

Supplementary information

Enhancing the Output Current of a CdTe Solar Cell *via* a CN-free Hydrocarbon Luminescent Down-Shifting Fluorophore with Intramolecular Energy Transfer and Restricted Internal Rotation Characteristics

Yilin Li^{a,§}, Joseph Olsen^{a,§} and Wen-Ji Dong^{a,b,*}

^a Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA 99164, United States;

^b Department of Integrative Physiology and Neuroscience, Washington State University, Pullman, WA 99164, United States.

§ These authors contributed equally.

* Corresponding author: Wen-Ji Dong, wdong@vetmed.wsu.edu.

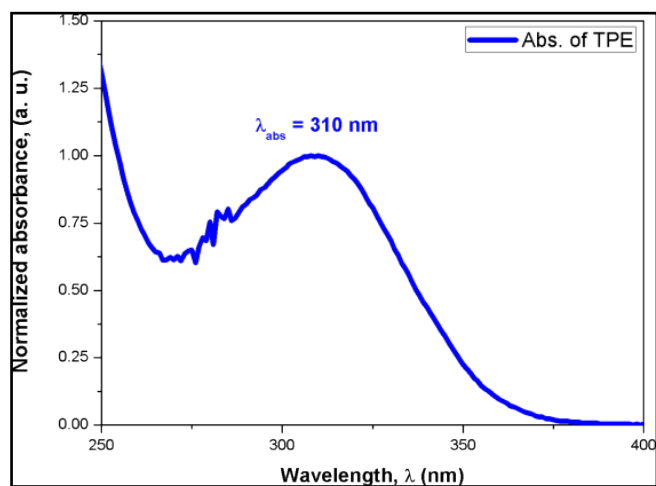


Figure S1. Absorption spectrum of TPE in THF.

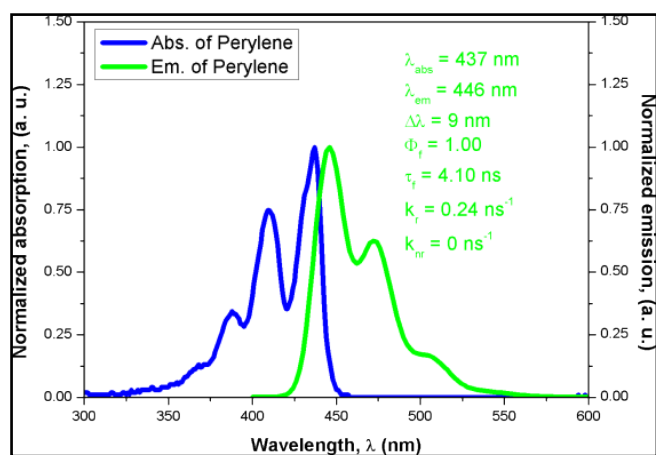


Figure S2. Absorption and emission spectra, and photophysical parameters of Perylene in THF

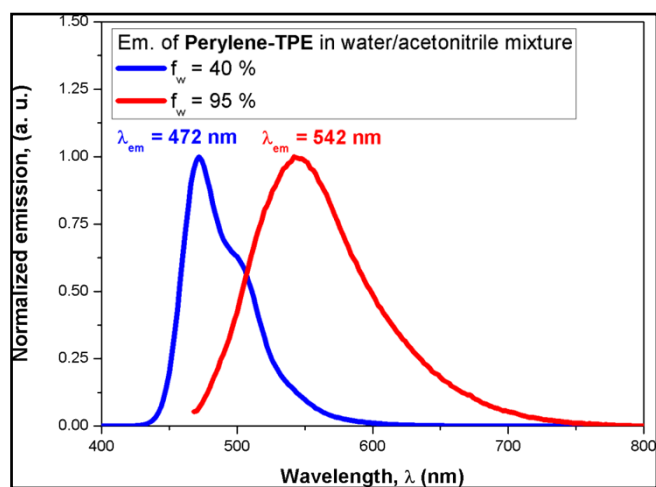


Figure S3. Emission spectra of Perylene-TPE in water/acetonitrile mixtures.

