Electronic Supplementary Material (ESI) for CrystEngComm.

Polymorphism and resulting luminescent properties of 1-acetylpyrene - Supporting Information

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Chapter 1

Methods

1.1 Methods

1.1.1 Synthesis of 1-acetylpyrene

Full NMR spectra of 1AP in Figure 1.1.

1.1.2 Photographs

The micrographs were taken using Olympus SZX16 stereoscopic microscope, equipped in motorized XY-stage. The photographed samples were illuminated either with UV (365 nm) or visible light. The VL-6 UV lamp removed from the CN-6 Vilber dark-room was used as an external UV source.

1.1.3 Differential Scanning Calorimetry

The DSC measurements were performed using Mettler-Toledo DSC1 STAR^e system at a heating rate of 10°C/min under a dry N_2 atmosphere and at a constant flow (60 ml/min) over a temperature range from 25 to 500°C. Obtained data were analyzed using the STARe software provided by Mettler Toledo. The total weight of each sample (7.12 and 5.27 mg in case of 1AP-γ and 1AP-α, respectively) was accurately weighted into open standard 40 μl aluminum crucibles using Mettler-Toledo XS105 DualRange balance. The DSC curves of 1AP-γ and 1AP-α were depicted in Fig. S1. The major endothermic peaks at the 90.83 and 91.38°C represent the melting points of 1AP-γ and 1AP-α, respectively. The value of enthalpy of this transition in case of 1AP-γ and 1AP-α is rescpectively -71.54 and -84.63 J/g.

1.1.4 Melting Points

As the amount of 1AP-β was insufficient to perform the DSC analysis, additional determination of the melting point temperatures was performed for single crystals of all three polymorphs of 1AP. The purity and quality of each single crystal was confirmed by a short X-ray diffraction experiment (unit cell determination). Single crystals of approximately the same size were placed on a siliconized glass wafer on a LinkamScientific TMS94 hot stage and then slowly heated at a rate of 5°C/min in air

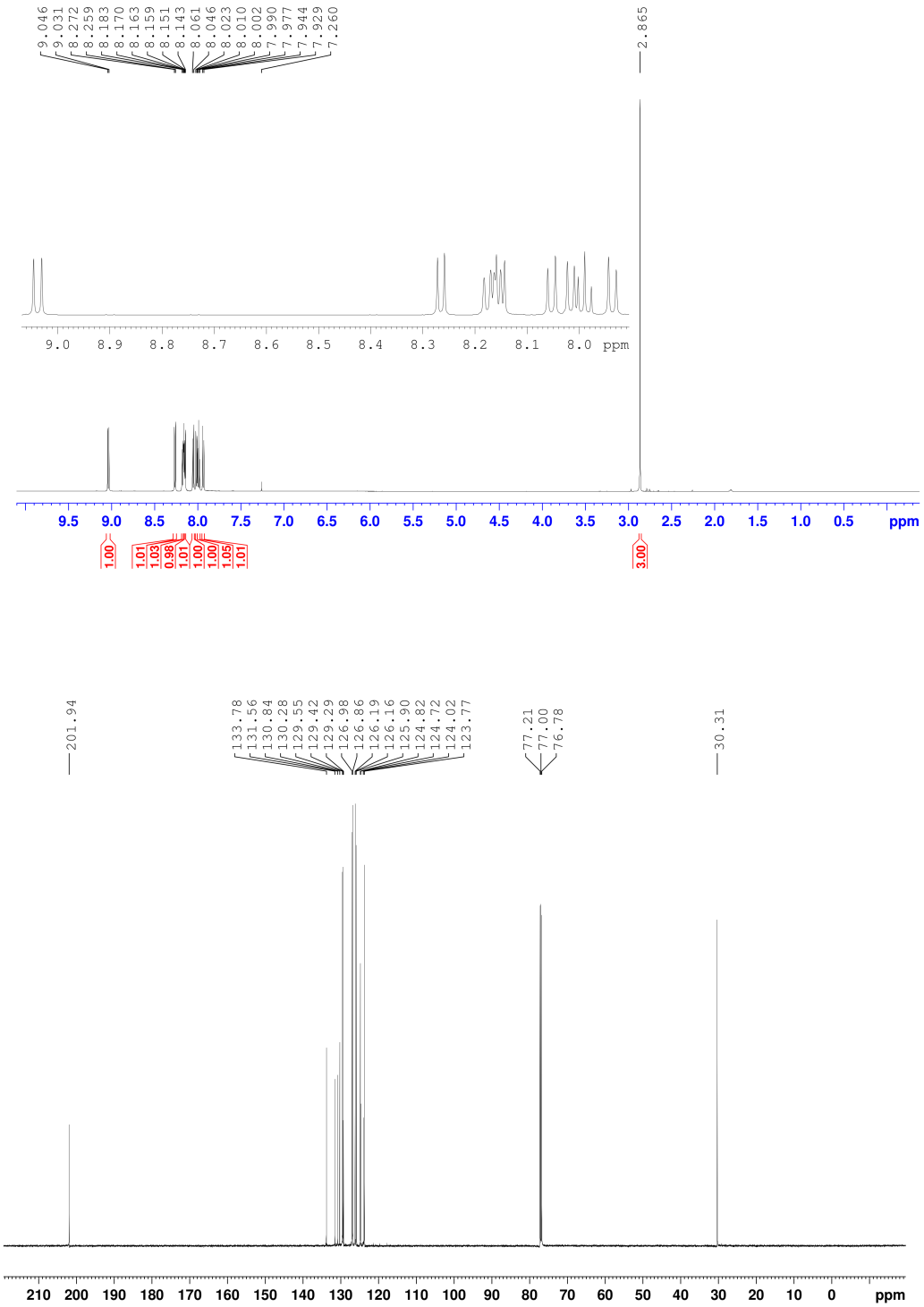


Figure 1.1: *1-HNMR (top) and 13-CNMR (bottom) spectra of 1AP after flash chromatography purification.*

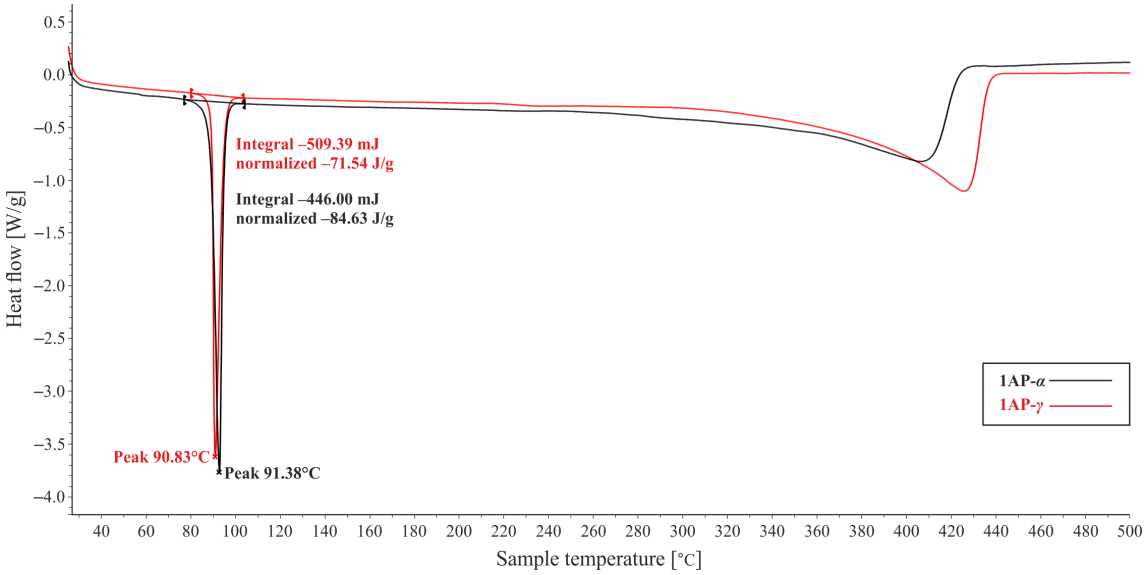


Figure 1.2: *The DSC curves of 1AP-α (black) and 1AP-γ (red).*

under a microscope. The 1AP-β transformed into 1AP-γ (single crystal to powder transformation, as confirmed by the change of luminescence and XRD analysis) at c.a. 74°C. The observed melting temperatures of 1AP-*alpha*, former 1AP-β and 1AP-γ were 88.2°C, 88.9°C and 88.9°C.

1.1.5 Theoretical Calculations

In order to obtain energies of cohesion, firstly the energy of the crystal bulk per unit cell was obtained from crystal geometry optimizations in periodic conditions, assuming temperature of 0K. Then the energy of a single, isolated molecule was calculated based on:

a) its **fixed geometry** obtained in the previous step or

b) **fully optimized geometry** of an isolated molecule in a gas phase.

