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Supporting Information

Quantum Mechanical and Experimental Validation that Cyclobis(paraquat-*p*-phenylene) Forms a 1:1 Inclusion Complex with Tetrathiafulvalene

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Marco Frasconi,^[a] Nema Hafezi,^[a] Sanjeev K. Dey,^[a] Amy A. Sarjeant,^[a] Charlotte L. Stern,^[a]
William A. Goddard, III,^{*,[b]} and J. Fraser Stoddart^{*,[a]}

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π - π Charge-Transfer Interactions: Comparisons of Theoretical Calculations with Experiment

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Supporting Information

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S1. Single Crystal X-Ray Crystallography

A single crystal of **Rt**•4PF₆ was grown from a mixture of *trans* and *cis* isomers in MeCN by vapour diffusion of diisopropyl ether at room temperature.

Crystal data for Rt •4PF₆: C₄₀H₅₆O₆S₄, P₄F₂₄, C₆H₁₄O, C₃₆H₃₂N₄, 3(C₂H₃N), green plate, *Mr* = 2086.96, crystal size 0.215 × 0.167 × 0.016 mm, triclinic, space group $P\bar{1}$, *a* = 11.2281(4), *b* = 13.1328(5), *c* = 19.9925(9) Å, α = 77.125(3), β = 85.321(3), γ = 65.056(3)°, *V* = 2605.57(18) Å³, *Z* = 1, ρ_{calc} = 1.330, *T* = 100(2) K, $R_1(F^2 > 2\sigma F^2)$ = 0.0851, wR_2 = 0.2094. Out of 17405 reflections a total of 8480 were unique. Crystallographic data (excluding structure factors) for the structures reported in this communication have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC–960538.

S2. Coordinates of TTF ⊂ CBPQT⁴⁺ Inclusion and Side-On Complexes

The geometries of TTF ⊂ CBPQT⁴⁺ complexes were optimised at the level of M06-2X/6-311G** with PCM model for MeCN (r_{probe} = 2.19 Å, $\epsilon_{optical}$ = 1.81 and ϵ_{static} = 37.5), as provided by the manual of Jaguar 7.9.^[1] M06-2X functional is recommended for applications involving main group elements.^[2] For TD-DFT calculations, a dense grid NRAD=125 was used to describe S atoms. Both geometry optimization and TD-DFT were carried out with GAMESS.

S2.1 TTF ⊂ CBPQT⁴⁺ Inclusion Complex-2CH₃CN

M06-2X/6-311G** in PCM: -3698.3894603666

M06-2X/6-311G(2df,p) in PCM: -3698.5435122102

H	0.1871455803	6.3297678835	0.5683544941
H	-0.8111526726	6.0410262299	2.0038433506
H	-0.5113302940	4.2355699283	3.2759593960
C	0.2185261216	3.7962720323	2.6117038507
H	4.3353096346	1.3233397983	1.1008091104
H	5.2964729846	-0.9404771302	1.3955053919
H	0.7322030052	2.1523352130	3.8494833300
N	0.4369873340	4.4540282429	1.4564588691
H	5.2671375120	-2.9875706001	2.2723630856
C	0.9110001822	2.6410736754	2.9016462866
C	3.7739731325	0.5774304697	1.6475514348
C	4.3268538812	-0.6770272041	1.7964870162
H	4.0364683187	-3.4563671002	3.4584660814
C	1.3466888165	4.0154465415	0.5714356093
C	1.8367360757	2.1415587539	1.9804778860
C	2.0654728536	2.8644533729	0.8095030357
C	2.5221083632	0.8496062673	2.2054348264
H	1.4891263033	4.5914201276	-0.3331277299
H	2.7683468730	2.5524883471	0.0485447741
N	3.6796367457	-1.6383447891	2.4805203603
C	1.8976232980	-0.1543083235	2.9476681597
H	0.9315015795	-0.0078531989	3.4090099175