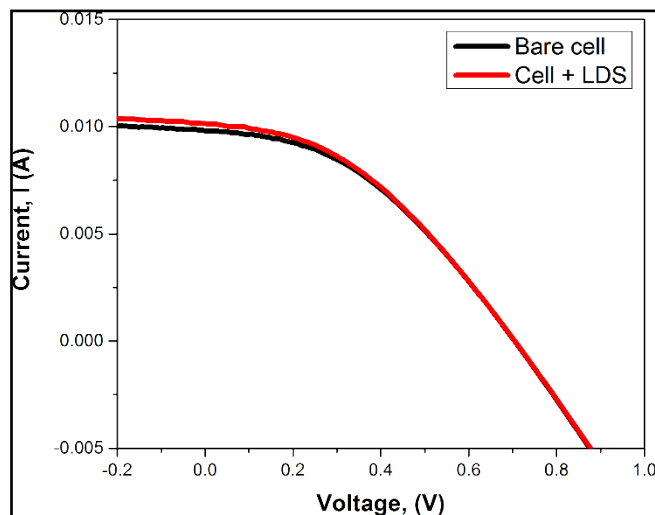


Figure S4. I-V curves for CdTe bare solar cell and CdTe solar cell with LDS film of **Perylene-TPE**.

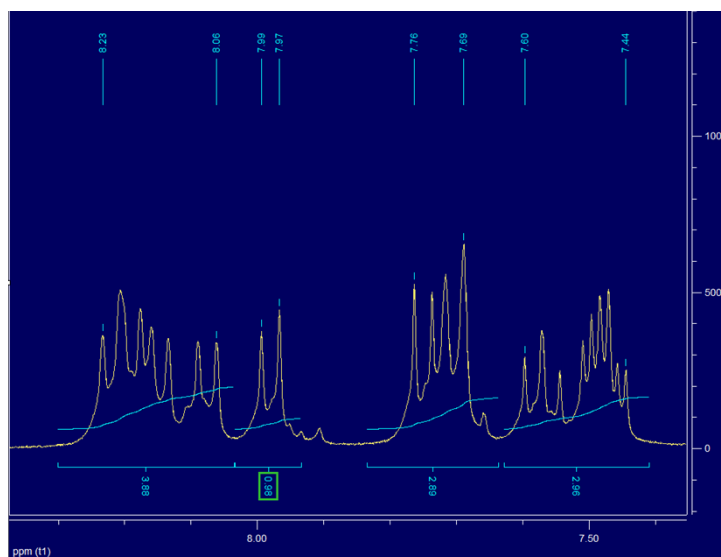
Table S1. Calculated charge distribution (%) on Perylene group and TPE group in **Perylene-TPE** molecule on HOMO and LUMO.

States	Perylene group	TPE group
HOMO	89 %	11 %
LUMO	92 %	8 %

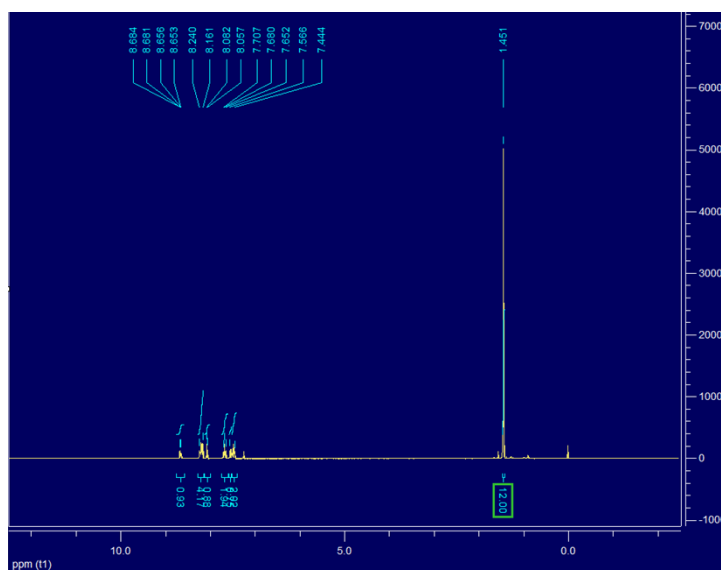
Table S2. Results of I-V measurements.

