

Electronic Supplementary Information for

**Induction of smectic polymorphism in bent-core derivatives of the
6-oxoverdazyl by partial fluorination of alkyl chains**

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1. Additional DSC data

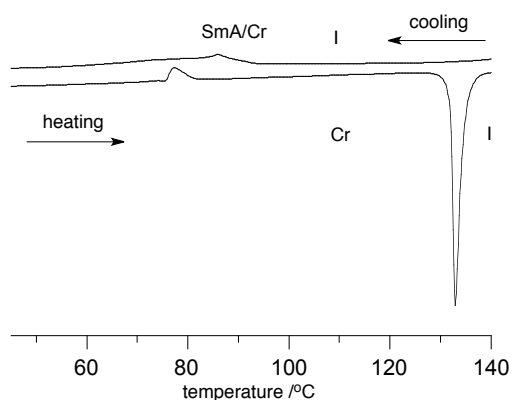


Fig. S1. DSC traces of **2[6,6]a**. The heating and cooling rates are 10 K min⁻¹.

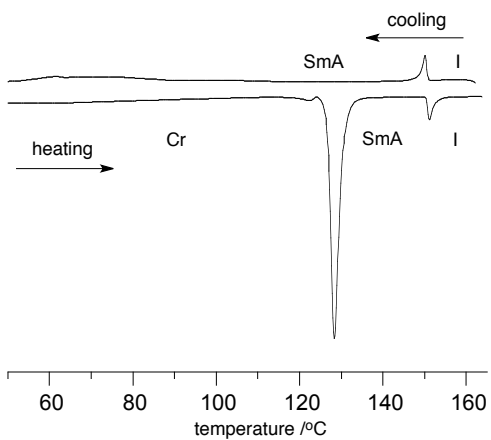


Fig. S2. DSC traces of **2[8,4]a**. The heating and cooling rates are 10 K min⁻¹.

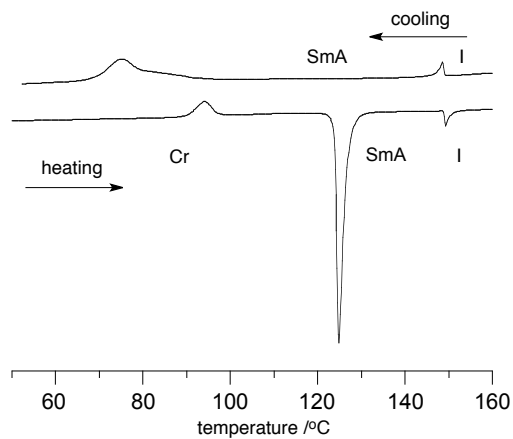


Fig. S3. DSC traces of **2[8,6]a**. The heating and cooling rates are 10 K min⁻¹.

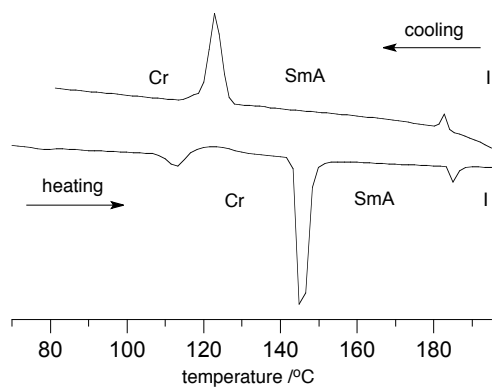


Fig. S4. DSC traces of **2[10,4]a**. The heating and cooling rates are 10 K min^{-1} .

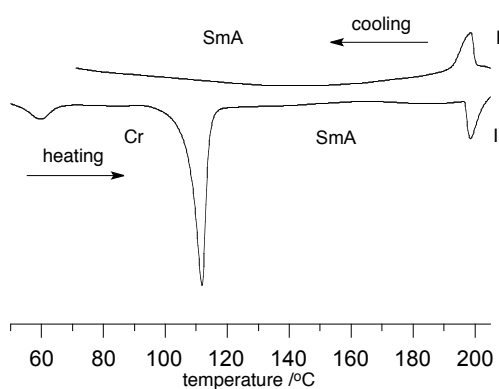


Fig. S5. DSC traces of **2[6,6]b**. The heating and cooling rates are 35 K min^{-1} .