C 2.4940970418 -1.3899683303 3.0629458380
C -0.4416799669 5.6023413688 1.0788101787
H 2.0271676049 -2.2069223829 3.5964183756
C 4.1978456183 -3.0401987656 2.4652720807
C -1.5499699748 5.0802252456 0.1951212096
H -0.4323887087 5.3338716519 -1.6339761167
C 3.4602569047 -3.8052054024 1.3923705682
H -2.9485476668 4.7848304150 1.8054931977
H 4.8955612284 -3.3667015729 -0.1520287026
H 1.8969089667 -4.4885982793 2.7117144135
C -1.3369127007 4.9467813292 -1.1768677480
C -2.7511955398 4.6407728198 0.7484645726
C 3.9307270250 -3.8053725318 0.0800939334
C 2.2527265047 -4.4348486250 1.6882977700
C -2.2843187823 4.3170781377 -1.9719573658
C -3.7019466613 4.0085144242 -0.0502088920
C 3.1630327429 -4.3620577647 -0.9391620789
C 1.4890416586 -4.9938511748 0.6723184620
H -2.1038318739 4.2222793639 -3.0369631820
H -4.6342849206 3.6666838314 0.3860032153
H 3.5361727616 -4.3528397450 -1.9583879107
C -3.4551779534 3.8124464425 -1.4077741514
H 0.5517233035 -5.4789957796 0.9210574648
C 1.9213801833 -4.9264764253 -0.6509937482
C -4.3866691099 2.9716358973 -2.2509037943
H -2.8157881227 2.0869989265 -4.1210604273
C 0.9990288951 -5.3669472710 -1.7634982761
C -2.9184660150 1.3411936899 -3.3450469819
N -3.7999921873 1.6028046069 -2.3631485690
H -4.4900313941 3.3569737804 -3.2637427661
H 1.2542668406 -3.4629182106 -3.5091533568
C -2.1968680358 0.1683956459 -3.3513051688
H -5.3750992550 2.8687948460 -1.8070519298
C -4.0123907527 0.7102877382 -1.3805124114
H -1.5140471669 0.0087644948 -4.1731000254
C 0.3599947062 -3.2986565474 -2.9223901749
N 0.0375613639 -4.2561071667 -2.0364640420
H -4.7391135625 0.9830493406 -0.6259131935
C -2.3729133694 -0.7669834828 -2.3251060159
C -0.4157894921 -2.1665206071 -3.0580724058
C -3.3270249773 -0.4857421319 -1.3422054795
C -1.5533477342 -2.0002751134 -2.2611069198
H -0.0892729521 -1.4228622641 -3.7721037287
C -1.0633451904 -4.1359130572 -1.2736859887
H -3.5247126256 -1.1525563341 -0.5105884565
H -1.2724891423 -4.9424057268 -0.5857552819

H 1.5344330150 -5.5682367581 -2.6887147659
 C -1.8740902985 -3.0257931306 -1.3634195734
 H 0.4157276845 -6.2449296533 -1.4934224557
 H -2.7406953446 -2.9883640182 -0.7172332133
 H 3.5787031862 -1.4496424267 -1.8324646407
 S -1.4341057416 1.6150729535 0.4049373051
 C 2.7005626465 -0.8549539888 -1.6230714407
 S 1.5772675745 -1.4771682443 -0.4197145530
 C 0.5193201537 -0.0681410231 -0.4954374909
 C -0.5137909854 0.1119114384 0.3548502318
 H -3.2315398048 1.7793241575 2.0707995568
 H 3.0172835469 0.7862318453 -2.9624809441
 C 2.4098640189 0.3041613013 -2.2085612414
 C -2.4876368506 1.0818315577 1.7082164789
 S 0.9096133040 1.0978757870 -1.7593508668
 S -1.0643815531 -1.1453896655 1.4637332297
 C -2.3198265578 -0.1505149599 2.1810022157
 H -2.9167516515 -0.5971611747 2.9633151718
 N 2.8019911862 3.7465086350 -2.2025151959
 C 3.0535317028 4.1047538786 -3.2652958306
 N -4.1485032381 -2.6677285625 1.1012704183
 C -4.6815224096 -3.2636449133 1.9262299702
 C -5.3556874886 -4.0192728007 2.9714636859
 H -5.7764401359 -4.9295038360 2.5449976370
 H -4.6405303289 -4.2793338602 3.7509230475
 H -6.1551902242 -3.4146610264 3.3976704365
 C 3.3755848596 4.5634125325 -4.6090546117
 H 4.4556239579 4.5438224601 -4.7506434609
 H 2.9016676755 3.9107116639 -5.3412141984
 H 3.0132777430 5.5828247092 -4.7397579097