	I_{sc} (mA)	V_{oc} (mV)	FF	η_{eff} (%)
CdTe solar cell	9.81	704	41.1	5.68
CdTe solar cell + LDS film	10.15	705	40.2	5.75
increase (+) / decrease (-)	+3.42 %	0.12 %	-2.21 %	1.26 %

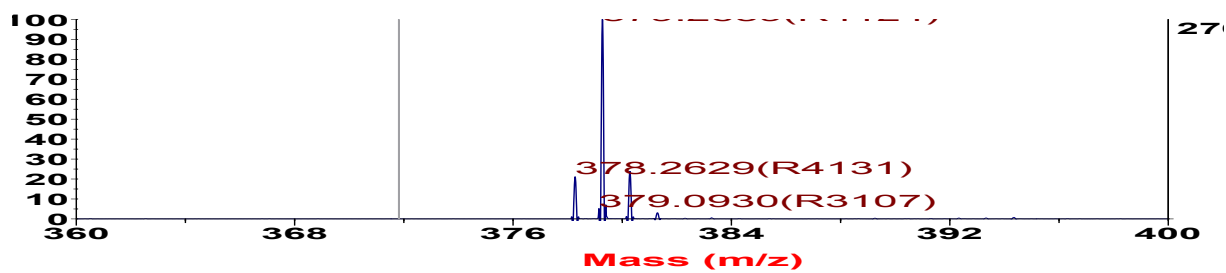
¹H-NMR of Perylene-Br



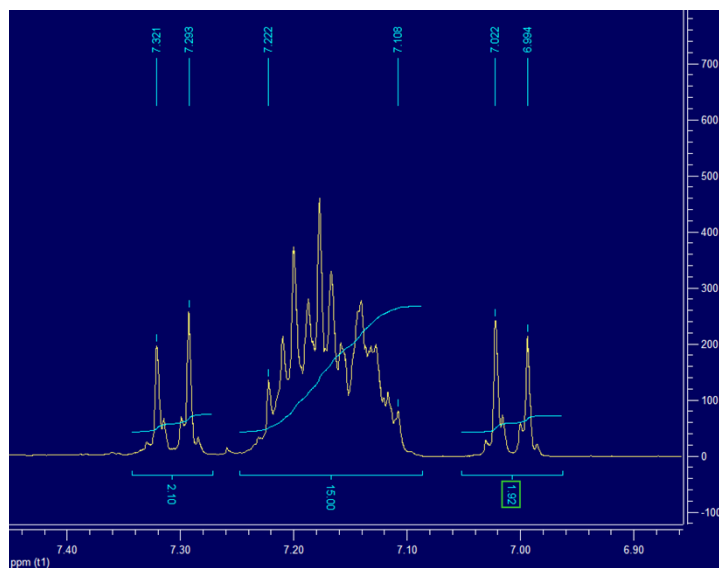
¹H-NMR of Perylene-Bpin



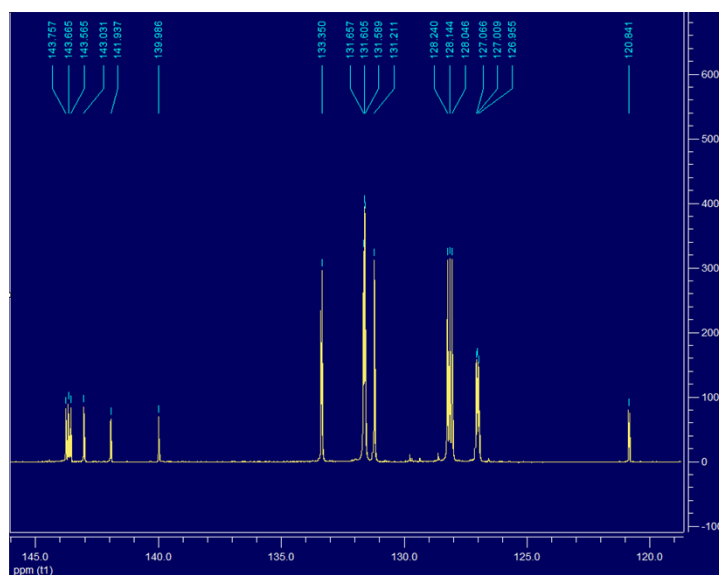
MALDI-MS of Perylene-Bpin



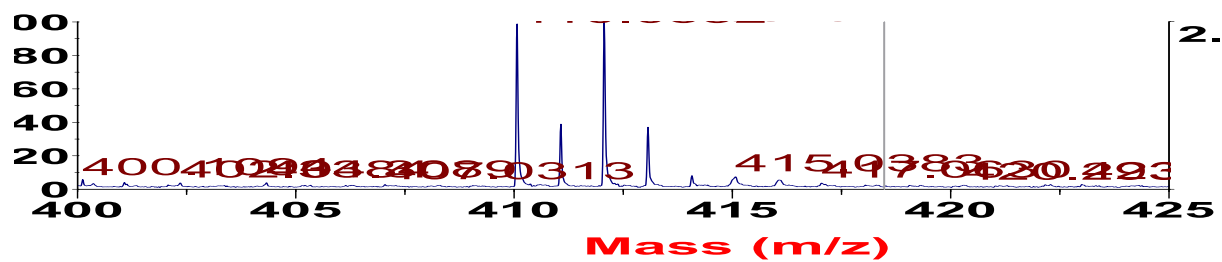
¹H-NMR of TPE-Br



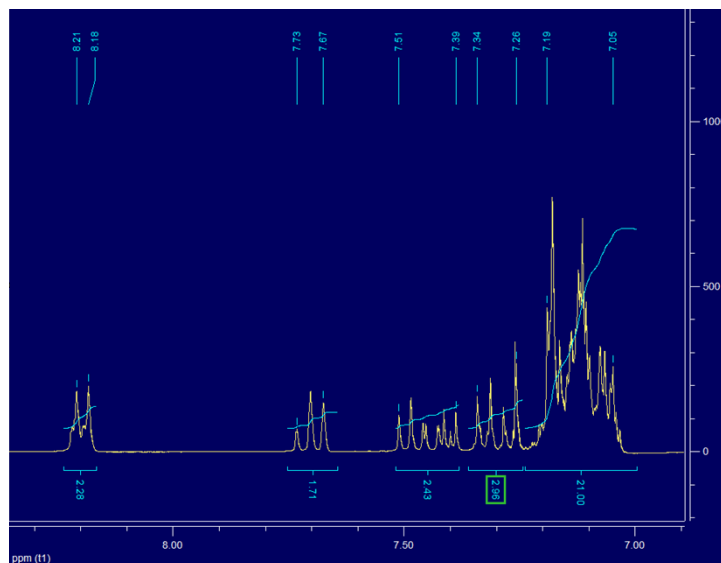
¹³C-NMR of TPE-Br



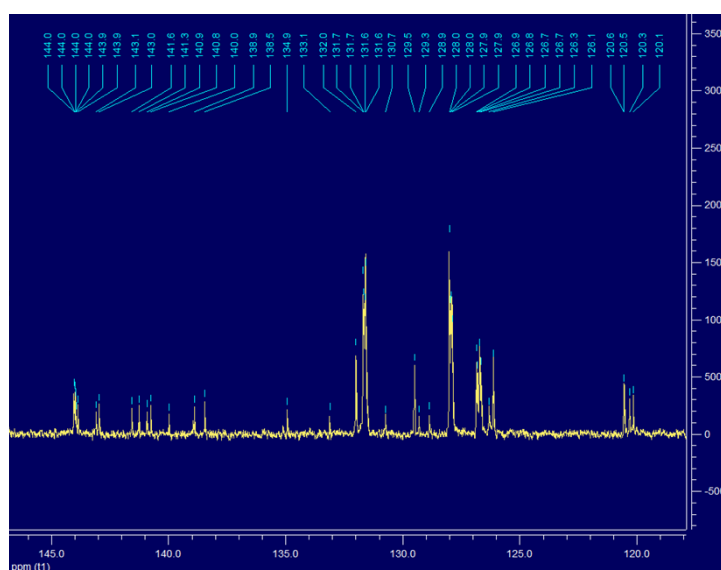
MALDI-MS of TPE-Br



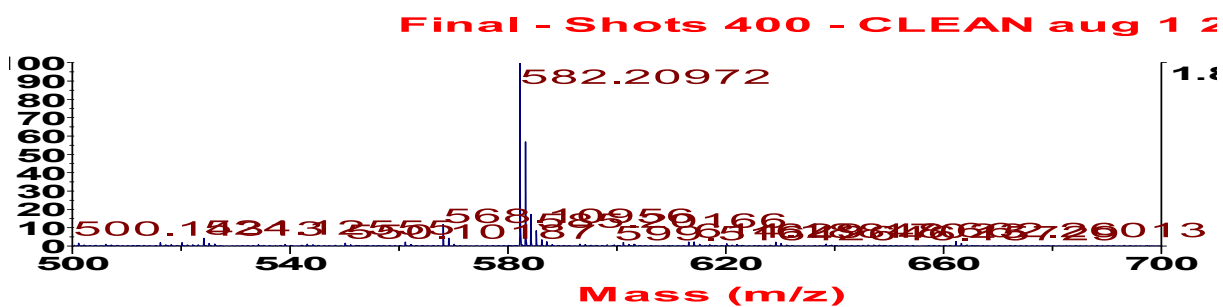
¹H-NMR of Perylene-TPE



¹³C-NMR of Perylene-TPE



MALDI-MS of Perylene-TPE



Optimal geometry of TPE at ground state

```
1\1\GINC-YILIN-SYSTEM-PRODUCT-NAME\FOpt\RB3LYP\6-31G(d)\C26H20\YILIN\0
7-Nov-2014\0\#\# opt b3lyp/6-31g(d)\Title Card Required\0,1\C,0.16046
79913,-0.6290201986,0.038401471\C,0.2362688963,-0.6884017511,1.4289592
901\C,1.1500079683,0.110899881,2.1384486748\C,1.9616741102,0.99629467,