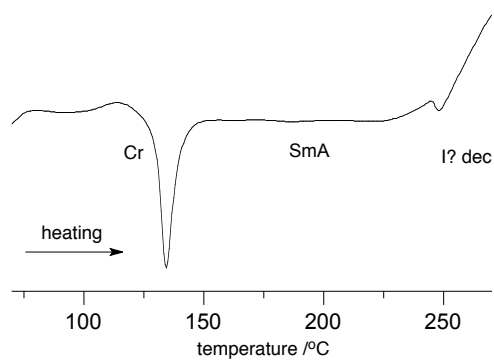


Fig. S6. DSC traces of **2[8,4]b**. The heating rate is 35 K min^{-1} .

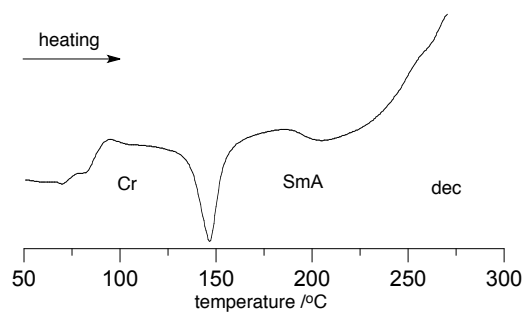


Fig. S7. DSC traces of **2[10,4]b**. The heating rate is 35 K min⁻¹.

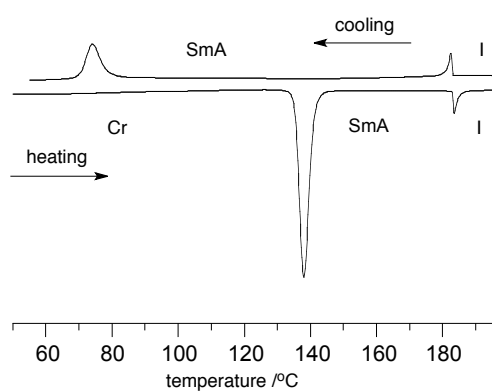


Fig. S8. DSC traces of **2[6,6]c**. The heating and cooling rates are 10 K min⁻¹.

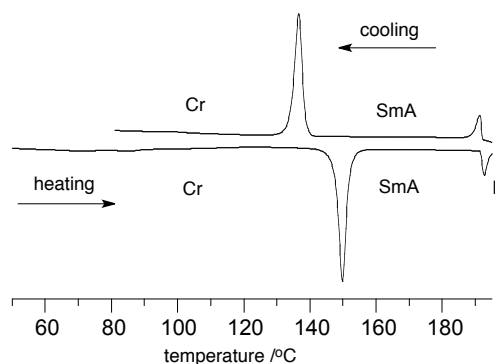


Fig. S9. DSC traces of **2[6,6]d**. The heating and cooling rates are 10 K min⁻¹.

2. Powder XRD measurements

X-ray diffraction experiments in broad angle range were performed with Bruker D8 GADDS (Cu K α radiation, Göbel mirror, point collimator, Vantec 2000 area detector) equipped with a modified Linkam heating stage. For small angle diffraction experiments Bruker Nanostar system was used (Cu K α radiation, cross-coupled Göbel mirrors, three

pinhole collimation, Vantec 2000 area detector). Samples were prepared in a form of a thin film or a droplet on a heated surface. The X-ray beam was incident nearly parallel to sample surface. Results are shown in Fig. S10 – S16.

Analysis demonstrated that the temperature dependence for **2[6,6]a**, **2[8,6]a**, **2[6,6]b**, **2[6,6]c** is well described by a quadratic function, e.g. $d_{01} = a \cdot T^2 + b$, while profiles for **2[8,4]a**, **2[10,4]a** and **2[6,6]d** are better described by cubic dependence on temperature ($d_{01} = a \cdot T^3 + b$). For comparison purposes, thermal expansion coefficients are obtained from fitting of the $d_{01}(T)$ data to the quadratic function $d_{01} = a \cdot T^2 + b$.