The lattice energy was estimated as a difference between total crystal energy and the energy of a single molecule in crystal-fixed geometry obtained in a), times the number N of molecules in the unit cell:

$E_{lattice} = E_{bulk} - N \cdot E_{molecule,a}$

The cohesive energy was estimated as a difference between total crystal energy and the energy of an isolated molecule optimized in b), times the number N of molecules in the unit cell:

$E_{cohesive} = E_{bulk} - N \cdot E_{molecule,b}$

The conformation energy was estimated as a difference between the energies of a single molecule obtained in a) and in b):

$E_{conformation} = E_{molecule,a} - E_{molecule,b}$

Chapter 2

Structure description

2.1 Structure description

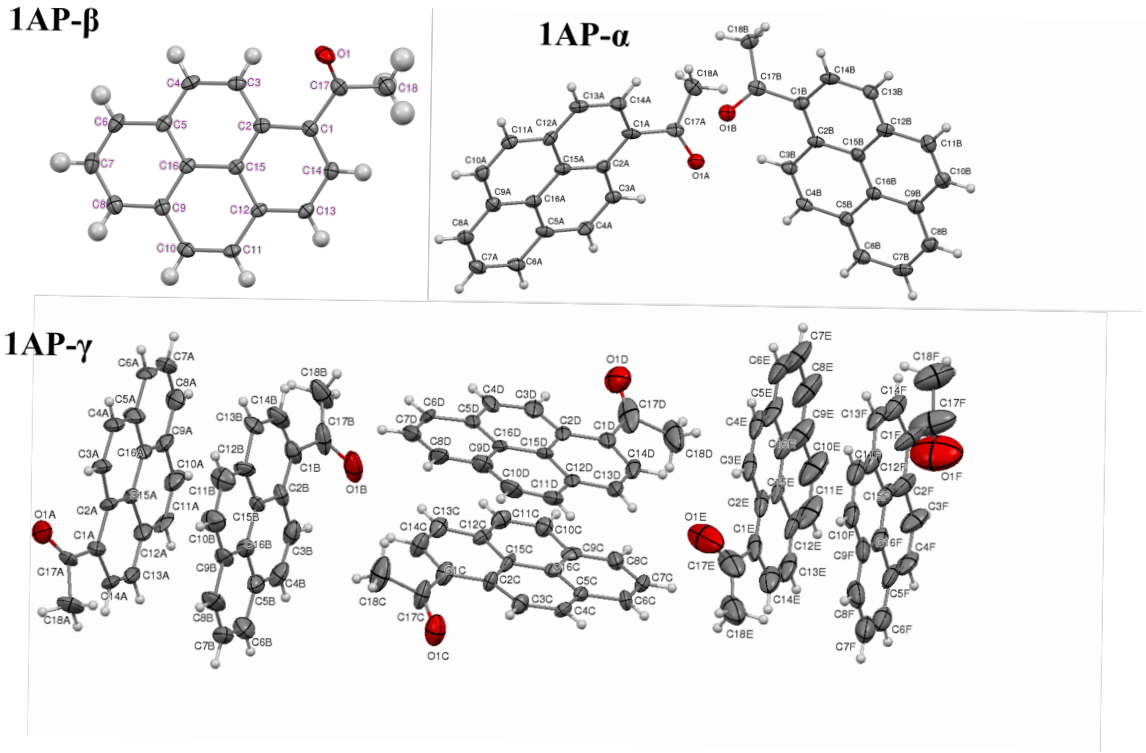


Figure 2.1: *ORTEP representations of the independent AP molecules present in its β, α and b) γ polymorphs, with atom numbering. H-atom labels derived from labels of connected carbon atoms. In the case of 1AP-α and 1AP-γ polymorphs, independent molecules are assigned labels A to B and A to F, respectively. Atomic displacement parameters drawn at 50% probability level.*

Figures presented further in this section have hydrogen atoms hidden for clarity.

A numerical comparison of Hirshfeld surfaces obtained for single molecules of 1-acetylpyrene confirms different nature of dominant interactions in 1AP-α and 1AP-γ or 1AP-β (Figure 2.5). The two latter cases feature a lot of π-stacking between

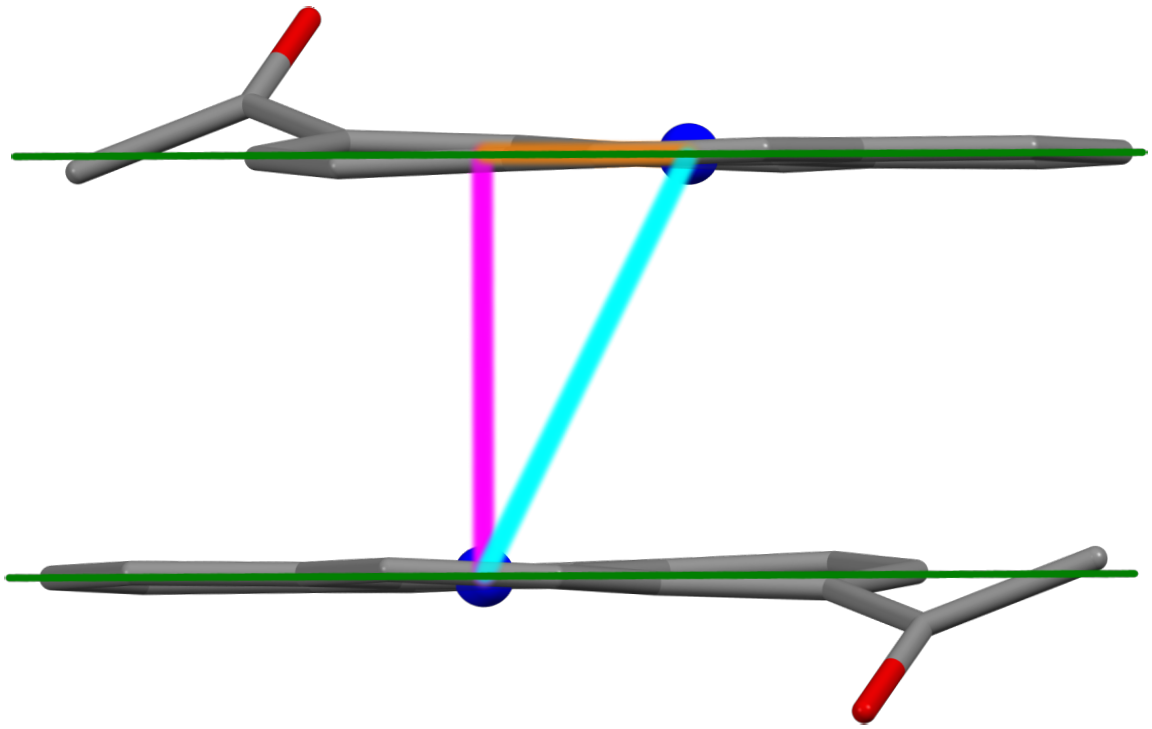
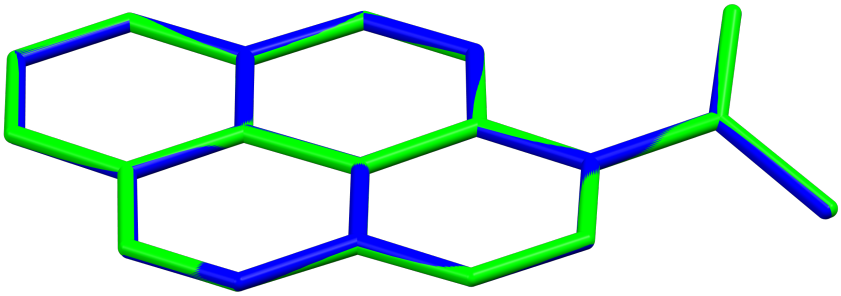


Figure 2.2: *Explanation of various definitions of distances between π-stacking rings. Both planes (green line) and centroids (blue spheres) are fitted to / averaged over all 16 carbon atoms contributing to the pyrene ring. The "total" distance (cyan) is a magnitude of vector between centroids; The "vertical" distance (magenta) is a distance between perpendicular planes. The "lateral" distance (orange) is the magnitude of vector resulting from projecting the cyan total distance vector onto the green average plane.*

multiple parallel aromatic rings, leading to direct carbon-carbon interactions. On the other side, 1AP-α's geometry suggests a much more significant role of $\mathrm{C-H}\cdots\pi$ contacts, and thus those are much more prominent here than in other two cases.

a)



b)