1.4091247468\C,1.877663015,1.0651001046,0.0192535957\C,0.9810594962,0.
2488700965,-0.6730608206\H,-0.5444475791,-1.2659251157,-0.4898750876\H
,-0.414599387,-1.3641544449,1.9767053415\H,2.6608195865,1.6341027954,1
.9408503541\H,2.5121754825,1.7612193802,-0.5232454651\H,0.9171012158,0
.3015278328,-1.7567054619\C,1.2047019468,0.0568031933,3.6318354578\C,2
.3775393993,-0.0539292224,4.3236676303\C,-0.1272488522,0.1334699281,4.
3072074191\C,-1.0660489871,1.1075622562,3.9237979281\C,-0.4998695519,-
0.7933272466,5.2955824171\C,-2.3193007543,1.1736887717,4.5303665762\H,
-0.8042611406,1.8199285787,3.1464346487\C,-1.7577073659,-0.7354089341,
5.8938890384\H,0.2051460846,-1.5636293777,5.5921182855\C,-2.6710616162
,0.2516523585,5.5184616623\H,-3.0241612594,1.9435930764,4.2269742585\H
,-2.0255423812,-1.4660630905,6.6527729754\H,-3.6508782906,0.2975640704
,5.9864381845\C,2.4658353754,0.1523045288,5.8020894551\C,3.1601134346,
-0.7657005849,6.6098296318\C,1.9129613536,1.2891967269,6.4157013231\C,