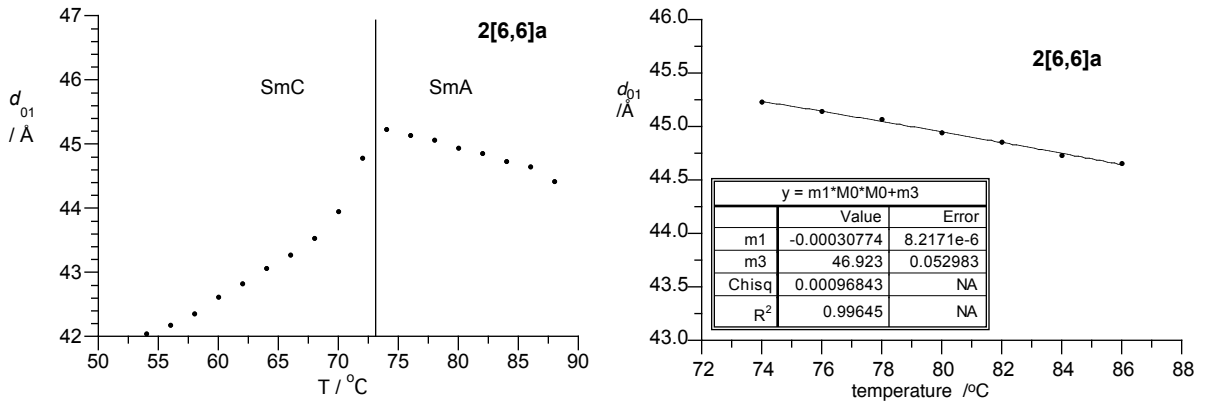


Fig. S10. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 86 °C – 74 °C to the function $d_{01} = a \cdot T^2 + b$.

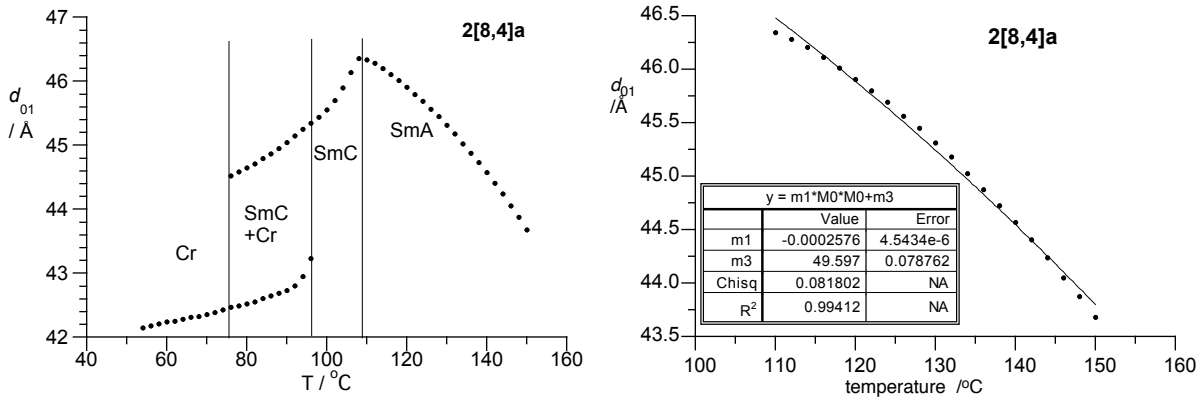


Fig. S11. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 150 °C – 110 °C to the function $d_{01} = a \cdot T^2 + b$.