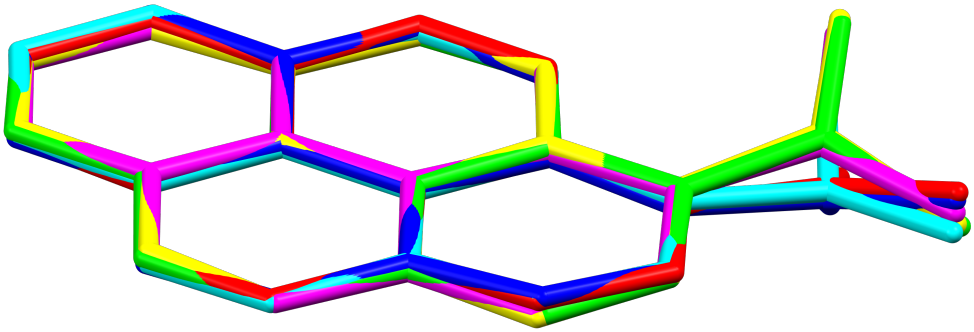


Figure 2.3: *An overlay of independent AP molecules present in its a) α and b) γ polymorphs. The graphics have been prepared by subsequent overlaying molecules B – F onto molecule A in Mercury [Macrae et al., 2008], using its native coloring scheme (A: green, B: blue, C: red, D: yellow, E: cyan, F: magenta). In the case of α RMSD is 0.0186Å^2 and maximum deviation of 0.0381Å when overlayed.*

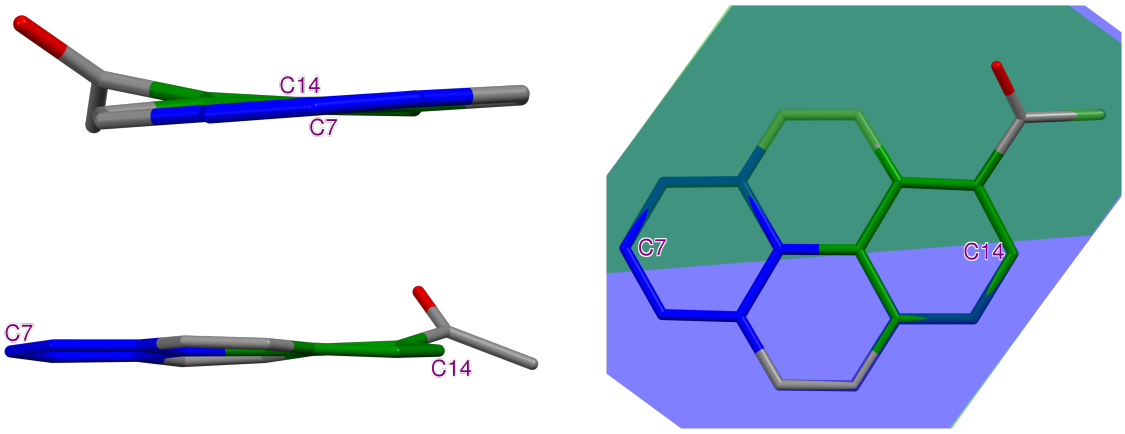


Figure 2.4: *Three perpendicular perspectives on the 1-acetylpyrene molecule, whose outer rings around C7 and C14 carbon atoms were colored blue and green. The side views presented on the left show a significant degree of twist roughly along the C7 – C14 axis. Fitting a plane to each of the individual rings on the right shows that the common line of the planes closely coincides with the above mentioned direction. The angle between the planes equals 5°.*

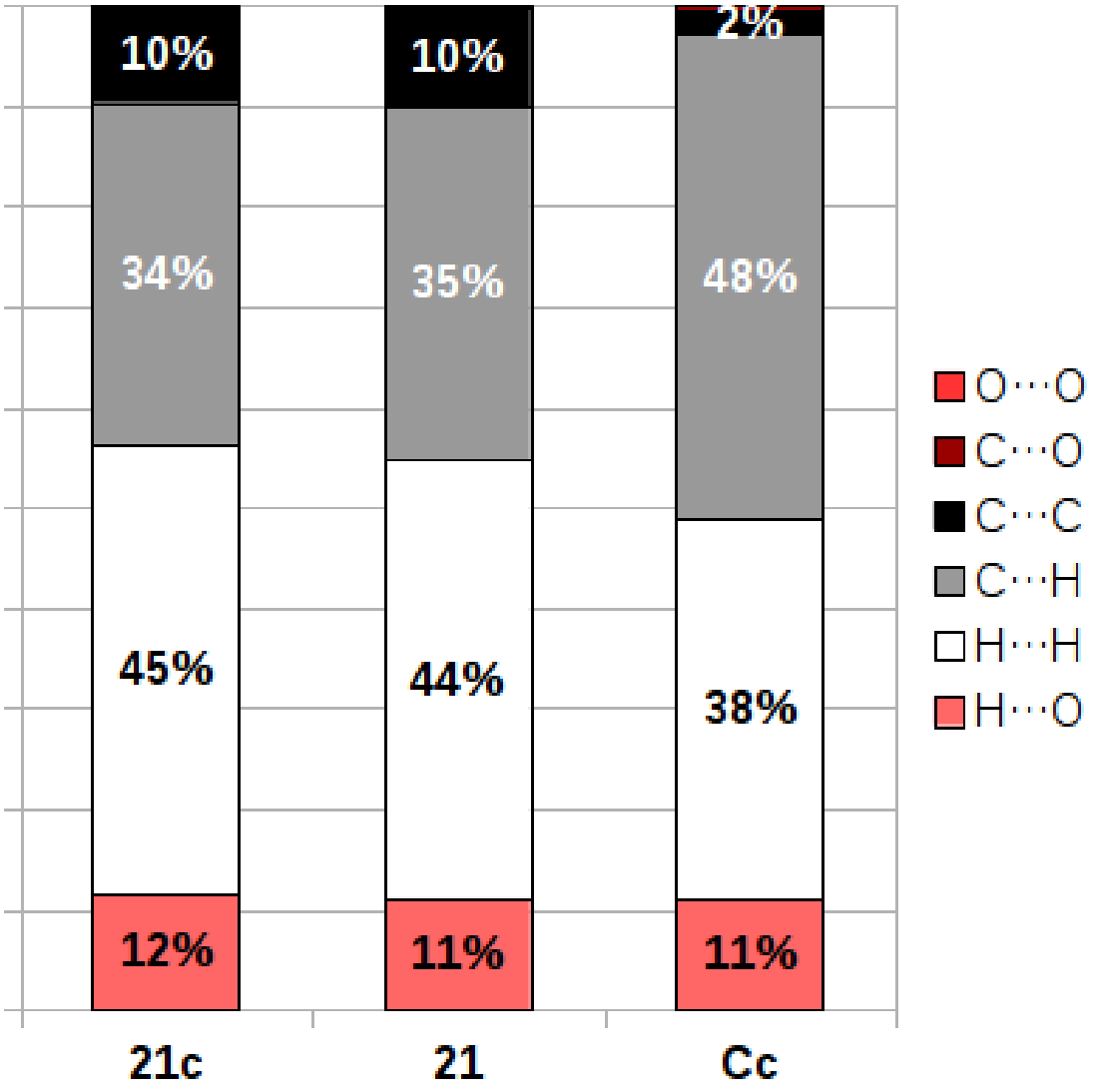


Figure 2.5: *Averaged participation of various intermolecular contacts observed on Hirshfeld surfaces of 1-acetylpyrene molecules in respective polymorphs.*