3.2686798236,-0.5713712036,7.9858345072\H,3.612578055,-1.6402563073,6.
1507862976\C,2.0318314126,1.4904379447,7.7900510528\H,1.3884719894,2.0
180512322,5.8057621833\C,2.7050147721,0.5585050802,8.5823825964\H,3.79
89440704,-1.3012049946,8.5922917804\H,1.600211215,2.3798719059,8.24183
36987\H,2.7959065457,0.714877975,9.6540332708\C,3.6760184794,-0.391010
3931,3.6630115278\C,4.8349056739,0.3528863584,3.947217965\C,3.78931159
78,-1.4871576959,2.7910642661\C,6.0555346949,0.0331126641,3.3549860196
\H,4.7718949127,1.1912583562,4.6353033643\C,5.0124464695,-1.815045255,
2.2080225756\H,2.9091126135,-2.0840070131,2.5734135479\C,6.1498666907,
-1.0532272872,2.4825185168\H,6.9355619733,0.6304372266,3.579449735\H,5
.0769738549,-2.6704061407,1.5404225997\H,7.1028255148,-1.3080861921,2.
0263759397\Version=EM64L-G09RevA.01\State=1-A\HF=-1002.805128\RMSD=3.
292e-09\RMSF=4.835e-06\Dipole=0.0000136,-0.0000097,-0.000068\Quadrupol
e=0.099861,-1.6973171,1.597456,-0.311817,-1.2815866,0.3564629\PG=C01 [
X(C26H20)]\@
```