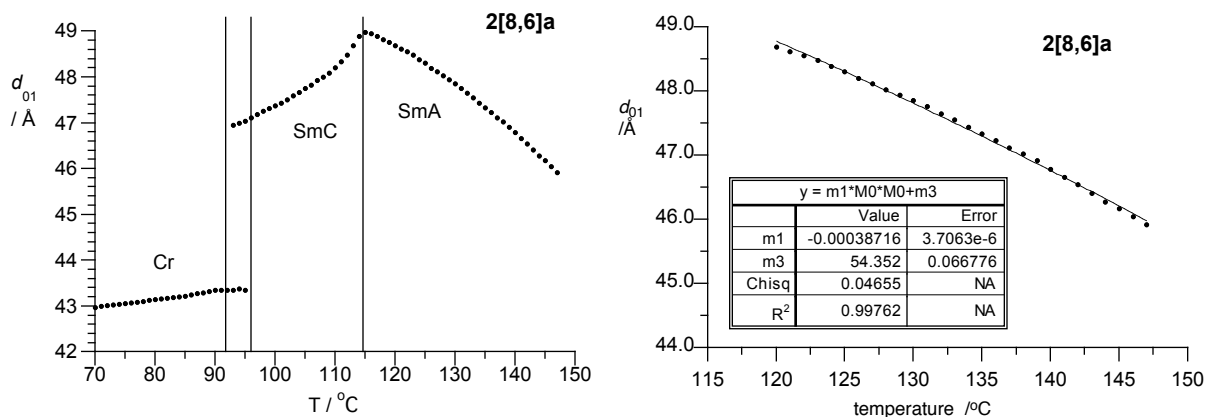


Fig. S12. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 147 °C – 120 °C to the function $d_{01} = a \cdot T^2 + b$.

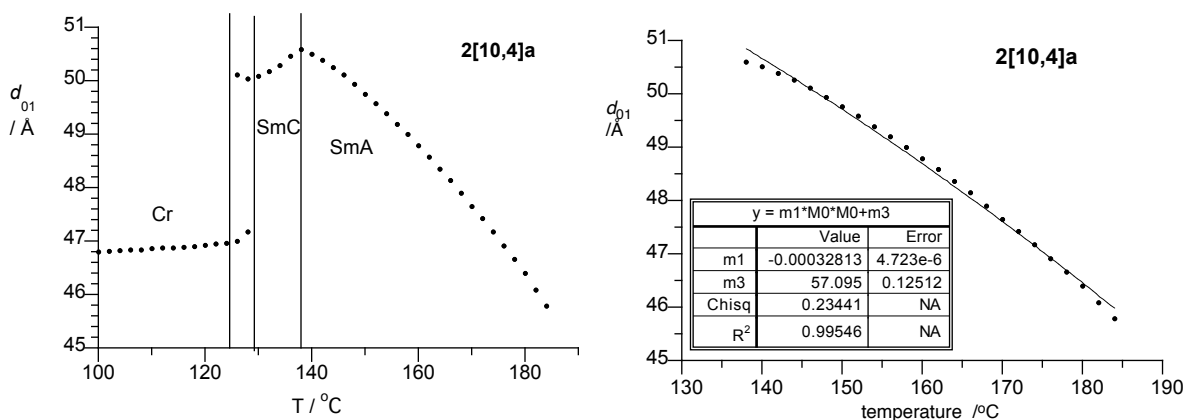


Fig. S13. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 184 °C – 138 °C to the function $d_{01} = a \cdot T^2 + b$.

