

Electronic Supplementary Information (ESI) for:

Air-stable organic semiconductors based on 6,6'-dithienylindigo and polymers thereof

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(5a_{vat}): A vat of DTI in 2M KOH was prepared by heating DTI powder in KOH solution with added sodium dithionite. Heating at 85 °C for about 30 minutes was necessary to achieve a 1 w% vat.

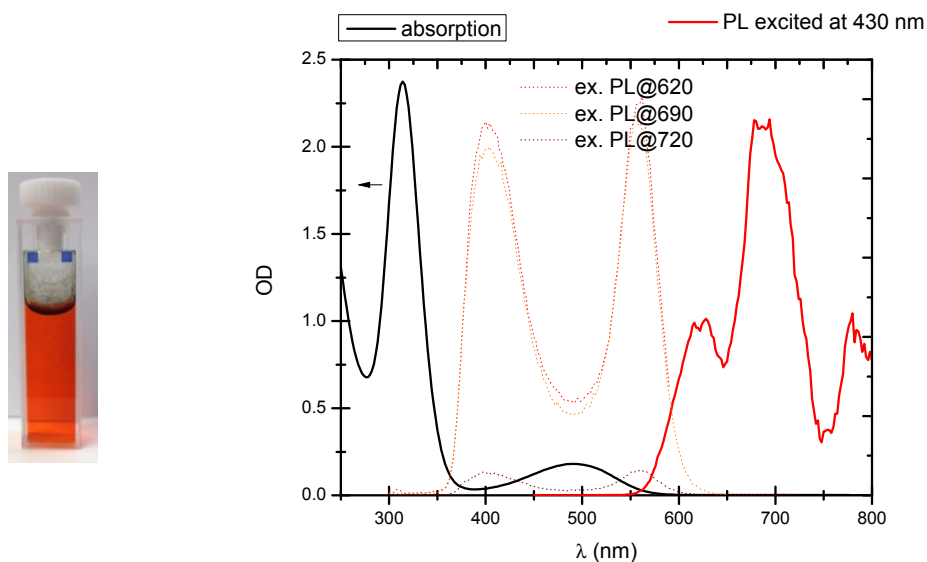


Figure S1: UV-Vis absorption spectra of a vat of DTI (5a_{vat}) together with emission and excitation spectra. The picture of the vat in a cuvette clearly shows the re-oxidized DTI material at the top of the cuvette caused by unavoidable entering of air before capping.

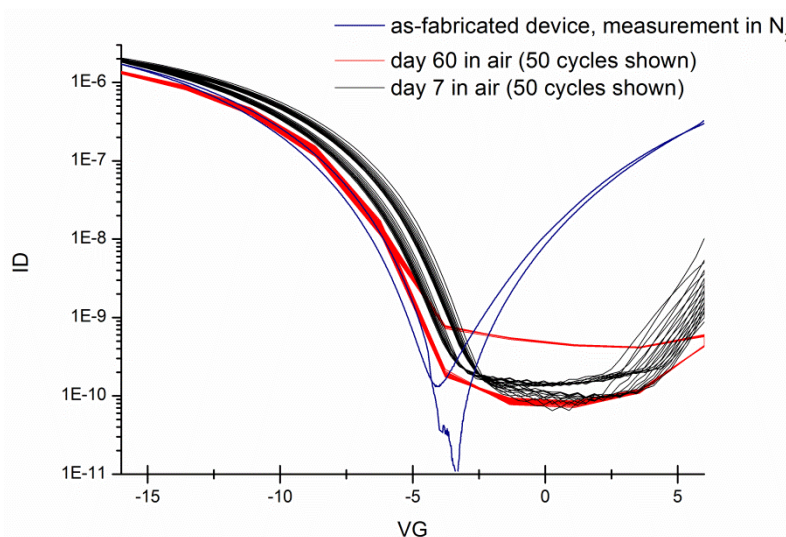


Figure S2. Transfer characteristics of a DTI FET device showing cyclic measurements in air (50 measurements out of 150 shown). $V_{SD} = -8V$ in all measurements.