Optimal geometry of Perylene at ground state

```
1\1\GINC-YILIN-SYSTEM-PRODUCT-NAME\FOpt\RB3LYP\6-31G(d)\C20H12\YILIN\0
7-Nov-2014\0\#\# opt b3lyp/6-31g(d)\Title Card Required\0,1\C,0.04845
37847,0.,0.1413814893\C,0.0491841347,0.,1.5479104541\C,1.2297033975,0.
,2.2846768248\C,2.4768956539,0.,1.5785390021\C,2.4711800068,0.,0.14324
77725\C,1.2358572406,0.,-0.5528422552\C,1.2356330392,0.,3.7613606763\C
,3.7296146973,0.,2.2746936578\C,3.7355438952,0.,3.7512669976\C,2.48845
```

```
59943,0.,4.4574596581\C,4.916176347,0.,4.4878593747\C,4.9042935803,0.,
1.5286434999\C,4.8938192043,0.,0.1222084269\C,3.7008945305,0.,-0.56257
78916\H,3.6819333326,0.,-1.6494969904\H,5.8372687863,0.,-0.4169245752\
H,-0.8993631319,0.,-0.3900411958\H,1.2464579171,0.,-1.6398676484\C,0.0
610687389,0.,4.5075839132\C,0.0716340981,0.,5.9140733855\C,1.264574500
1,0.,6.5987388307\C,2.4942672038,0.,5.8927505039\H,-0.8718844537,0.,6.
4530907508\H,1.2839046209,0.,7.6856440365\C,4.9169972404,0.,5.89433321
13\H,5.8647461181,0.,6.4258720834\C,3.7296104829,0.,6.5886776989\H,3.7
19378829,0.,7.6757140219\H,5.8669769306,0.,2.0269944477\H,5.8748264487
,0.,3.9817932894\H,-0.9095845463,0.,2.0537384628\H,-0.901731275,0.,4.0
094719866\Version=EM64L-G09RevA.01\State=1-A1\HF=-769.4061198\RMSD=4.
537e-09\RMSF=1.411e-05\Dipole=0.0000038,0.,0.\Quadrupole=5.5155843,-10
.8480662,5.3324818,0.,-0.0007353,0.\PG=C02V [SGV(C20H12)]\@
```