Chapter 3

Lattice interactions

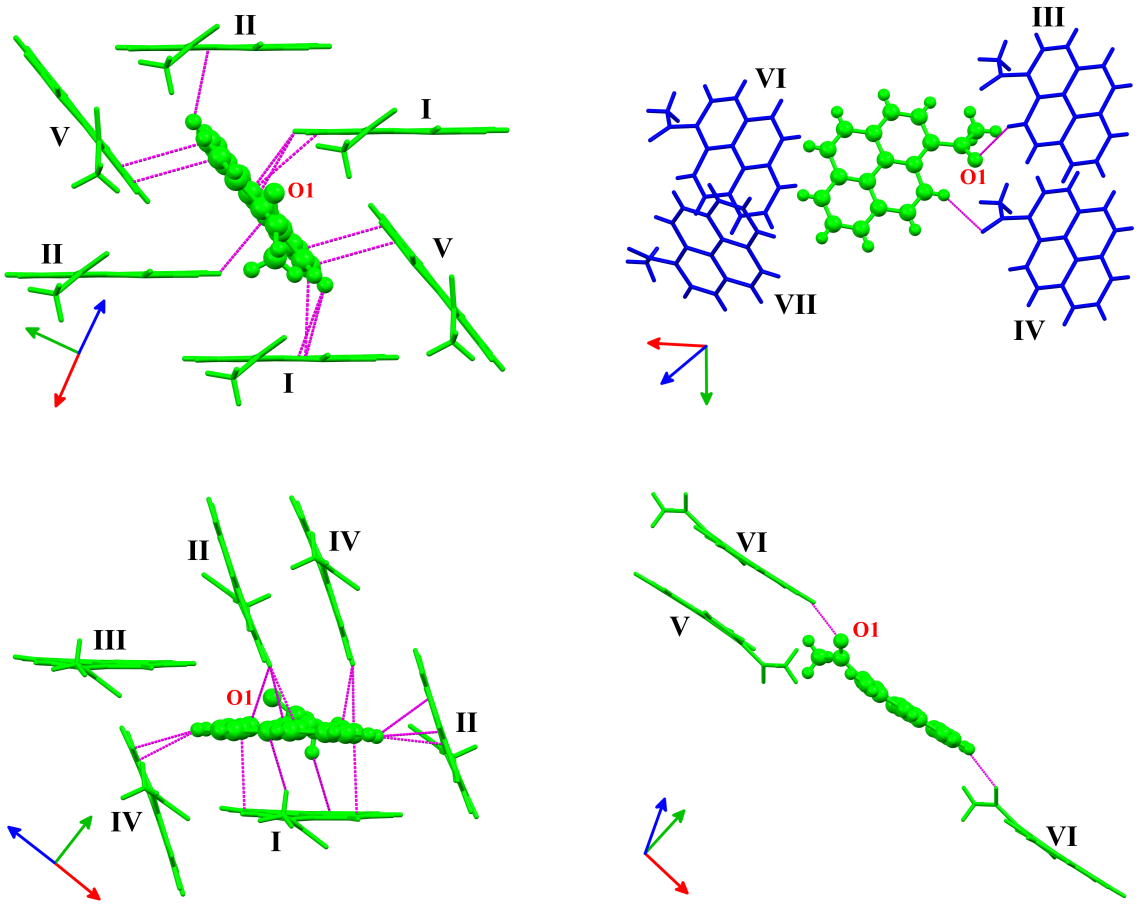


Figure 3.1: *Visualization of strongest interactions within (left) and between (right) individual layers in 1AP-α (top) and 1AP-β (bottom). Crystallographic directions* ***[100]****,* ***[010]****and* ***[001]****represented in red, green and blue accordingly.*

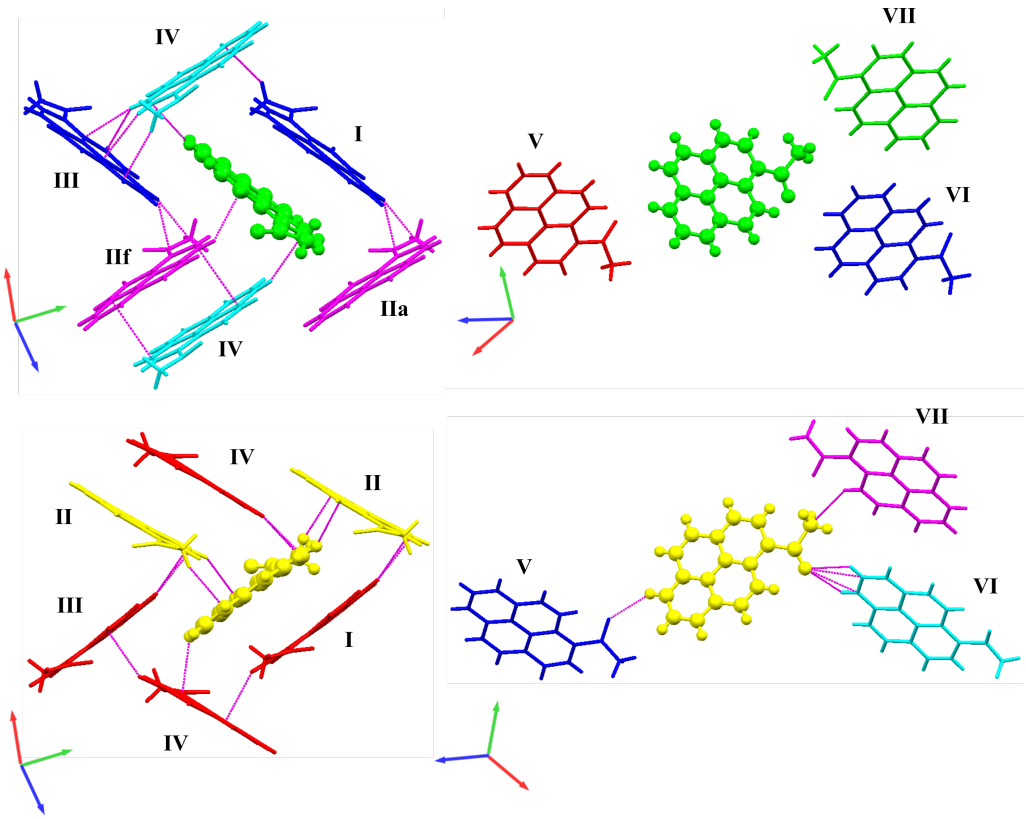


Figure 3.2: *Visualization of the strongest interactions within (left) and between (right) individual layers in in 1AP-γ for molecules A (top) and D (bottom), representing two layers in the crystal structure. Intermolecular interactions in 1AP-γ are similar to those of 1AP-β and thus inherit some of the labels. Crystallographic directions* ***[100]****,* ***[010]****and* ***[001]****represented in red, green and blue accordingly.*

Table 3.1: *The strongest intermolecular interactions in 1-acetylpyrene polymorphs according to energies estimated by Crystal Explorer. Labels of interactions, expressed using Roman numerals, are common for this Table and Figures 3.1 & 3.2.*

	main interaction		energy /kJ mol^{-1}		
1AP-α	edge-to-edge		mol A	mol B	
I	C – H $\cdots$ π	edge-to-edge	-33.5	-33.1	
II	C – H $\cdots$ π	edge-to-edge	-22.1	-22.1	
III	C – H $\cdots$ O		-17.9	-18.6	
IV	C – H $\cdots$ O		-18.6	-17.9	
V	H $\cdots$ H	'edge over edge'	-18.1	-18.3	
VI	C – H $\cdots$ π		-8.9	-12.2	
VII	C – H $\cdots$ π		-7.9	-7.9	
1AP-β			mol A		
I	$\pi \cdots \pi$		-56.1		
II	C – H $\cdots$ π	edge-to-face	-33.1		
III	H $\cdots$ H	edge-over-edge	-18.1		
IV	C – H $\cdots$ π	edge-to-edge	-16.6		
V	C – H $\cdots$ O	donor: CH_3	-16.1		
VI	C – H $\cdots$ O	donor: CH	-12.3		
1AP-γ			mol A	mol B	mol C
I	$\pi \cdots \pi$		-48.3	-48.3	-52.3
II	C – H $\cdots$ π	edge-to-face	-31.1, -24.7	-31.8, -25.4	-29.7
III	H $\cdots$ H	edge-over-edge	-16.2	-16.2	-15.2
IV	C – H $\cdots$ π	edge-to-edge	-18.6, -12.5	-15.6, -15.1	-17.9, -15.2
V	C – H $\cdots$ O	donor: CH_3	-10.7	-11.4	-11.4
VI	C – H $\cdots$ O	donor: CH	-10.9, -10.3	-11.2, -10.9	-10.8, -10.3
VII	H $\cdots$ H	edge-over-edge	-9.7	-14.2	-14.2
			mol D	mol E	mol F
I	$\pi \cdots \pi$		-52.3	-58.3	-58.3
II	C – H $\cdots$ π	edge-to-face	-30.2	-31.1, -24.7	-31.8, -25.4
III	H $\cdots$ H	edge-over-edge	-15.2	-13.9	-13.9
IV	C – H $\cdots$ π	edge-to-edge	-17.9, -14.7	-15.6, -15.1	-18.6, -12.5
V	C – H $\cdots$ O	donor: CH_3	-10.5	10.5	-9.4
VI	C – H $\cdots$ O	donor: CH	-11.2, -11.8	-10.9, -10.8	-10.9, -5.2
VII	H $\cdots$ H	edge-over-edge	-9.7	-4.0	-6.9