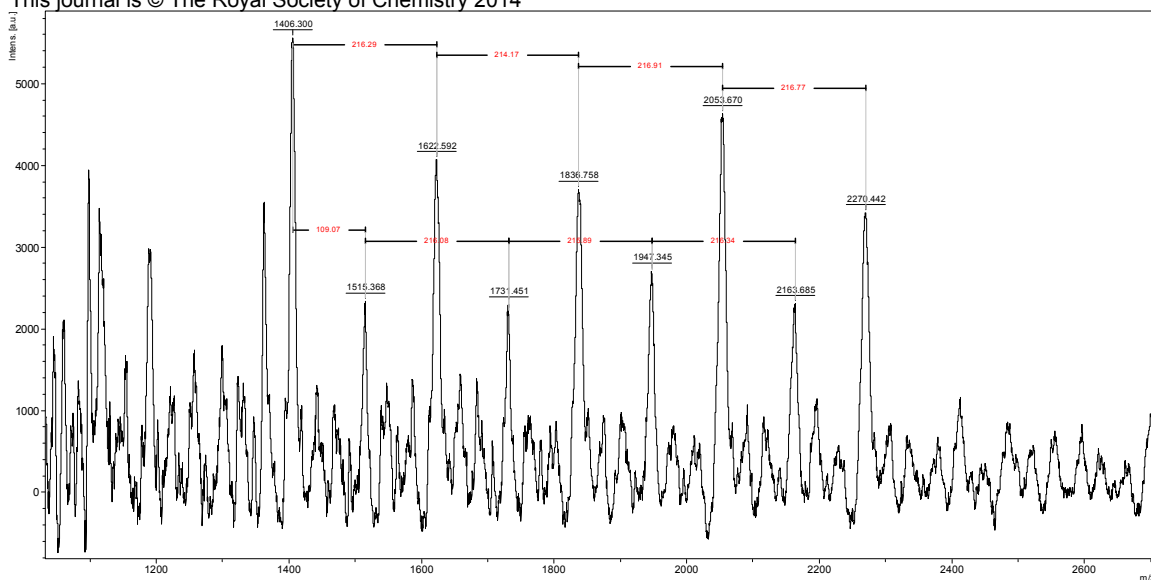


Figure S3. MALDI spectrum of **6a**. The repeating unit clearly visible here is the 6-thienylindole. Various oligomers can be seen, with the largest corresponding to 5 repeating 6,6'-dithienylindole units.

X-ray diffraction

Data collections were performed at the X-ray diffraction beamline (XRD1) of the Elettra Synchrotron, Trieste (Italy) with a monochromatic wavelength of 0.700 Å through the rotating crystal method. Complete datasets were collected at 100 K (nitrogen stream supplied through an Oxford Cryostream 700) Images were acquired using a Pilatus 2M image plate detector. The crystals of compound **5a** were dipped in N-paratone and mounted on the goniometer head with a nylon loop. The unit cell and space group have also been determined at room temperature and no phase change has been detected. The structures were solved by direct methods using SIR2014,^[2S] Fourier analyzed and refined by the full-matrix least-squares based on F^2 implemented in SHELXL-2014.^[3S] The Coot program was used for modeling.^[4S] Anisotropic thermal motion modeling was then applied to atoms with full occupancy. Hydrogen atoms were included (except for disordered water molecules) at calculated positions with isotropic $U_{\text{factors}} = 1.2 U_{\text{eq}}$.

The **5a** molecule shows an inversion center which is located on an inversion center of the triclinic $P2_1/c$ cell. The asymmetric units therefore contains half **5a** molecule only. No disorder and no solvent molecules are present in this crystal form.

Essential crystal and refinement data are reported below.

	5a
Moiety Formula	$\text{C}_{24}\text{H}_{14}\text{N}_2\text{O}_2\text{S}_2$
Empirical Formula	$\text{C}_{24}\text{H}_{14}\text{N}_2\text{O}_2\text{S}_2$
Formula weight (Da)	426.50
Temperature (K)	100(2)
Wavelength (Å)	0.700
Crystal system	Monoclinic
Space Group	$P2_1/c$
a (Å)	6.7320(9)
b (Å)	4.7810(2)
c (Å)	28.098(1)
α (°)	90
β (°)	91.932(9)
γ (°)	90
V (Å ³)	903.84(13)
Z	2
ρ (g·cm ⁻³)	1.567

F(000)	440.0
μ (mm ⁻¹)	0.304
θ min,max (°)	2.9 28.2
Resolution (Å)	0.74
Total refl. collectd	13053
Independent refl.	2875
Obs. Refl. [Fo>4 σ (Fo)]	1988
I/ σ (I) (all data)	16.1
I/ σ (I) (max resltn)	11.8
Completeness (all data)	0.99
Completeness (max resltn)	0.99
Rmerge (all data)	0.070
Rmerge (max resltn,)	0.087
Multiplicity (all data)	5.6
Multiplicity (max resltn)	5.1
Data/restraint/parameters	2252/0/137
Goof	1.066
R[I>2.0 σ (I)], wR2 [I>2.0 σ (I)]	0.0431, 0.1202
R (all data), wR2 (all data)	0.0469, 0.1238