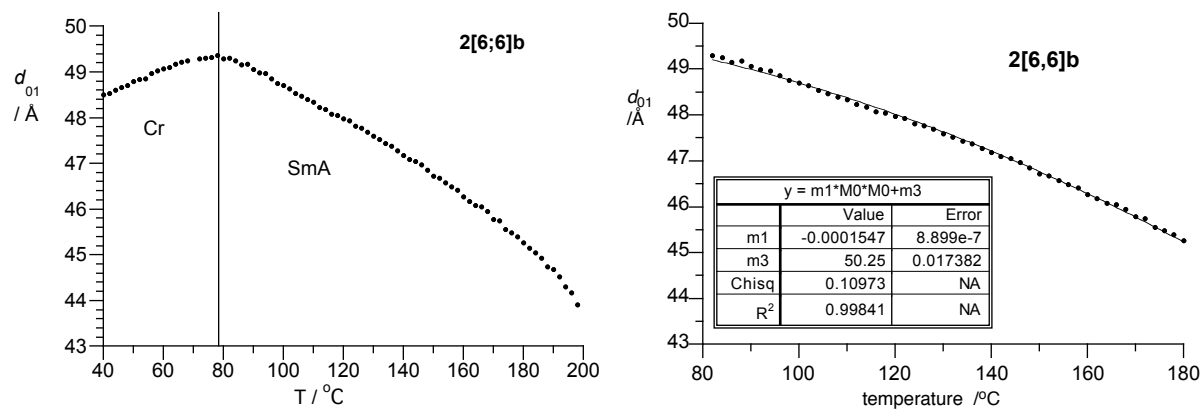


Fig. S14. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 180 – 82 °C to the function $d_{01} = a \cdot T^2 + b$.

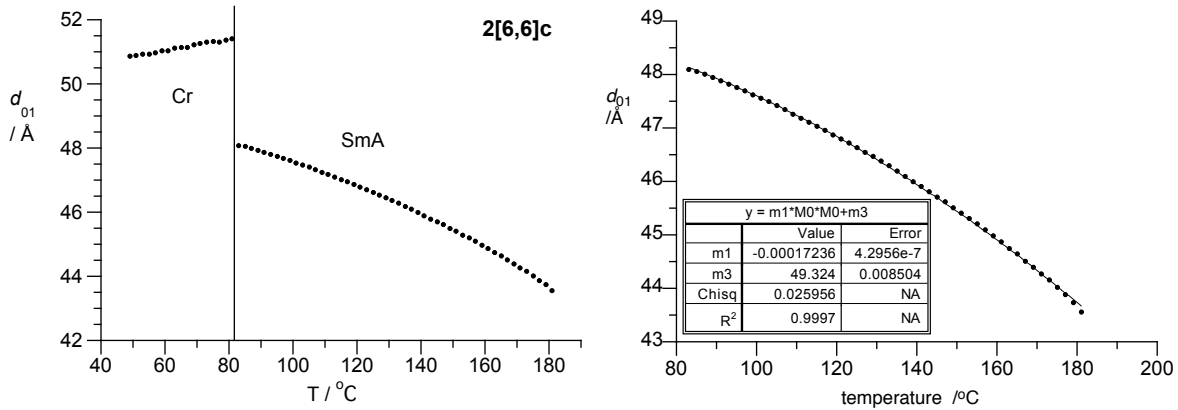


Fig. S15. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 182 – 82 °C to the function $d_{01} = a \cdot T^2 + b$.