Chapter 4

Theoretical calculations

4.1 Theoretical calculations

4.1.1 Optimized structures

Table 4.1: *Coordinates of independent atoms in 1AP-α's unit cell as optimized in CRYSTAL17 (excerpt from output).*

```
*******************************************************************************
CRYSTALLOGRAPHIC CELL (VOLUME=       2383.75411139)
A              B              C           ALPHA      BETA       GAMMA
9.85660000     7.11030000    34.36100000    90.000000  98.160000  90.000000

COORDINATES IN THE CRYSTALLOGRAPHIC CELL
ATOM                X/A                 Y/B                 Z/C
*******************************************************************************
     1 T   6 C    -3.432291385554E-01  4.160028982205E-01 -3.644493625639E-02
     3 T   6 C    -2.725783793120E-01  2.803792557835E-01 -5.658639146974E-02
     5 T   6 C    -2.289142546164E-01  1.004063306495E-01 -4.006153327074E-02
     7 T   1 H    -2.499479131630E-01  6.444662027936E-02 -1.097334874326E-02
     9 T   6 C    -1.612427668835E-01 -2.505602953170E-02 -6.033500213416E-02
    11 T   1 H    -1.301583290376E-01 -1.600951277247E-01 -4.730533714671E-02
    13 T   6 C    -1.313921733829E-01  1.416938838948E-02 -9.916718674004E-02
    15 T   6 C    -5.993757059700E-02 -1.133163344930E-01 -1.199913150100E-01
    17 T   1 H    -2.698940867210E-02 -2.465056836568E-01 -1.065031386607E-01
    19 T   6 C    -3.203713704528E-02 -7.018471592718E-02 -1.576176902794E-01
    21 T   1 H     2.417461141863E-02 -1.700545034847E-01 -1.730813455777E-01
    23 T   6 C    -7.623582891058E-02  9.971664194670E-02 -1.754497549391E-01
    25 T   1 H    -5.359000768216E-02  1.317582373939E-01 -2.047842446656E-01
    27 T   6 C    -1.493756809996E-01  2.305872533746E-01 -1.558045462977E-01
    29 T   6 C    -1.962617108589E-01  4.071006369837E-01 -1.732746797783E-01
    31 T   1 H    -1.748476491092E-01  4.395667314287E-01 -2.026887808564E-01
    33 T   6 C    -2.654067957840E-01 -4.674001209831E-01 -1.534562285749E-01
    35 T   1 H    -2.996581235871E-01 -3.339029555447E-01 -1.667022759124E-01
    37 T   6 C    -2.926663903472E-01  4.945766288390E-01 -1.141946585375E-01
    39 T   6 C    -3.616990649566E-01 -3.757041350896E-01 -9.337411591761E-02
    41 T   1 H    -3.935272563504E-01 -2.421182632044E-01 -1.068163324842E-01
    43 T   6 C    -3.871497575733E-01 -4.154083886343E-01 -5.549664432199E-02
    45 T   1 H    -4.369126086725E-01 -3.093611483310E-01 -3.986783425730E-02
    47 T   6 C    -2.475836215078E-01  3.208896363186E-01 -9.581963737416E-02
```

```
 49 T   6 C    -1.769224483644E-01  1.884578316456E-01 -1.169800445343E-01
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 53 T   6 C    -4.976940512541E-01  4.609499423679E-01  1.791219574904E-02
 55 T   1 H     4.604765222785E-01 -4.137144685764E-01  2.486908515050E-03
 57 T   1 H    -4.812419711391E-01  4.864001306625E-01  4.950476978946E-02
 59 T   1 H     4.240057803154E-01  3.508308218556E-01  1.240916437474E-02
 61 T   8 O    -2.823108995777E-01  3.060668776463E-01  2.927103312150E-02
 63 T   6 C     2.242009473914E-01  8.484991732774E-02  1.030666025133E-01
 65 T   6 C     3.140563777080E-01  2.207807289468E-01  1.233939502080E-01
 67 T   6 C     3.426423336788E-01  4.002731123174E-01  1.068472132749E-01
 69 T   1 H     2.945221864715E-01  4.355247657891E-01  7.754213289224E-02
 71 T   6 C     4.294188438174E-01 -4.738706388440E-01  1.273665161605E-01
 73 T   1 H     4.485814542081E-01 -3.392703885422E-01  1.142922345909E-01
 75 T   6 C     4.953938330491E-01  4.879271098662E-01  1.665088719716E-01
 77 T   6 C    -4.135028689969E-01 -3.842674450039E-01  1.876169854143E-01
 79 T   1 H    -3.926149792507E-01 -2.517190465812E-01  1.740720800497E-01
 81 T   6 C    -3.507867635780E-01 -4.264338503770E-01  2.255714872880E-01
 83 T   1 H     2.209216335802E-01  1.729515797279E-01 -2.588106596307E-01
 85 T   6 C     1.206462813377E-01 -9.543990850435E-02 -2.565507442659E-01
 87 T   1 H     1.699065491872E-01 -1.272251222801E-01 -2.269826120790E-01
 89 T   6 C    -4.709260487664E-01  2.734237890394E-01  2.235008803544E-01
 91 T   6 C     4.984468439377E-01  9.747305910826E-02  2.410175480188E-01
 93 T   1 H     4.752292800933E-02 -4.332507327316E-01 -2.293113144804E-01
 95 T   6 C     4.113849087969E-01 -2.885884430681E-02  2.208120090511E-01
 97 T   1 H     3.893614870310E-01 -1.624673971482E-01  2.338589852378E-01
 99 T   6 C     3.475920473927E-01  8.073001632837E-03  1.812742153208E-01
101 T   6 C     2.588550152451E-01 -1.221137709087E-01  1.602581839145E-01
103 T   1 H     2.392589823118E-01 -2.551989073788E-01  1.737643810836E-01
105 T   6 C     1.978922352434E-01 -8.321658814683E-02  1.221492154247E-01
107 T   1 H     1.330964547234E-01 -1.893780487312E-01  1.064009459518E-01
109 T   6 C     3.756635534073E-01  1.812157324964E-01  1.628803361406E-01
111 T   6 C     4.660681085295E-01  3.141826182183E-01  1.843255209430E-01
113 T   6 C     1.611586534473E-01  1.109596019977E-01  6.106229707549E-02
115 T   6 C     1.743155327119E-02  3.971676870770E-02  4.834215311416E-02
117 T   1 H    -8.731381965742E-03 -8.743020326413E-02  6.324476676662E-02
119 T   1 H     2.467534222095E-03  1.733858025068E-02  1.665276907434E-02
121 T   1 H    -5.563001030839E-02  1.485413847382E-01  5.439726027638E-02
123 T   8 O     2.223202953629E-01  1.937466029684E-01  3.732812952771E-02
```

Table 4.2: *Coordinates of independent atoms in 1AP-β's unit cell as optimized in CRYSTAL17 (excerpt from output).*

```
*******************************************************************************
LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=  1215.553437 - DENSITY  1.312 g/cm^3
A              B              C           ALPHA      BETA       GAMMA
10.47890000    11.52780000    10.37860000    90.000000 104.174000  90.000000
*******************************************************************************
ATOMS IN THE ASYMMETRIC UNIT   31 - ATOMS IN THE UNIT CELL:  124
ATOM                X/A                 Y/B                 Z/C
*******************************************************************************
     1 T   6 C     2.761170635914E-01  1.445473714791E-01 -1.591710346800E-03
     5 T   6 C     3.766256624785E-01  9.637962787876E-02  1.015912578893E-01
     9 T   6 C     3.489548449689E-01  2.682655755682E-02  2.060393580484E-01
    13 T   1 H     2.462160322185E-01  8.843388500872E-03  2.050883289409E-01
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 17 T   6 C     4.463723415999E-01 -1.924849628072E-02  3.045148159700E-01
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 25 T   6 C    -4.176521329288E-01  1.888402502944E-03  3.085955385899E-01
 29 T   6 C    -3.148586542279E-01 -4.524472160144E-02  4.079447043811E-01
 33 T   1 H    -3.385662121498E-01 -9.906518756508E-02  4.844737604514E-01
 37 T   6 C    -1.840514255380E-01 -2.500474723382E-02  4.066881680475E-01
 41 T   1 H    -1.056901891199E-01 -6.416092325034E-02  4.823216361684E-01
 45 T   6 C    -1.526683634375E-01  4.406454657309E-02  3.083536572432E-01
 49 T   1 H    -5.100096834006E-02  5.785090083706E-02  3.051641914671E-01
 53 T   6 C    -2.523807331300E-01  9.387071540594E-02  2.079538471009E-01
 57 T   6 C    -2.232104151448E-01  1.655886041816E-01  1.054541551266E-01
 61 T   1 H    -1.204926775593E-01  1.833489158241E-01  1.103185689769E-01
 65 T   6 C    -3.207227471431E-01  2.077258738153E-01  4.471725688153E-03
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 73 T   6 C    -4.566613992980E-01  1.836975971565E-01 -1.611822654857E-03
 77 T   6 C     4.411578379531E-01  2.231884378528E-01 -1.061194092512E-01
 81 T   1 H     4.649118551040E-01  2.695003462372E-01 -1.878166266518E-01
 85 T   6 C     3.101362375702E-01  2.045850972485E-01 -1.057482596750E-01
 89 T   1 H     2.339489248921E-01  2.383107104103E-01 -1.874238081005E-01
 93 T   6 C    -4.891226276936E-01  1.170635471272E-01  1.020287978310E-01
 97 T   6 C    -3.866492310075E-01  7.151608856427E-02  2.066320591880E-01
101 T   6 C     1.373885114341E-01  1.333486247734E-01  2.718687487973E-03
105 T   6 C     2.635606167672E-02  1.744143615366E-01 -1.135327589428E-01
109 T   1 H     3.798896833734E-02  2.668864239213E-01 -1.304828064210E-01
113 T   1 H    -7.053917426812E-02  1.599080456168E-01 -9.536040517638E-02
117 T   1 H     3.168784946962E-02  1.253775349245E-01 -2.020718797685E-01
121 T   6 C     8.867937818005E-02  9.265033778935E-02  9.894867130598E-02
```