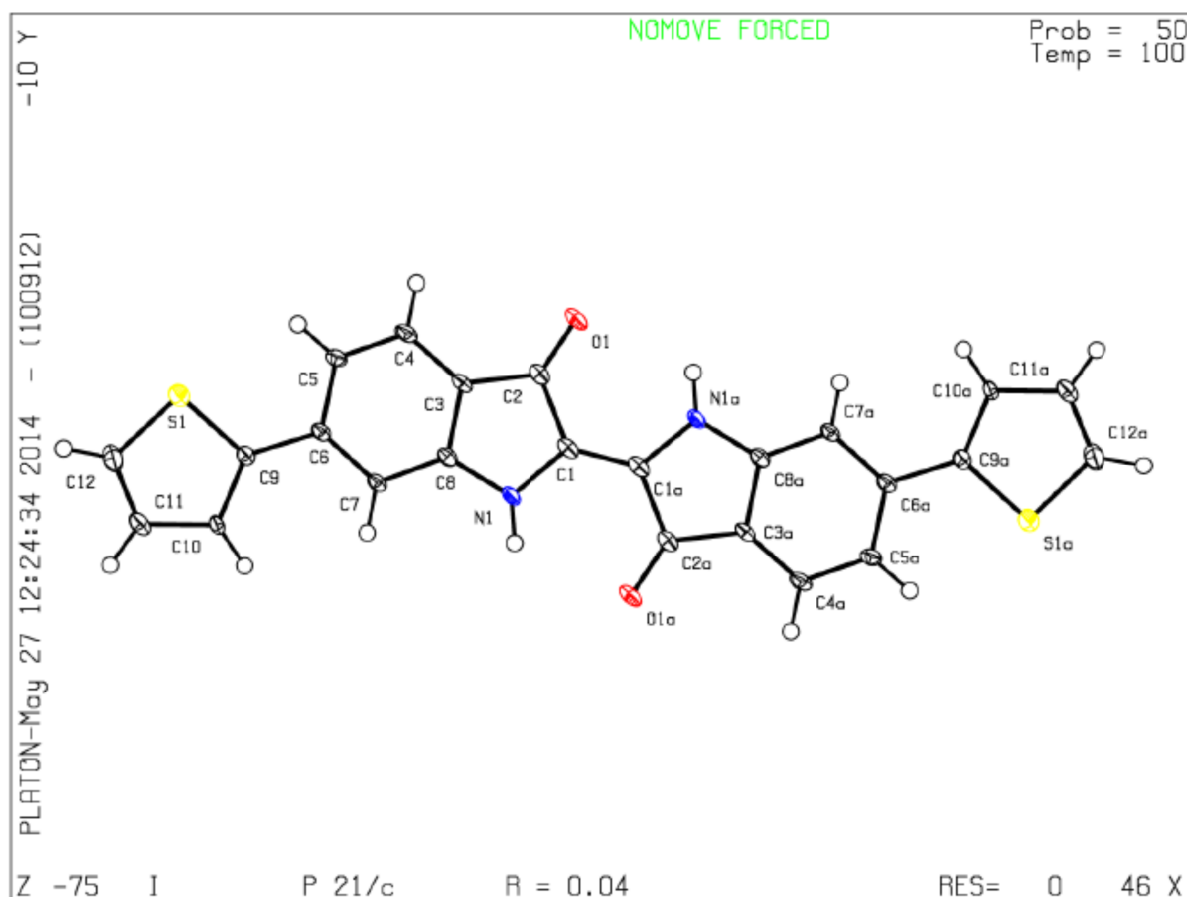


Figure S4. 50% probability ellipsoid structure of **5a**.

Computational details:

Gaussian09 program was used in the calculations.¹ All quantum-chemical calculations have been carried out using density functional theory (DFT) based method with hybrid B3LYP² functional. 6-31G(d,p) basis has been used through the calculations. The obtained geometries were verified to correspond to a real minimum by establishing an absence of imaginary IR

frequencies. Initial coordinates of **4** were taken from the corresponding X-ray molecular structure.³ Initial coordinates of **5b** were obtained by replacing the bromine atom in **4** by a thienyl group. For the cut-out segments of **6a,b**, the optimized core-structures of the substituted and non-substituted indigo-moieties were used, whereas the thienyl-moieties were added from the template set of the GaussView 5 program. To reduce calculation costs, **6b** were optimized in C_2 -symmetry.

xyz-coordinates of the optimized structures of:

- **4:**

O	0.37620100	-2.57371900	-0.78342500
O	-0.37619600	2.57368600	-0.78344400
O	-0.98544600	-1.87759800	1.58591700
O	2.94986600	2.45809200	0.58348700
O	0.98545300	1.87763600	1.58582500
N	-1.78191000	-0.60624000	-0.10969300
N	1.78191900	0.60622000	-0.10974000
C	-5.09775400	0.63320100	-1.33202700
C	-4.73064400	1.94709200	-1.65426100
C	-4.20903200	-0.31166500	-0.81454400
C	-3.41412400	2.34636000	-1.45090600
C	-2.89583000	0.11379300	-0.62199500
C	-2.50422000	1.42390800	-0.93727600
C	3.41412400	-2.34640200	-1.45091500
C	-1.08212400	1.58828800	-0.61592600
C	4.73064000	-1.94713500	-1.65429100
C	1.08213000	-1.58831900	-0.61592500
C	-0.64365600	0.22403300	-0.15661200
C	2.50422300	-1.42394300	-0.93729200
C	5.09775200	-0.63323800	-1.33208500
C	0.64366700	-0.22405900	-0.15662100
C	2.89583500	-0.11382200	-0.62203800
C	4.20903400	0.31163700	-0.81461000
C	-0.90957300	-4.35179500	1.74204400
C	-0.93563300	-3.03404900	2.51950900
C	1.96522800	1.75813800	0.69623800
C	-2.11982900	-2.94366900	3.48519300
C	0.38813000	-2.79971800	3.24846200
C	0.90957700	4.35183900	1.74183600
C	-0.38814100	2.79983400	3.24831300
C	0.93563000	3.03413000	2.51936300
C	2.11981600	2.94379600	3.48506400
H	-5.46744300	2.62951500	-2.06002400
H	-4.52027600	-1.31790700	-0.57973300
H	-3.08576200	3.35362500	-1.68629600
H	3.08576100	-3.35367200	-1.68628500
H	5.46743600	-2.62956400	-2.06005000
H	-1.85634000	-4.53134200	1.23270400
H	-0.10911400	-4.34119400	0.99910800
H	4.52027800	1.31788300	-0.57982000
H	-3.06631100	-3.07355500	2.95945100
H	-0.72817600	-5.17227600	2.44383800
H	0.10912600	4.34120200	0.99889100
H	1.22756200	-2.84001700	2.54915500
H	-2.12509100	-1.97647200	3.99725600
H	-1.22756600	2.84010300	2.54899600
H	-2.03043900	-3.72862700	4.24266400
H	1.85635000	4.53136300	1.23249800
H	0.53466600	-3.57244400	4.00844500
H	0.39212200	-1.82333900	3.74119500
H	0.72817100	5.17235300	2.44358900
H	-0.39214000	1.82347800	3.74109100
H	-0.53468300	3.57259600	4.00825900
H	3.06630400	3.07365500	2.95932600
H	2.12507100	1.97662300	3.99717400
H	2.03041900	3.72879100	4.24249600
Br	-6.90675100	0.10195000	-1.62315300
Br	6.90674600	-0.10198800	-1.62323800
C	-1.96521600	-1.75813500	0.69632000

- **5a:**

C	-0.09633800	2.91482100	-0.01630700
C	1.29726500	2.69308600	0.10339500
C	2.17346600	3.77670000	0.16807200
C	1.65805000	5.06535700	0.12043000
C	0.26433300	5.29197300	-0.00129600
C	-0.62196800	4.20043900	-0.07837300
C	0.15061500	0.66320000	0.00999500
C	1.51929400	1.24436000	0.12686700
H	3.24085500	3.60352300	0.26383500
H	2.32770700	5.91494700	0.20159200
H	-1.68603200	4.36295400	-0.21042300
C	-0.15061500	-0.66320000	-0.00999500
C	-1.51929400	-1.24436000	-0.12686700
C	0.09633800	-2.91482100	0.01630700
C	-1.29726500	-2.69308600	-0.10339500
C	0.62196800	-4.20043900	0.07837300
C	-2.17346600	-3.77670000	-0.16807200
C	-0.26433300	-5.29197300	0.00129600
H	1.68603200	-4.36295400	0.21042300
C	-1.65805000	-5.06535700	-0.12043000
H	-3.24085500	-3.60352300	-0.26383500
H	-2.32770700	-5.91494700	-0.20159200
O	2.55995300	0.58719300	0.21915200
O	-2.55995300	-0.58719300	-0.21915200
N	0.76022900	-1.69755000	0.07238500
H	1.75328600	-1.52531500	0.15866400
N	-0.76022900	1.69755000	-0.07238500
H	-1.75328600	1.52531500	-0.15866400
C	-0.27323400	6.65530900	-0.04351100
C	-1.52699600	7.09378200	0.32443500
S	0.68788200	8.00606300	-0.61934000
C	-1.71741200	8.49328800	0.15343100
H	-2.28122700	6.43400900	0.73720600
C	-0.60880500	9.12066400	-0.34676000
H	-2.63687100	9.01167400	0.39943200
H	-0.47588700	10.16879900	-0.57570200
C	0.27323400	-6.65530900	0.04351100
C	1.52699600	-7.09378200	-0.32443500
S	-0.68788200	-8.00606300	0.61934000
C	1.71741200	-8.49328800	-0.15343100
H	2.28122700	-6.43400900	-0.73720600
C	0.60880500	-9.12066400	0.34676000
H	2.63687100	-9.01167400	-0.39943200
H	0.47588700	-10.16879900	0.57570200

- **5b:**

O	-2.55874600	0.47907200	-0.68325700
O	2.55874600	-0.47907200	-0.68325700
O	-1.44827300	1.53480200	1.68687200
O	1.38538900	-3.57731300	0.67620600
O	1.44827300	-1.53480200	1.68687200
N	0.00358700	1.88250400	-0.01461700
N	-0.00358700	-1.88250400	-0.01461700
C	2.25444800	4.66327800	-1.22165700
C	3.36842700	3.85046300	-1.53877300
C	1.07885500	4.08252900	-0.70052500
C	3.32754500	2.47779900	-1.34138500
C	1.04840600	2.70539000	-0.52479000
C	2.15988300	1.90647100	-0.83671000
C	-3.32754500	-2.47779900	-1.34138500
C	1.85464500	0.51007200	-0.51869500
C	-3.36842700	-3.85046300	-1.53877300
C	-1.85464500	-0.51007200	-0.51869500
C	0.42082300	0.53624800	-0.06320700
C	-2.15988300	-1.90647100	-0.83671000

