.040645
6	1.349519	4.321092	0.327863
6	2.017543	3.117131	0.079704
6	3.405413	3.211629	-0.183991
6	-0.017838	2.602079	0.442487
1	-0.946539	2.062409	0.582960
6	-1.066623	4.890627	0.821634
1	-1.898012	4.295967	1.216827
1	-0.740096	5.589396	1.599241
6	-1.474837	5.649539	-0.443693
1	-1.799026	4.952171	-1.225677
1	-2.303275	6.332194	-0.218435
1	-0.626397	6.234498	-0.816571

Dimer Fig. 5d

7	5.07253183	-2.32038103	-0.53432574
7	3.47257475	-0.58335477	-0.03751648
7	7.37258485	-1.99002099	-0.50412506
1	7.49448851	-2.97157220	-0.70777179
1	8.17735237	-1.41615354	-0.29900430
7	6.72436262	0.89346179	0.32019771
7	4.56798211	1.54375319	0.53646132
6	3.83702587	-1.82744647	-0.37784283
1	3.02657889	-2.53142540	-0.55011237
6	4.53652280	0.21695880	0.16213015
6	5.87892492	-0.16204374	0.03614550
6	6.12310577	-1.50139731	-0.33355554
6	5.90611267	1.87955107	0.60748687
1	6.21295980	2.87965475	0.88831944
6	3.42668187	2.43750589	0.74928255
1	3.75324885	3.21352637	1.44919079
1	2.64310542	1.85677597	1.24333580

6	2.90433383	3.05417913	-0.54989654
1	3.67856246	3.65326637	-1.04239787
1	2.04942291	3.70440219	-0.33341060
1	2.57005526	2.27552897	-1.24207889
53	0.52134216	-0.31875066	0.02752555
9	-1.54376662	2.13467265	-0.42676486
9	-1.80183973	-2.52658129	0.46403430
6	-1.58241817	-0.20223205	0.01768034
6	-2.24399806	1.00480765	-0.21033623
6	-2.37306451	-1.33079426	0.23521389
53	-6.50553703	0.06072417	-0.03037788
9	-4.46616385	-2.38321263	0.44507136
9	-4.20991909	2.27589752	-0.45372933
6	-4.42022668	-0.04998052	-0.00772715
6	-3.76414439	-1.25967130	0.22447396
6	-3.63452309	1.08318477	-0.22448560