Table 4.3: *Coordinates of independent atoms in 1AP-γ's unit cell as optimized in CRYSTAL17 (excerpt from output).*

```
*******************************************************************************
LATTICE PARAMETERS (ANGSTROMS AND DEGREES) - BOHR = 0.5291772083 ANGSTROM
PRIMITIVE CELL - CENTRING CODE 1/0 VOLUME=  3608.388832 - DENSITY  1.348 g/cm^3
A              B              C           ALPHA      BETA       GAMMA
12.55560000    10.95470000    26.24400000    90.000000  91.529000  90.000000
*******************************************************************************
ATOMS IN THE ASYMMETRIC UNIT  186 - ATOMS IN THE UNIT CELL:  372
ATOM                X/A                 Y/B                 Z/C
*******************************************************************************
     1 T   8 O     4.631496148436E-01 -6.059526298284E-02  2.473388646771E-02
     3 T   6 C    -4.819753272192E-01  6.877177025117E-02  9.379610296652E-02
     5 T   6 C    -4.031872520016E-01 -9.229634473521E-03  1.165584661648E-01
     7 T   6 C    -3.528173014491E-01 -1.075463244906E-01  8.979011889587E-02
     9 T   1 H    -3.769809115804E-01 -1.241303705608E-01  5.059704074362E-02
    11 T   6 C    -2.770515856207E-01 -1.792797190968E-01  1.129049144299E-01
    13 T   1 H    -2.402127944878E-01 -2.526531908965E-01  9.177370039613E-02
    15 T   6 C    -2.447770869118E-01 -1.622710250420E-01  1.652315803678E-01
    17 T   6 C    -1.684125660327E-01 -2.371712104983E-01  1.897995602447E-01
    19 T   1 H    -1.321844504324E-01 -3.108040686557E-01  1.687306124557E-01
    21 T   6 C    -1.393392349351E-01 -2.176702530594E-01  2.407904794918E-01
    23 T   1 H    -7.883879461450E-02 -2.747156365597E-01  2.589461705173E-01
    25 T   6 C    -1.858729126049E-01 -1.238612379717E-01  2.683964795407E-01
    27 T   1 H    -1.624716172396E-01 -1.108149764645E-01  3.081917755047E-01
    29 T   6 C    -2.620229503814E-01 -4.645284606974E-02  2.451284507080E-01
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31 T   6 C    -3.111297875108E-01  5.108060983149E-02  2.724199334622E-01
33 T   1 H    -2.904970902450E-01  6.179731793877E-02  3.125392862931E-01
35 T   6 C    -3.822238948569E-01  1.278659229670E-01  2.489609108109E-01
37 T   1 H    -4.177822765581E-01  2.024592600160E-01  2.697894769870E-01
39 T   6 C    -4.130158684158E-01  1.122735353308E-01  1.962697070789E-01
41 T   6 C    -4.852013412740E-01  1.916577904734E-01  1.714565415702E-01
43 T   1 H     4.835583044270E-01  2.695495199967E-01  1.917713060584E-01
45 T   6 C     4.820839472188E-01  1.703418863519E-01  1.213478062232E-01
47 T   1 H     4.246432733905E-01  2.323900536830E-01  1.039097085010E-01
49 T   6 C    -3.694145225793E-01  1.277108396855E-02  1.683355015121E-01
51 T   6 C    -2.921478707304E-01 -6.505184117638E-02  1.928105151449E-01
53 T   6 C     4.664639833768E-01  4.301418334000E-02  4.301129631497E-02
55 T   6 C     4.124675268161E-01  1.476534377352E-01  1.451533262278E-02
57 T   1 H     3.947789198552E-01  1.185331384795E-01 -2.450015248672E-02
59 T   1 H     4.613542087223E-01  2.302479046209E-01  1.442004331283E-02
61 T   1 H     3.371898767761E-01  1.713226903312E-01  3.231060103927E-02
63 T   8 O     4.861279456375E-02  3.055726898607E-01  3.264932864525E-01
65 T   6 C    -1.900879489025E-02  1.781135580393E-01  2.592022005306E-01
67 T   6 C    -9.787488434707E-02  2.590466518700E-01  2.386300994929E-01
69 T   6 C    -1.406012278047E-01  3.602695632111E-01  2.665995676870E-01
71 T   1 H    -1.107189669403E-01  3.762574486637E-01  3.049560470895E-01
73 T   6 C    -2.164110186497E-01  4.352576094127E-01  2.455181483215E-01
75 T   1 H    -2.475134825180E-01 -4.894192496181E-01  2.676017524928E-01
77 T   6 C    -2.552962809824E-01  4.195298864212E-01  1.940872934320E-01
79 T   6 C    -3.305235947470E-01  4.986778803999E-01  1.713319088293E-01
81 T   1 H    -3.613771537609E-01 -4.258711786127E-01  1.931953275338E-01
83 T   6 C    -3.652296699192E-01  4.817217358568E-01  1.209514001610E-01
85 T   1 H    -4.245221331134E-01 -4.569607626280E-01  1.044671909565E-01
87 T   6 C    -3.248709062324E-01  3.864146112279E-01  9.195764435188E-02
89 T   1 H    -3.521776119392E-01  3.755615751748E-01  5.256438616492E-02
91 T   6 C    -2.496357195946E-01  3.048076413133E-01  1.133194423612E-01
93 T   6 C    -2.054303059623E-01  2.066757648574E-01  8.443699455030E-02
95 T   1 H    -2.280083205289E-01  1.985902842410E-01  4.440131085870E-02
97 T   6 C    -1.350372693851E-01  1.262747389071E-01  1.061455779883E-01
99 T   1 H    -1.022648717637E-01  5.265983749812E-02  8.377729635123E-02
101 T   6 C    -1.002859434519E-01  1.383045880243E-01  1.584560818242E-01
103 T   6 C    -2.810752278430E-02  5.582469037049E-02  1.814085600741E-01
105 T   1 H    -1.219837134699E-03 -2.252975179933E-02  1.599834261687E-01
107 T   6 C     1.085090041291E-02  7.537058941623E-02  2.306907676663E-01
109 T   1 H     6.860119653777E-02  1.145092919583E-02  2.465805865958E-01
111 T   6 C    -1.381783202108E-01  2.386521135117E-01  1.877420270822E-01
113 T   6 C    -2.146712777504E-01  3.203999368093E-01  1.651938727464E-01
115 T   6 C     3.862971860849E-02  2.020811737661E-01  3.086652360168E-01
117 T   6 C     8.995054256612E-02  9.477853418157E-02  3.364178001591E-01
119 T   1 H     1.659391364095E-01  7.201699432359E-02  3.191345105113E-01
121 T   1 H     4.048041657003E-02  1.272609413721E-02  3.350765367905E-01
123 T   1 H     1.060209249064E-01  1.208523176704E-01  3.759465171705E-01
125 T   8 O    -2.206436469669E-02 -1.839431311406E-01  3.805567651538E-01
127 T   6 C     4.115220057825E-02 -2.931947374022E-01  4.544023560958E-01
129 T   6 C     1.152924464653E-01 -2.045868098851E-01  4.735484093881E-01
131 T   6 C     1.550842920927E-01 -1.052000180022E-01  4.435887545785E-01
133 T   1 H     1.269209116339E-01 -9.726734466872E-02  4.045388626183E-01
135 T   6 C     2.265307621703E-01 -2.289848812947E-02  4.632420368869E-01
137 T   1 H     2.560503502201E-01  5.018405513475E-02  4.394683346242E-01
139 T   6 C     2.656809377732E-01 -3.043926009373E-02 -4.850554377248E-01
141 T   6 C     3.393046916633E-01  5.372556958217E-02 -4.642313202839E-01
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143 T   1 H     3.667728105131E-01  1.280376023330E-01 -4.877656833119E-01
145 T   6 C     3.781037588886E-01  4.113224560438E-02 -4.142310003026E-01
147 T   1 H     4.373261162472E-01  1.040788482562E-01 -3.988718229443E-01
149 T   6 C     3.438579710525E-01 -5.513936490112E-02 -3.840051947431E-01
151 T   1 H     3.750371655817E-01 -6.397128054592E-02 -3.451748401363E-01
153 T   6 C     2.708507160446E-01 -1.416331040282E-01 -4.034516368345E-01
155 T   6 C     2.370903668286E-01 -2.436639595657E-01 -3.737109566109E-01
157 T   1 H     2.676376835489E-01 -2.512389008291E-01 -3.348416397375E-01
159 T   6 C     1.682760654951E-01 -3.284423930650E-01 -3.933971600207E-01
161 T   1 H     1.440407766176E-01 -4.061904468145E-01 -3.708291328290E-01
163 T   6 C     1.262146778904E-01 -3.184541778896E-01 -4.445987881809E-01
165 T   6 C     5.688802902118E-02 -4.067412092726E-01 -4.655124043148E-01
167 T   1 H     3.610024242328E-02 -4.857647484174E-01 -4.429339258063E-01
169 T   6 C     1.602298399878E-02 -3.939285985075E-01  4.851966123305E-01
171 T   1 H    -3.826012972032E-02 -4.632737165172E-01  4.707353048888E-01
173 T   6 C     1.567669511262E-01 -2.172074071508E-01 -4.753156254766E-01
175 T   6 C     2.303792657878E-01 -1.295453072681E-01 -4.545873798820E-01
177 T   6 C    -1.495017690935E-02 -2.816298261775E-01  4.037594363140E-01
179 T   6 C    -6.854009911820E-02 -3.942025351630E-01  3.808943272827E-01
181 T   1 H    -1.414077115785E-01 -4.161024332995E-01  4.010775068093E-01
183 T   1 H    -1.724582837401E-02 -4.748357505758E-01  3.829130689300E-01
185 T   1 H    -9.047672346224E-02 -3.743975409387E-01  3.412692305508E-01
187 T   8 O    -4.341513101817E-01 -4.612674750568E-01 -3.460866876852E-01
189 T   6 C     4.993717032743E-01 -3.410826400201E-01 -4.158804348429E-01
191 T   6 C     4.251975316761E-01 -4.272976005828E-01 -4.368142525858E-01
193 T   6 C     3.861701620398E-01  4.690330214078E-01 -4.090962451869E-01
195 T   1 H     4.164669729487E-01  4.543216179857E-01 -3.706873476716E-01
197 T   6 C     3.124436403041E-01  3.912390633307E-01 -4.301725458526E-01
199 T   1 H     2.830036671190E-01  3.150830694473E-01 -4.080676147241E-01
201 T   6 C     2.731434050279E-01  4.055694783181E-01 -4.816155116448E-01
203 T   6 C     1.999948401223E-01  3.239736475196E-01  4.955671732357E-01
205 T   1 H     1.712467399531E-01  2.474539723672E-01 -4.825621946625E-01
207 T   6 C     1.645345569668E-01  3.402275471293E-01  4.452645927133E-01
209 T   1 H     1.061740225900E-01  2.785162849063E-01  4.282879942858E-01
211 T   6 C     2.025430874982E-01  4.371453059708E-01  4.164287370636E-01
213 T   1 H     1.751046899320E-01  4.470536438574E-01  3.770592628156E-01
215 T   6 C     2.748841514737E-01 -4.781565141148E-01  4.379015387392E-01
217 T   6 C     3.132439812450E-01 -3.757061193679E-01  4.096076451995E-01
219 T   1 H     2.902222042743E-01 -3.683789318384E-01  3.696260366885E-01
221 T   6 C     3.775448702641E-01 -2.899802420827E-01  4.319922241671E-01
223 T   1 H     4.036165817734E-01 -2.106769839487E-01  4.108136053420E-01
225 T   6 C     4.141085626990E-01 -3.029446500851E-01  4.840059203721E-01
227 T   6 C     4.811911868666E-01 -2.159995650233E-01 -4.925931876148E-01
229 T   1 H    -4.982960343605E-01 -1.343196987536E-01  4.866881792678E-01
231 T   6 C    -4.773014933775E-01 -2.352176333995E-01 -4.438300381973E-01
233 T   1 H    -4.234280027286E-01 -1.674737121258E-01 -4.277310123506E-01
235 T   6 C     3.834227938357E-01 -4.078711237849E-01 -4.875168784320E-01
237 T   6 C     3.105204712552E-01 -4.932891840967E-01  4.896922402631E-01
239 T   6 C    -4.434125358131E-01 -3.599020648409E-01 -3.660724699006E-01
241 T   6 C    -3.919901447956E-01 -2.500543696857E-01 -3.400096822430E-01
243 T   1 H    -3.728578946731E-01 -2.739236206435E-01 -3.004922460860E-01
245 T   1 H    -4.425381787595E-01 -1.688191889532E-01 -3.412435324117E-01
247 T   1 H    -3.176328462328E-01 -2.260792817568E-01 -3.585735249708E-01
249 T   8 O    -4.531966124942E-01  6.178894712429E-02 -3.025249334893E-01
251 T   6 C    -4.295894731628E-01  1.346290416618E-01 -2.165088239006E-01
253 T   6 C    -3.658418044423E-01  3.620151092521E-02 -1.969554029942E-01
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255 T   6 C    -3.253445253366E-01 -6.082700703384E-02 -2.280248305105E-01
257 T   1 H    -3.440034313010E-01 -5.812769682422E-02 -2.683427916696E-01
259 T   6 C    -2.637280707524E-01 -1.522266132142E-01 -2.077730983467E-01
261 T   1 H    -2.323669478973E-01 -2.226139885483E-01 -2.323975796434E-01
263 T   6 C    -2.361627729204E-01 -1.572110955449E-01 -1.545186394629E-01
265 T   6 C    -1.698930795951E-01 -2.487484834912E-01 -1.335932851061E-01
267 T   1 H    -1.386813832606E-01 -3.183412730979E-01 -1.584585479724E-01
269 T   6 C    -1.418914449935E-01 -2.485896599503E-01 -8.187367428685E-02
271 T   1 H    -8.699844563182E-02 -3.160284043619E-01 -6.617169675550E-02
273 T   6 C    -1.811988637423E-01 -1.582867760335E-01 -4.985509112238E-02
275 T   1 H    -1.588604979446E-01 -1.587094312171E-01 -9.560344084728E-03
277 T   6 C    -2.471686097952E-01 -6.467562089209E-02 -6.921718414324E-02
279 T   6 C    -2.849849993078E-01  3.181704392084E-02 -3.736587507832E-02
281 T   1 H    -2.645518441437E-01  2.878868937613E-02  3.057757303505E-03
283 T   6 C    -3.434180595408E-01  1.256851384371E-01 -5.738901581811E-02
285 T   1 H    -3.697566862351E-01  2.004943386045E-01 -3.368646570408E-02
287 T   6 C    -3.713386424104E-01  1.300633673308E-01 -1.108023127706E-01
289 T   6 C    -4.307325180152E-01  2.271150491063E-01 -1.316081767593E-01
291 T   1 H    -4.541488526322E-01  3.011780070718E-01 -1.069464264646E-01
293 T   6 C    -4.592874285664E-01  2.283112623847E-01 -1.829948513858E-01
295 T   1 H     4.940719924139E-01  3.046758587761E-01 -1.972064665887E-01
297 T   6 C    -3.379539621058E-01  3.409939067851E-02 -1.435948355957E-01
299 T   6 C    -2.747474251892E-01 -6.294142136890E-02 -1.224386544952E-01
301 T   6 C    -4.692601724436E-01  1.419857844604E-01 -2.706945929770E-01
303 T   6 C     4.646216494182E-01  2.522095812062E-01 -2.870236738488E-01
305 T   1 H     4.456427701185E-01  2.434951003874E-01 -3.276392059613E-01
307 T   1 H    -4.928562051898E-01  3.380454879924E-01 -2.803226902515E-01
309 T   1 H     3.901323857158E-01  2.568943074509E-01 -2.663769827417E-01
311 T   8 O    -2.824217935986E-02  1.711967195019E-01 -9.404107627042E-03
313 T   6 C    -3.031606651455E-02  1.072174313535E-01 -9.699411375002E-02
315 T   6 C    -9.231568734837E-02  2.049500212696E-01 -1.183730744659E-01
317 T   6 C    -1.326442560739E-01  3.050974833909E-01 -8.903658658236E-02
319 T   1 H    -1.151499233149E-01  3.055041951384E-01 -4.859713122134E-02
321 T   6 C    -1.937954571303E-01  3.947562623692E-01 -1.109481037335E-01
323 T   1 H    -2.250195719008E-01  4.676893150333E-01 -8.757643670891E-02
325 T   6 C    -2.203999616740E-01  3.951329175105E-01 -1.643434629767E-01
327 T   6 C    -2.865817563597E-01  4.844657735355E-01 -1.869672493699E-01
329 T   1 H    -3.195064970007E-01 -4.444017008236E-01 -1.633808152077E-01
331 T   6 C    -3.117369237740E-01  4.806833679305E-01 -2.389221345845E-01
333 T   1 H    -3.654613846857E-01 -4.529148064630E-01 -2.562158347385E-01
335 T   6 C    -2.699154925012E-01  3.892056827836E-01 -2.695738932561E-01
337 T   1 H    -2.906639654029E-01  3.879160493036E-01 -3.100090083771E-01
339 T   6 C    -2.040919997347E-01  2.976077335583E-01 -2.484475297206E-01
341 T   6 C    -1.632027212496E-01  1.999048037772E-01 -2.787970957833E-01
343 T   1 H    -1.791597643305E-01  2.020164324542E-01 -3.196202416776E-01
345 T   6 C    -1.070354495256E-01  1.063036794195E-01 -2.570691774549E-01
347 T   1 H    -7.927742857002E-02  3.010189376311E-02 -2.796771587125E-01
349 T   6 C    -8.290593371050E-02  1.052574205676E-01 -2.032310057819E-01
351 T   6 C    -2.524854271070E-02  9.403679456488E-03 -1.805361581796E-01
353 T   1 H    -1.362230462863E-03 -6.683972458171E-02 -2.037091502959E-01
355 T   6 C     1.020863026681E-03  1.145276247345E-02 -1.289966356493E-01
357 T   1 H     4.583169288042E-02 -6.469371865710E-02 -1.133641857854E-01
359 T   6 C    -1.174438567246E-01  2.036466934125E-01 -1.720105431864E-01
361 T   6 C    -1.797353631530E-01  2.991783920956E-01 -1.949164419244E-01
363 T   6 C     2.340464659664E-03  9.921713477052E-02 -4.202329688562E-02
365 T   6 C     7.786908532849E-02 -2.692580922435E-03 -2.543025617076E-02
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```
367 T   1 H     9.764225077650E-02  1.004257721846E-02  1.489803697716E-02
369 T   1 H     1.509696818837E-01 -2.342741663634E-03 -4.722784361264E-02
371 T   1 H     4.105357717899E-02 -9.259570005451E-02 -3.059193105841E-02
```