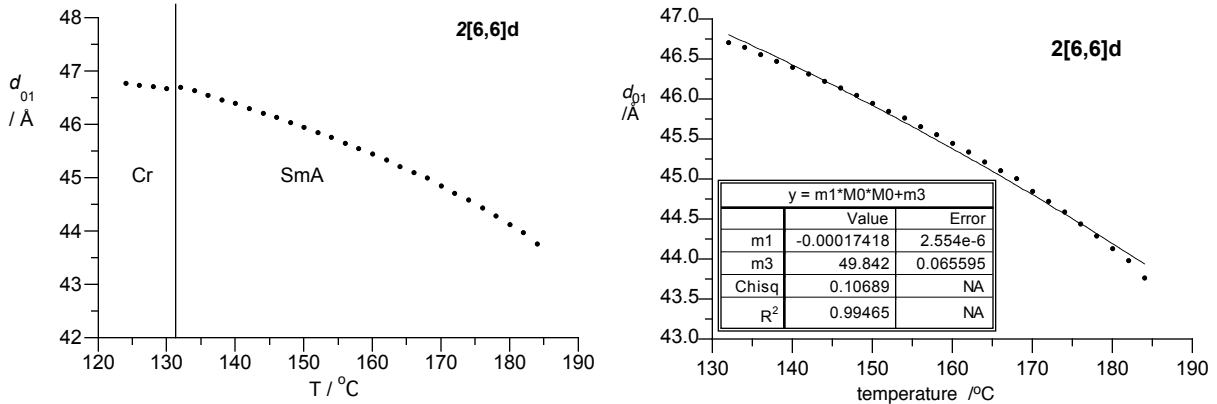


Fig. S16. Left: Layer thickness d_{01} as a function of temperature. Right: fitting the SmA datapoints in a range of 184 – 132 °C to the function $d_{01} = a \cdot T^2 + b$.

3. Archive for DFT results

2[6,6]a

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2[8,4]a

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2[8,6]a

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2[10,4]a

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7\F,26.4936417751,-3.9026123896,-1.1455141651\F,24.5279359534,-5.09166
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2039407382,-0.150510242,-0.8200924675\F,-17.3919388349,-2.1589471739,-
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17,-5.6136805745,-0.3113874497\C,27.1534640374,-5.8301771164,0.0405798
077\C,28.6702201648,-5.5771795295,0.2578783737\F,-28.8827346867,-5.238

3319818,-1.573689795\F,-29.1007344647,-4.6623358284,0.5197812148\F,-29.3199356408,-6.748575621,-0.070469647\F,-26.6999630278,-6.677660977,-1.0692081604\F,-26.9964222746,-6.483539719,1.1087505386\F,27.0052321121,-6.4551872744,-1.1475550738\F,26.7269954325,-6.6470455644,1.0330160577\F,29.1077393562,-4.6260182517,-0.5787909615\F,28.9084595204,-5.1984294015,1.5175427111\F,29.338952352,-6.7102371003,0.013952157\\Version=ES64L-G09RevD.01\State=2-A\HF=-7429.5885965\S2=0.769119\S2-1=0.\S2A=0.750186\RMSD=1.531e-09\RMSF=8.823e-07\Dipole=-0.0144035,-1.366898,0.0547187\Quadrupole=18.4050823,-27.7624088,9.3573265,-0.3293776,-21.3853485,0.9198822\PG=C01 [X(C57H32F45N4O7)]\\