S2.2 TTF ⊂ CBPQT⁴⁺ Side-On Complex-2CH₃CN

M06-2X/6-311G** in PCM: -3698.3728296208

M06-2X/6-311G(2df,p) in PCM: -3698.5270797703

H 4.7881912934 6.2760816213 -4.2475270293
 H 3.7325023914 5.9325979502 -2.8656153302
 H 3.6930184754 3.7848604613 -1.9322471651
 C 4.6023451756 3.5222059762 -2.4567842056
 H 8.5250634636 0.9748156696 -4.4257530026
 H 9.4109641447 -1.3035227111 -4.2376358413
 H 4.9012790078 1.7119733703 -1.4273333817
 N 5.0171976786 4.3751151490 -3.4117549238
 H 9.7046375036 -3.2282446847 -2.9389558057
 C 5.2886310637 2.3580404120 -2.2013919532
 C 8.1339894146 0.3329166499 -3.6496507161
 C 8.6559973041 -0.9371394178 -3.5545795308

H 8.5221619630 -3.6402607952 -1.6848484512
C 6.1514258400 4.1363051476 -4.0922239288
C 6.4250026460 2.0326639572 -2.9529195951
C 6.8681011782 2.9757829757 -3.8895089553
C 7.1013978899 0.7305795624 -2.7908498535
H 6.4562139650 4.8867224765 -4.8106304323
H 7.7615525029 2.8360851927 -4.4805028673
N 8.2017704090 -1.8051065109 -2.6323598407
C 6.7092341257 -0.1718394716 -1.7935938533
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C 4.1465268440 5.5286160127 -3.7875912531
H 7.0264188113 -2.1470010250 -0.9654016187
C 8.6461507851 -3.2288275032 -2.6849141021
C 3.0824411757 5.0343869643 -4.7344768991
H 4.3043613363 5.2906435944 -6.4948511134
C 7.8119581985 -3.9442831369 -3.7179740073
H 1.6043820871 4.7410584846 -3.1971338152
H 9.2725151115 -3.7260336705 -5.2839691198
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C 3.3648588714 4.9217835520 -6.0965695179
C 1.8476513788 4.6195988718 -4.2471753118
C 8.2717043471 -4.0543125567 -5.0254984249
C 6.5407408624 -4.4166730693 -3.3884488023
H 11.9517854480 0.0907140644 -1.8187983506
S 7.5758482354 4.5296881872 -0.8013893368
C 11.2294328709 0.8948038179 -1.8344156757
S 9.8935156879 0.7845054068 -0.6998270913
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H 7.8150008212 -4.6636737019 -7.0299202598
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H 4.7276997650 -5.3015109516 -4.1063170799
C 6.1607691915 -5.0046179383 -5.6949099381
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H 1.6826592956 2.0829638856 -9.2966494880
C 5.2185935529 -5.4371033397 -6.7906380459
C 1.5779296239 1.3611409922 -8.4983045984
N 0.8020859844 1.7116776911 -7.4567975065
H 0.2505517182 3.5127482221 -8.3650973830
H 5.8364970433 -3.3264864258 -8.1070576862
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H -0.7266942371 3.0542895777 -6.9604751874
C 0.5961329699 0.8704008099 -6.4297471442
H 2.7995122062 -0.1228915485 -9.3871574287
C 4.8180807340 -3.2357766434 -7.7559823479
N 4.3092428558 -4.2890725652 -7.0952381150
H -0.0393539150 1.2230119475 -5.6283782642
C 2.0365553920 -0.7453455363 -7.4495234280
C 4.0753285369 -2.0900415947 -7.9275958234
C 1.1956908792 -0.3697458650 -6.4028598625
C 2.7935506966 -2.0168092987 -7.3850823186
H 4.5387676254 -1.2570870105 -8.4385918968
C 3.0520982828 -4.2719512793 -6.6129529295
H 1.0371783230 -0.9968405062 -5.5361579763
H 2.7024060015 -5.1883161161 -6.1592773016
H 5.7492694761 -5.6786372675 -7.7090102677
C 2.2706141898 -3.1421581414 -6.7437928249
H 4.5926298832 -6.2799076968 -6.5034540681
H 1.2594139024 -3.1595626962 -6.3585440772
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N 3.4004904322 1.4800589193 -4.8144972593
C 5.2050851758 1.6307902153 -6.6921396512
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H 3.0988456372 -2.1437149745 -3.9752593949
H 4.2966926081 -2.1954021537 -2.6724586217