Optimal geometry of Perylene-TPE at ground state

```
1\1\GINC-YILIN-SYSTEM-PRODUCT-NAME\FOpt\RB3LYP\6-31G(d)\C46H30\YILIN\1
2-Aug-2014\0\#\ opt b3lyp/6-31g(d)\Title Card Required\0,1\C,1.16891
5031,-1.5963591045,-0.463159052\C,1.1108082219,-1.7636796212,0.9321373
782\C,1.8456375468,-0.9634314289,1.8024096228\C,2.681253003,0.05820464
09,1.2468509308\C,2.7417438825,0.2230759626,-0.1774878335\C,1.96935195
4,-0.6223502464,-1.0133329549\C,1.7919119686,-1.1387679907,3.268407001
3\C,3.4596648958,0.9179191941,2.0869912956\C,3.3866263226,0.7551039529
,3.5512327916\C,2.5732338212,-0.282000987,4.1138466674\C,4.0832612769,
1.5865870966,4.4202189455\C,4.2649308808,1.8818204632,1.4868323863\C,4
.3227219693,2.0390586627,0.0904845884\C,3.5741899925,1.2283733857,-0.7
311795126\H,3.6110246201,1.342894493,-1.8115788627\H,4.9651347185,2.80
69721375,-0.3318908855\H,0.5759966806,-2.2459614851,-1.1013327986\H,2.
0225965666,-0.4866294697,-2.0905895322\C,0.9924034019,-2.1114225593,3.
8591007383\C,0.9229878504,-2.2622763877,5.2525448725\C,1.6675729795,-1
.4536282605,6.0802053126\C,2.5234733501,-0.457527163,5.5421519641\H,0.
2684207496,-3.0197785245,5.6752262904\H,1.5935115439,-1.5613823264,7.1
558035063\C,4.0411553392,1.4105695841,5.8097884173\H,4.6316271042,2.06
74455537,6.4424958601\C,3.3002059909,0.3975235346,6.394191804\H,4.8761
901664,2.5386771279,2.0950750988\H,4.6949367048,2.3940544741,4.0343739
088\H,0.3894635813,-2.7711779073,3.2459865681\H,0.4687243259,-2.546394
1706,1.3192561133\C,3.3393330332,0.2409583494,7.8734545959\C,3.0466909
208,1.3305304543,8.7098203121\C,3.7331239192,-0.9633687642,8.482815287
3\C,3.1223463118,1.2174852282,10.095342727\H,2.7434749946,2.2742749807
,8.264447376\C,3.825255732,-1.0706571414,9.8672978927\H,3.9936598114,-
1.8158801627,7.861677483\C,3.5022352192,0.0109893498,10.7056345879\H,2
.8812576841,2.074457039,10.7165262401\H,4.1540462857,-2.0069007978,10.
3096539144\C,3.6242363778,-0.1085571491,12.1899348684\C,2.6374775603,0
.2975521445,13.0438261097\C,4.910922929,-0.7047674543,12.6637193786\C,
4.9301324903,-1.7545783283,13.5976970757\C,6.1377559695,-0.2627460627,
```


12.1376122341\C,6.1335017808,-2.3272523017,14.0066217545\H,3.991963954
2,-2.1213236074,14.002345897\C,7.342121806,-0.8272948346,12.5545719484
\H,6.1423003182,0.534328319,11.3993152186\C,7.3452781612,-1.8627972592
,13.491435232\H,6.1233855612,-3.1414503704,14.7266407955\H,8.279196871
7,-0.4605782329,12.1435009371\H,8.2832777642,-2.3085386529,13.81170616
87\C,2.8484991356,0.4304186843,14.5178336207\C,3.9470126746,1.13624445
27,15.0373389615\C,1.914041002,-0.1019604832,15.4237597863\C,4.1163463
449,1.2865722243,16.4128386377\H,4.6694334285,1.5707364354,14.35350270
57\C,2.0891945853,0.0376229177,16.7995941629\H,1.0468739145,-0.6331486
168,15.0413496557\C,3.1917048627,0.7331015559,17.3005581473\H,4.971073
5394,1.8413335326,16.7911859882\H,1.3605153495,-0.393609684,17.4812527
174\H,3.3249250424,0.8489484859,18.3729159135\C,1.2594555441,0.6418546
403,12.5769261166\C,0.5368132027,-0.2222882785,11.7367362472\C,0.62813
48245,1.8179462305,13.018952101\C,-0.7615858957,0.0882470621,11.335415
7799\H,1.0004358622,-1.1446705985,11.400881433\C,-0.6657060784,2.13494
81126,12.6083090494\H,1.1621378835,2.4886979043,13.686295681\C,-1.3668
750321,1.2709680527,11.7644753994\H,-1.3029949926,-0.5980798265,10.689
3966481\H,-1.1288040972,3.0562479446,12.9522718157\H,-2.3784018086,1.5
13758934,11.4500125638\\Version=EM64L-G09RevA.01\State=1-A\HF=-1771.01
63184\RMSD=4.963e-09\RMSF=3.900e-06\Dipole=0.0054641,0.0017747,0.15998
47\Quadrupole=-3.0224529,-2.9417629,5.9642157,7.0529903,1.9388596,-0.7
59481\PG=C01 [X(C46H30)]\@