2[6,6]b

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(d)\C56H43F26N4O7S1(2)\PIOTR\12-Fe b-2016\0\#\# UB3LYP/6-31G* FOpt geom=(nodistance,noangle) fcheck SCF=direct\\1,5-(4-F(CF2)(CH2)6O-C6H4COOC6H4)-3-Thienyl oxoverdazyl, C2 pseudosymm\\0,2\O,-0.0573161635,-0.3178778888,0.283930584\C,-0.0503152232,0.8959865389,0.1837926619\N,1.1212355327,1.6508707287,0.0277001495\N,1.1452130494,3.0156683987,-0.0455415696\C,-0.0414381067,3.6207158082,-0.0183606854\N,-1.2374199433,3.0375149392,0.0862071444\N,-1.2169456346,1.6758277035,0.2097049494\C,-2.5123917859,1.0600004405,0.260508776\C,-2.7642261847,-0.0597384219,1.0615862076\C,-4.045114967,-0.6035417899,1.0945744554\C,-5.0697405144,-0.0320975671,0.3425028085\C,-4.8302389393,1.0941476806,-0.445807337\C,-3.5488063079,1.6344013714,-0.4849233216\C,2.4137976812,1.0267482188,0.0279769903\C,3.4859276797,1.7188690882,0.6033675988\C,4.7680379871,1.1772275611,0.5924184213\C,4.972441341,-0.0721329552,0.0040650588\C,3.9099088418,-0.7639679968,-0.5764703923\C,2.6297624134,-0.2199462901,-0.5722951247\O,6.2201925551,-0.6690442135,-0.1326100027\O,-6.3329760037,-0.5925065027,0.4988270672\C,7.1628434121,-0.6284969411,0.8674484474\O,6.988306722,-0.0839326907,1.9358997879\O,-6.802312077,-0.6075877776,-1.7336047808\C,-7.1353272358,-0.8400405198,-0.5922291213\C,8.3992810116,-1.3354221531,0.463598859\C,9.4559489453,-1.3820389528,1.3811216557\C,8.5573098191,-1.9568351166,-0.788570392\C,10.6488215193,-2.0295961981,1.0730458409\C,9.739745509,-2.6041798533,-1.1060083822\C,10.79540948,-2.6470680646,-0.1785532068\C,-8.4335772785,-1.4219719799,-0.1849805656\C,-9.3442794275,-1.7557459985,-1.1948157968\C,-8.7908551587,-1.6487775812,1.1565075884\C,-10.5867990813,-2.3033885433,-0.8907911673\C,-10.0259985601,-2.1913206423,1.4710807477\C,-10.934888842,-2.5229509572,0.4509322083\C,-0.0352333863,5.0821333166,-0.1150774094\C,-1.1099431744,5.936713788,-0.041701825\S,1.4559380368,5.9618083409,-0.3489666763\C,-0.7410731541,7.3049225937,-0.1730184907\C,0.6075404261,7.4725360883,-0.3435966761\O,11.9083432275,-3.3076450593,-0.5885582955\O,-12.1173917146,-3.0467595942,0.8645200575\C,13.0324738981,-3.3987394321,0.2899293159\C,14.1113606333,-4.1959859004,-0.4302976904\C,-13.0996079097,-3.4028097611,-0.1114234034\C,-14.3181237585,-3.9361574963,0.6292993814\H,-3.3455150406,2.5103039926,-1.0889285054\H,-5.6261181331,1.5325786621,-1.0334521579\H,-4.2602849858,-1.4711053679,1.7097320068\H,-1.9712670632,-0.5078420803,1.6435880083\H,1.8110170855,-0.7626547734,-1.0226273489\H,4.0970505303,-1.7273269336,-1.0394772042\H,5.5894154118,1.7126652684,1.0482823095\H,3.3125917161,2.6903361679,1.0496598783\H,9.3276282042,-0.9006535614,2.3451415958\H,7.7473117

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\F,24.254070435,-10.003502434,0.9794470871\F,23.2327024042,-8.80340677
71,-1.097259532\F,22.8060501871,-6.4577975004,1.4780706187\F,22.057519
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43F26N4O7S1)]\

2[6,6]c

1\1\GINC-LOCALHOST\FOpt\UB3LYP\6-31G(d)\C58H45F26N4O7(2)\PIOTR\12-Aug-
2016\0\#\#P UB3LYP/6-31G* FOpt geom=(nodistance,noangle) fcheck SCF=dir
ect\1,5-(4-F(CF2)(CH2)6O-C6H4COOC6H4)-3-Ph oxoverdazyl, C2 pseudosymm
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75734,-0.1332556265\N,-1.1337599732,5.3398415453,0.0640821703\N,-1.144
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\O,6.289990078,3.0481510012,-0.5940296551\C,-7.2108007615,3.129076931,
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8,2.9769281932,1.6296678814\C,7.1074769063,2.7694233892,0.4779684195\C
, -8.444321571,2.4221226144,-0.3099621538\C,-9.5183826447,2.4011740701,
-1.2080591936\C,-8.5830478011,1.7761066364,0.9320294585\C,-10.70964306
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3\C,-10.836897289,1.1130363316,0.3505823068\C,8.3952873762,2.188787308
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,1.9903486299,-1.3148745981\C,10.5537844891,1.2788351332,0.6882477726\
C,9.9565186185,1.447744833,-1.6612466449\C,10.8793446914,1.0878461415,
-0.6634499707\O,-11.9462885229,0.4513646272,0.7681154242\O,12.05209033
28,0.566844779,-1.1074478442\C,-13.087460616,0.385040183,-0.0904678165
\C,-14.1576018871,-0.419880375,0.6342542458\C,13.0478972001,0.18497873
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\H,4.1879842737,2.2095112598,-1.7843137467\H,1.9080464105,3.1879567999
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2[6,6]d

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