C	-2.25444800	-4.66327800	-1.22165700
C	-0.42082300	-0.53624800	-0.06320700
C	-1.04840600	-2.70539000	-0.52479000
C	-1.07885500	-4.08252900	-0.70052500
C	-3.81855900	2.24697100	1.84296900
C	-2.55874600	1.85516800	2.61861300
C	1.02766400	-2.42246100	0.78962100
C	-2.09698600	2.95110700	3.58287800
C	-2.75662000	0.52665300	3.35042800
C	3.81855900	-2.24697100	1.84296900
C	2.75662000	-0.52665300	3.35042800
C	2.55874600	-1.85516800	2.61861300
C	2.09698600	-2.95110700	3.58287800
H	4.25634900	4.30524500	-1.96555500
H	0.22808600	4.68740900	-0.42627800
H	4.17543000	1.84425700	-1.58148200
H	-4.17543000	-1.84425700	-1.58148200
H	-4.25634900	-4.30524500	-1.96555500
H	-3.69007600	3.20281700	1.33521600
H	-4.05886500	1.48540500	1.09801100
H	-0.22808600	-4.68740900	-0.42627800
H	-1.92001500	3.88844000	3.05449800
H	-4.65443200	2.33172300	2.54511400
H	4.05886500	-1.48540500	1.09801100
H	-3.06366400	-0.25723400	2.65292300
H	-1.17709200	2.65012200	4.09370800
H	3.06366400	0.25723400	2.65292300
H	-2.86833400	3.11743700	4.34155200
H	3.69007600	-3.20281700	1.33521600
H	-3.53353900	0.63444200	4.11274000
H	-1.83063200	0.21248500	3.84036800
H	4.65443200	-2.33172300	2.54511400
H	1.83063200	-0.21248500	3.84036800
H	3.53353900	-0.63444200	4.11274000
H	1.92001500	-3.88844000	3.05449800
H	1.17709200	-2.65012200	4.09370800
H	2.86833400	-3.11743700	4.34155200
C	-1.02766400	2.42246100	0.78962100
O	-1.38538900	3.57731300	0.67620600
C	-2.29546800	-6.11261300	-1.43510800
C	-1.24017000	-6.98398100	-1.60046500
S	-3.81400200	-6.99134000	-1.50732700
C	-1.63880000	-8.33625000	-1.78825300
H	-0.20679200	-6.65841800	-1.61351300
C	-2.99777500	-8.49654400	-1.76318400
H	-0.94402100	-9.15379600	-1.94144100
H	-3.56934500	-9.40724000	-1.87543400
C	2.29546800	6.11261300	-1.43510800
C	1.24017000	6.98398100	-1.60046500
S	3.81400200	6.99134000	-1.50732700
C	1.63880000	8.33625000	-1.78825300
H	0.20679200	6.65841800	-1.61351300
C	2.99777500	8.49654400	-1.76318400
H	0.94402100	9.15379600	-1.94144100
H	3.56934500	9.40724000	-1.87543400

- Cut-out segment of 6b:

C	-2.90344600	-0.10088800	0.30834200
C	-2.57177100	1.18629000	0.79857500
C	-3.57164100	2.02440700	1.29218900
C	-4.88558500	1.57592500	1.30059800
C	-5.22302900	0.28924900	0.80941600
C	-4.21697500	-0.55571600	0.30005100
C	-0.66052600	0.07952100	0.04926700
C	-1.12323300	1.36006600	0.65575700
H	-3.31339300	3.00833500	1.67117700
H	-5.66517700	2.20799300	1.71238800
H	-4.46793500	-1.52630500	-0.11347800
C	0.62599800	-0.23228300	-0.26456800
C	1.09035600	-1.51735500	-0.86361600
C	2.87123600	-0.05958000	-0.50985600
C	2.53955100	-1.34811500	-0.99613800
C	4.18518500	0.39158000	-0.49070900
C	3.54232400	-2.19197700	-1.47487800
C	5.19497200	-0.45950400	-0.98390800
H	4.43480800	1.36347000	-0.07945100
C	4.85761200	-1.74795500	-1.47129800