Table 4.4: *Coordinates of atoms in single flat molecule of 1AP optimized in CRYSTAL17 (excerpt from output).*

```
*****************************************************************************
ATOMS IN THE ASYMMETRIC UNIT   31 - ATOMS IN THE UNIT CELL:   31
ATOM             X(ANGSTROM)         Y(ANGSTROM)         Z(ANGSTROM)
*****************************************************************************
1 T   8 O    -3.706729449568E-01  1.869554592867E+00 -2.535090293646E-01
2 T   6 C     4.526274991576E-02  1.086291816676E+00 -1.098916859443E+00
3 T   6 C    -3.131791455510E-01  1.168077300080E+00 -2.551159495335E+00
4 T   6 C     9.783328387555E-01 -3.224464946055E-02 -6.439450480384E-01
5 T   6 C     1.552303109174E-01  1.522504153792E-01 -3.404129585345E+00
6 T   6 C    -1.102604579859E+00  2.220739327260E+00 -3.106100018746E+00
7 T   1 H     1.158106733832E+00  1.020606077668E-01  4.227819627859E-01
8 T   1 H     1.932373434802E+00 -6.520634517698E-03 -1.180467751070E+00
9 T   1 H     5.311090240400E-01 -1.018314532367E+00 -8.095679407249E-01
10 T   1 H     7.537529907385E-01 -6.522956534358E-01 -2.995764972849E+00
11 T   6 C    -1.240480581670E-01  1.338725304305E-01 -4.760342388620E+00
12 T   6 C    -1.386016232605E+00  2.204507753410E+00 -4.512767015966E+00
13 T   6 C    -1.630929876711E+00  3.314838448735E+00 -2.331747878797E+00
14 T   1 H     2.530511003738E-01 -6.715960954139E-01 -5.384002123124E+00
15 T   6 C    -8.932823356567E-01  1.150811346549E+00 -5.342217636807E+00
16 T   6 C    -2.167090685909E+00  3.243189785719E+00 -5.108077944525E+00
17 T   1 H    -1.423883942991E+00  3.328312661694E+00 -1.272708313106E+00
18 T   6 C    -2.373015844120E+00  4.301691460803E+00 -2.907608284306E+00
19 T   6 C    -1.192537148462E+00  1.155296061769E+00 -6.746217457335E+00
20 T   6 C    -2.671446583527E+00  4.308783769476E+00 -4.307786302932E+00
21 T   6 C    -2.449601333152E+00  3.225448195398E+00 -6.508271178524E+00
22 T   1 H    -2.756455304829E+00  5.114249873238E+00 -2.295793785154E+00
23 T   1 H    -8.072218455417E-01  3.419854440867E-01 -7.354864131577E+00
24 T   6 C    -1.936918028050E+00  2.147185101710E+00 -7.304992940982E+00
25 T   6 C    -3.436126974179E+00  5.321790775070E+00 -4.909046863008E+00
26 T   6 C    -3.217801269231E+00  4.257988469239E+00 -7.067766262654E+00
27 T   1 H    -2.156640122930E+00  2.140828486587E+00 -8.369263524203E+00
28 T   1 H    -3.816813833780E+00  6.130549967425E+00 -4.291353159149E+00
29 T   6 C    -3.705615013945E+00  5.295470080660E+00 -6.275034230399E+00
30 T   1 H    -3.429366042265E+00  4.238800306244E+00 -8.133433981081E+00
31 T   1 H    -4.298361211704E+00  6.086210450483E+00 -6.725015992672E+00
```