2.3 TTF⁻CBPQT⁴⁺ Side-On Complex-2CH₃CN

M06-2X/6-311G** in PCM: -3432.867612915

H 5.0401336287 6.2495420321 -4.5377000485
H 3.9335787278 5.9361578252 -3.1899230495
H 3.9908421071 3.9642100238 -2.0596367560

C 4.8272813452 3.5943232967 -2.6355995233
H 9.0391195619 1.1145273966 -4.0132685248
H 9.9111202230 -1.1812446745 -3.7834578298
H 5.1440010081 1.8561996784 -1.4842346484
N 5.2144813338 4.3567721000 -3.6747155232
H 9.7667012645 -3.2593594052 -3.1014437474
C 5.4881214449 2.4247828937 -2.3374796638
C 8.4479490208 0.3838816887 -3.4770233003
C 8.9556684515 -0.8932690778 -3.3687742166
H 8.6921600108 -3.6616673232 -1.7515239956
C 6.2860183316 4.0159942810 -4.4150152742
C 6.5669073224 2.0065059331 -3.1245087390
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H 7.8044204912 2.6149236291 -4.8160270833
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C 6.5570577091 -0.3121953472 -2.1838092736
H 5.5953208421 -0.1573951945 -1.7158715801
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C 3.3332754799 5.0259211502 -5.0732991221
H 4.4620200925 5.5994279478 -6.8158198007
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H 8.6399492677 -3.1320308659 -5.4864691466
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C 3.5760057731 5.0977860737 -6.4423124296
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 C 1.2745123476 3.8479695289 -5.5072589523
 C 6.9450545392 -4.3620182970 -5.9229682843
 C 5.9281143384 -5.4845476487 -4.0469250572
 H 2.8779882210 4.5900212784 -8.4063534684
 H 0.3730757302 3.3750282043 -5.1336373601
 H 6.9854171721 -4.1561363455 -6.9873735725
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 H 5.1760037298 -6.1536304860 -3.6435334083
 C 5.9463144989 -5.1907621526 -5.4057246401
 C 0.6498929403 3.1243679996 -7.8329570029
 H 2.5680445860 2.0392291673 -9.1820692640
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 N 1.0436438541 1.6823249959 -7.8226244067
 H 0.7512972999 3.4785941508 -8.8574817135
 H 4.4417827845 -4.6852937988 -8.6942922567
 C 2.6179569947 0.0199367629 -8.4164638480
 H -0.4000305087 3.1690260664 -7.5496550220
 C 0.4049553743 0.8238297576 -7.0082576374
 H 3.5080852130 -0.2448365392 -8.9710798638
 C 3.9318941665 -4.0817748977 -7.9559124625
 N 3.9812963743 -4.5149003884 -6.6850557357
 H -0.4606557207 1.2056934698 -6.4863875801
 C 2.0127297768 -0.8717554509 -7.5296034761
 C 3.2539537274 -2.9215698650 -8.2756528523
 C 0.8680466165 -0.4645810563 -6.8463858251
 C 2.6276340508 -2.1941791465 -7.2662079778
 H 3.2355085234 -2.5991984757 -9.3083678577
 C 3.3367615890 -3.8595461268 -5.7015510555
 H 0.3370083046 -1.1252891117 -6.1749244991
 H 3.4236545990 -4.2705851972 -4.7038036572
 H 5.2167324413 -6.1065360991 -7.2389261826
 C 2.6470184132 -2.6998723811 -5.9642732636
 H 4.2010180740 -6.4099420948 -5.8168811682
 H 2.1826494232 -2.1724919092 -5.1425121217

S2.4 TTF ⊂ CBPQT⁴⁺ Inclusion Complex-2CH₃CN

M06-2X/6-311G** in PCM: -3432.8937621033

H 5.1978338015 6.3488790130 -4.3384621221
 H 4.1795386747 6.0702549025 -2.9163618479
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