H	3.28525200	-3.17738100	-1.85085100
H	5.63968800	-2.38527700	-1.87004800
O	-0.39086600	2.31028900	0.94667400
O	0.35644000	-2.46650200	-1.15383900
N	1.72108800	0.58717200	-0.07937500
H	1.63119100	1.51122900	0.32239900
N	-1.75611400	-0.74136600	-0.13536100
H	-1.66479600	-1.66716300	-0.53276700
C	-6.60908300	-0.17837000	0.82679400
C	-7.07910100	-1.47613700	0.83049400
S	-7.95601400	0.94664400	0.84095400
C	-8.48936000	-1.57690800	0.86292000
H	-6.42262200	-2.33794300	0.85120700
C	-9.13123300	-0.35357800	0.88178000
H	-9.02209700	-2.52030100	0.90130400
C	6.58199700	0.00263200	-0.98619700
C	7.05703200	1.29829700	-0.99070900
S	7.92648000	-1.12711000	-0.97446200
C	8.46805200	1.39436700	-1.00306400
H	6.40405700	2.16244300	-1.02545000
C	9.10685200	0.16909800	-1.00478500
H	9.00426600	2.33591300	-1.03718500
C	10.52258600	-0.11798900	-1.01281100
C	11.16987200	-1.30424000	-1.29290500
S	11.69566000	1.12778800	-0.61769200
C	12.58126600	-1.21688800	-1.21234300
H	10.64219300	-2.20719200	-1.57909700
C	13.04565800	0.03504100	-0.86958300
H	13.24258400	-2.04541900	-1.43777000
C	-10.54752100	-0.07128200	0.91861100
C	-11.18987600	1.10925600	1.23931400
S	-11.72212000	-1.30727300	0.51059400
C	-12.59987100	1.02301700	1.17284200
H	-10.65788300	2.00379100	1.54271800
C	-13.06922300	-0.22155000	0.80433400
H	-13.25733500	1.84510500	1.43000700
C	-14.45549000	-0.66238900	0.65033500
C	-14.79914800	-2.03317200	0.76583700
C	-15.45626900	0.29462500	0.38836400
C	-16.11451700	-2.45601400	0.62815400
H	-14.02345700	-2.75734400	0.99101900
C	-16.77078900	-0.13902000	0.26539200
H	-15.19977000	1.34026400	0.25889100
C	-17.10909800	-1.50972400	0.38040900
H	-16.37805100	-3.50509200	0.71986800
C	-18.55762600	-1.63053400	0.18954500
C	-19.01319100	-0.22939400	-0.04291800
C	14.43168400	0.47662100	-0.69691700
C	15.42777000	-0.44458800	-0.33159200
C	14.80715500	1.82825100	-0.89459400
C	16.74070300	-0.01169900	-0.18894600
H	15.18419300	-1.48437400	-0.13955000
C	16.11505200	2.27959300	-0.74298200
H	14.04646200	2.54291400	-1.19465000
C	17.08932300	1.34512500	-0.38970100
C	17.96804900	-0.73461700	0.17910900
H	16.36320500	3.32333900	-0.90614000
C	19.02758100	0.31283700	0.16545100
C	20.34418100	0.11538700	0.44685900
C	21.40328000	1.16816700	0.43657200
C	22.28669900	-0.90612500	1.01137100
C	22.63021500	0.45125100	0.80688000
C	23.25166600	-1.84354000	1.37815800
C	23.94636800	0.88534100	0.96729100
C	24.56306000	-1.38999000	1.53418700
H	22.99609100	-2.88627000	1.53709700
C	24.91646000	-0.04497400	1.33362100
H	24.19280200	1.93031200	0.80638300
H	25.33173100	-2.10233300	1.81974700
H	25.94789800	0.26457700	1.46552300
C	-20.29650600	0.16366800	-0.26601100
C	-20.74937900	1.56683500	-0.49112400
C	-22.54150800	0.08354800	-0.56117100
C	-22.20207700	1.45303800	-0.67474100
C	-23.86437500	-0.34014600	-0.69016700
C	-23.18418600	2.41342800	-0.91875800
C	-24.83246000	0.63572400	-0.93394200
H	-24.13357700	-1.38806800	-0.60457400
C	-24.50741400	1.99812200	-1.04861600
H	-22.90556400	3.45938300	-1.00269000
H	-25.86917700	0.32842500	-1.03773900
H	-25.29187500	2.72320200	-1.23844300
N	18.44759400	1.51888400	-0.17868000
H	18.98912300	2.37123300	-0.23963900

N	20.92592300	-1.08552200	0.79193100
H	20.38723200	-1.93856800	0.86326700
N	-17.91406000	0.60452900	0.01080900
H	-17.99889100	1.60422900	-0.11870400
N	-21.39786500	-0.66590300	-0.31955900
H	-21.31770700	-1.66579000	-0.18984400
O	18.15047200	-1.92397400	0.44672400
O	21.21258200	2.35599100	0.16748700
O	-19.29502600	-2.61993300	0.20445900
O	-20.00976600	2.55399400	-0.50515400

- **Cut-out segment of 6b:**

O	-2.56785500	-0.42685600	0.58537300
O	2.56785500	0.42685600	0.58537300
O	-1.88914900	0.94579700	2.95437700
O	2.52452800	-2.88987000	1.94733500
O	1.88914900	-0.94579700	2.95437700
N	-0.64237800	1.76965400	1.25403000
N	0.64237800	-1.76965400	1.25403000
C	0.51555400	5.15026200	0.03531500
C	1.84237400	4.76879800	-0.27880700
C	-0.38947700	4.20175400	0.55953900
C	2.27505600	3.46650100	-0.07717300
C	0.05594300	2.89972900	0.74106200
C	1.37470800	2.53037900	0.43054900
C	-2.27505600	-3.46650100	-0.07717300
C	1.56714200	1.11450100	0.75024100
C	-1.84237400	-4.76879800	-0.27880700
C	-1.56714200	-1.11450100	0.75024100
C	0.21139400	0.64805300	1.20594600
C	-1.37470800	-2.53037900	0.43054900
C	-0.51555400	-5.15026200	0.03531500
C	-0.21139400	-0.64805300	1.20594600
C	-0.05594300	-2.89972900	0.74106200
C	0.38947700	-4.20175400	0.55953900
C	-4.36106200	0.80929000	3.11039400
C	-3.04285000	0.86771100	3.88593500
C	1.79558700	-1.92504500	2.05929700
C	-2.98127400	2.05379900	4.85211600
C	-2.77709200	-0.44992800	4.61567300
C	4.36106200	-0.80929000	3.11039400
C	2.77709200	0.44992800	4.61567300
C	3.04285000	-0.86771100	3.88593500
C	2.98127400	-2.05379900	4.85211600
H	2.52079900	5.49871600	-0.70822400
H	-1.39725300	4.47587600	0.83158800
H	3.28891900	3.16210300	-0.31655400
H	-3.28891900	-3.16210300	-0.31655400
H	-2.52079900	-5.49871600	-0.70822400
H	-4.56788000	1.75359200	2.60680500
H	-4.32857500	0.01447300	2.36215700
H	1.39725300	-4.47587600	0.83158800
H	-3.13312900	2.99652600	4.32545400
H	-5.17478800	0.60054000	3.81261900
H	4.32857500	-0.01447300	2.36215700
H	-2.79781600	-1.29024800	3.91664600
H	-2.01419700	2.08234400	5.36370800
H	2.79781600	1.29024800	3.91664600
H	-3.76361200	1.94650500	5.61009000
H	4.56788000	-1.75359200	2.60680500
H	-3.54557200	-0.61408700	5.37644800
H	-1.80030700	-0.43041500	5.10728100
H	5.17478800	-0.60054000	3.81261900
H	1.80030700	0.43041500	5.10728100
H	3.54557200	0.61408700	5.37644800
H	3.13312900	-2.99652600	4.32545400
H	2.01419700	-2.08234400	5.36370800
H	3.76361200	-1.94650500	5.61009000
C	-1.79558700	1.92504500	2.05929700
O	-2.52452800	2.88987000	1.94733500
C	-0.05594300	-6.52101600	-0.18324300
C	1.23865000	-6.98108200	-0.31989900
S	-1.18449100	-7.86042700	-0.30499000
C	1.33248100	-8.37472000	-0.53633500
H	2.10005100	-6.32437000	-0.29985500
C	0.10819100	-9.01537100	-0.56616600
H	2.27111800	-8.89406200	-0.69277100
C	0.05594300	6.52101600	-0.18324300
C	-1.23865000	6.98108200	-0.31989900
S	1.18449100	7.86042700	-0.30499000
C	-1.33248100	8.37472000	-0.53633500
H	-2.10005100	6.32437000	-0.29985500

C	-0.10819100	9.01537100	-0.56616600
H	-2.27111800	8.89406200	-0.69277100
O	-2.47268800	19.06283800	-1.42388600
O	2.59224900	19.80443200	-2.35469000
O	-1.49654700	20.96758000	0.41524000
O	2.80475300	16.93432800	-0.21131200
O	2.28239900	19.07956400	0.35618500
N	-0.51113900	21.32913500	-1.59079100
N	0.82427000	17.87885400	-0.89189300
C	0.42560500	24.25762300	-3.75568600
C	1.69166400	23.80716600	-4.15851400
C	-0.39788300	23.51432600	-2.90476000
C	2.16701500	22.58017300	-3.70492600
C	0.08922100	22.28605700	-2.45936500
C	1.35447200	21.82810600	-2.85703100
C	-2.21555900	15.95065400	-1.34544200
C	1.61371400	20.52907600	-2.22454000
C	-1.78984100	14.63239800	-1.27503300
C	-1.44574000	18.42273400	-1.23330700
C	0.34554800	20.21559100	-1.47874300
C	-1.27194800	16.96898300	-1.21464200
C	-0.42560400	14.31992000	-1.06146300
C	-0.04873600	18.96677900	-1.09886900
C	0.08362400	16.66757000	-1.00670100
C	0.52469700	15.35449500	-0.91885500
C	-3.92077400	20.92429800	0.93351800
C	-2.50981600	21.13841900	1.48655800
C	2.08146600	17.90936000	-0.24303700
C	-2.33094700	22.51855000	2.12437300
C	-2.13042700	20.02669700	2.46618500
C	4.74660700	19.20900000	0.11925500
C	3.36927900	20.83020100	1.47402400
C	3.55446300	19.36792000	1.06581100
C	3.65374600	18.46172600	2.29580400
H	2.29316200	24.41429000	-4.82733500
H	-1.37288200	23.86850400	-2.60415400
H	3.14074200	22.19704100	-3.99335000
H	-3.25823500	16.20217400	-1.51102100
H	-2.50690500	13.82957500	-1.41193000
H	-4.20553800	21.72535000	0.25144900
H	-3.97932200	19.97357600	0.39925700
H	1.56511000	15.14019100	-0.72842300
H	-2.56510400	23.31171200	1.41363300
H	-4.62920100	20.90562500	1.76814000
H	4.58965500	19.79264400	-0.79037600
H	-2.23619300	19.04516500	1.99648800
H	-1.30322800	22.64766800	2.47785200
H	3.27181900	21.46884100	0.59204200
H	-3.00075100	22.61085300	2.98517600
H	4.89774900	18.16567300	-0.15781800
H	-2.78516600	20.06325900	3.34163000
H	-1.09577300	20.14218900	2.80148400
H	5.64859100	19.57267000	0.62216600
H	2.47368900	20.94988700	2.09028900
H	4.23535900	21.16733700	2.05069200
H	3.74549400	17.41484600	2.00490700
H	2.77067900	18.57963800	2.93138900
H	4.53452800	18.74014200	2.88310100
C	-1.54003700	21.70204200	-0.69365600
O	-2.28690700	22.62875200	-0.93174500
C	0.02473400	12.93052000	-0.99330100
C	1.29662000	12.42889900	-1.18592900
S	-1.08633000	11.62210900	-0.62457800
C	1.38441000	11.02374800	-1.06041900
H	2.14150800	13.05503900	-1.44630700
C	0.17873400	10.41662300	-0.76365700
H	2.30210300	10.46608900	-1.20907700
H	0.06340900	25.21496200	-4.11922600
O	-2.59224900	-19.80443200	-2.35469000
O	2.47268800	-19.06283800	-1.42388600
O	-2.28239900	-19.07956400	0.35618500
O	2.28690700	-22.62875200	-0.93174500
O	1.49654700	-20.96758000	0.41524000
N	-0.82427000	-17.87885400	-0.89189300
N	0.51113900	-21.32913500	-1.59079100
C	0.42560400	-14.31992000	-1.06146300
C	1.78984100	-14.63239800	-1.27503300
C	-0.52469700	-15.35449500	-0.91885500
C	2.21555900	-15.95065400	-1.34544200
C	-0.08362400	-16.66757000	-1.00670100
C	1.27194800	-16.96898300	-1.21464200
C	-2.16701500	-22.58017300	-3.70492600
C	1.44574000	-18.42273400	-1.23330700
C	-1.69166400	-23.80716600	-4.15851400

C	-1.61371400	-20.52907600	-2.22454000
C	0.04873600	-18.96677900	-1.09886900
C	-1.35447200	-21.82810600	-2.85703100
C	-0.42560500	-24.25762300	-3.75568600
C	-0.34554800	-20.21559100	-1.47874300
C	-0.08922100	-22.28605700	-2.45936500
C	0.39788300	-23.51432600	-2.90476000
C	-4.74660700	-19.20900000	0.11925500
C	-3.55446300	-19.36792000	1.06581100
C	1.54003700	-21.70204200	-0.69365600
C	-3.65374600	-18.46172600	2.29580400
C	-3.36927900	-20.83020100	1.47402400
C	3.92077400	-20.92429800	0.93351800
C	2.13042700	-20.02669700	2.46618500
C	2.50981600	-21.13841900	1.48655800
C	2.33094700	-22.51855000	2.12437300
H	2.50690500	-13.82957500	-1.41193000
H	-1.56511000	-15.14019100	-0.72842300
H	3.25823500	-16.20217400	-1.51102100
H	-3.14074200	-22.19704100	-3.99335000
H	-2.29316200	-24.41429000	-4.82733500
H	-4.89774900	-18.16567300	-0.15781800
H	-4.58965500	-19.79264400	-0.79037600
H	1.37288200	-23.86850400	-2.60415400
H	-3.74549400	-17.41484600	2.00490700
H	-5.64859100	-19.57267000	0.62216600
H	3.97932200	-19.97357600	0.39925700
H	-3.27181900	-21.46884100	0.59204200
H	-2.77067900	-18.57963800	2.93138900
H	2.23619300	-19.04516500	1.99648800
H	-4.53452800	-18.74014200	2.88310100
H	4.20553800	-21.72535000	0.25144900
H	-4.23535900	-21.16733700	2.05069200
H	-2.47368900	-20.94988700	2.09028900
H	4.62920100	-20.90562500	1.76814000
H	1.09577300	-20.14218900	2.80148400
H	2.78516600	-20.06325900	3.34163000
H	2.56510400	-23.31171200	1.41363300
H	1.30322800	-22.64766800	2.47785200
H	3.00075100	-22.61085300	2.98517600
C	-2.08146600	-17.90936000	-0.24303700
O	-2.80475300	-16.93432800	-0.21131200
C	-0.02473400	-12.93052000	-0.99330100
C	-1.29662000	-12.42889900	-1.18592900
S	1.08633000	-11.62210900	-0.62457800
C	-1.38441000	-11.02374800	-1.06041900
H	-2.14150800	-13.05503900	-1.44630700
C	-0.17873400	-10.41662300	-0.76365700
H	-2.30210300	-10.46608900	-1.20907700
H	-0.06340900	-25.21496200	-4.11922600

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- ¹ Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.
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