Table 4.5: *Coordinates of atoms in single twisted molecule of 1AP optimized in CRYSTAL17 (excerpt from output). This molecule features total energy 0.1 kJ mol^{-1} higher than the flat one.*

```
*****************************************************************************
ATOMS IN THE ASYMMETRIC UNIT   31 - ATOMS IN THE UNIT CELL:   31
ATOM             X(ANGSTROM)         Y(ANGSTROM)         Z(ANGSTROM)
*****************************************************************************
1 T   6 C    -3.288505153402E+00  2.835353147931E+00 -1.251676450826E+00
2 T   6 C    -3.660463245016E+00  4.021765095781E+00 -1.909063390294E+00
3 T   6 C    -2.434063266135E+00  1.913288740131E+00 -1.927997137798E+00
```

```
 4 T   6 C    -3.811300445247E+00  2.605317185669E+00  1.330873251177E-01
 5 T   1 H    -4.307439417097E+00  4.729240280836E+00 -1.405485459251E+00
 6 T   6 C    -3.219190182988E+00  4.332549735086E+00 -3.184513342597E+00
 7 T   6 C    -1.989028028046E+00  2.229154827837E+00 -3.254968211539E+00
 8 T   6 C    -2.002045885997E+00  6.622359573913E-01 -1.358773286298E+00
 9 T   8 O    -3.422792882658E+00  1.698890309445E+00  8.599434150505E-01
10 T   6 C    -4.883943158475E+00  3.549496635945E+00  6.677891054201E-01
11 T   1 H    -3.522376720230E+00  5.263557421148E+00 -3.654886712392E+00
12 T   6 C    -2.382134430247E+00  3.451045689016E+00 -3.882410774218E+00
13 T   6 C    -1.143513935467E+00  1.326075318923E+00 -3.971060461833E+00
14 T   1 H    -2.327465399147E+00  4.246258105251E-01 -3.575516160441E-01
15 T   6 C    -1.199578584532E+00 -1.947386174988E-01 -2.049878848337E+00
16 T   1 H    -4.491496212733E+00  4.563803630384E+00  7.994428234721E-01
17 T   1 H    -5.206475414918E+00  3.168784481272E+00  1.637118101076E+00
18 T   1 H    -5.742814042738E+00  3.611485972735E+00 -7.872872537429E-03
19 T   6 C    -1.917892411026E+00  3.747527728591E+00 -5.208156221053E+00
20 T   6 C    -7.385114385863E-01  9.741216332257E-02 -3.373614002258E+00
21 T   6 C    -6.982121032203E-01  1.642942012128E+00 -5.290891549669E+00
22 T   1 H    -8.925017692096E-01 -1.132243035289E+00 -1.593501061209E+00
23 T   1 H    -2.228806320797E+00  4.684161367259E+00 -5.662478494489E+00
24 T   6 C    -1.112612269513E+00  2.883350732907E+00 -5.882708953927E+00
25 T   6 C     8.952460237232E-02 -7.799076752107E-01 -4.092769536182E+00
26 T   6 C     1.289400429263E-01  7.375006513159E-01 -5.973208651833E+00
27 T   1 H    -7.681199215405E-01  3.117729382309E+00 -6.886344806799E+00
28 T   1 H     3.935982911754E-01 -1.714790704995E+00 -3.629919611087E+00
29 T   6 C     5.179403499463E-01 -4.618308769687E-01 -5.379170859318E+00
30 T   1 H     4.644023000303E-01  9.840095515650E-01 -6.976935239505E+00
31 T   1 H     1.157715457136E+00 -1.150987798813E+00 -5.922190588291E+00
```

4.2 Band gaps

Table 4.6: *Energy levels of Highest Occupied Crystalline Orbital (HOCO), Lowest Unoccupied Crystalline Orbital (LUCO), band gap extent and peak absorption wavelength (from HOCO – LUCO gap) calculated in CRYSTAL17. Approximate experimental emission maxima, obtained using recursive fitting of a Gaussian function in a 40nm range, provided for reference.*

		1AP-α	1AP-β	1AP-γ
E_{HOMO}	/ Hartree	-0.193439	-0.190872	-0.187023
E_{LUMO}	/ Hartree	-0.083063	-0.082877	-0.081520
Band Gap	/ Hartree	0.110376	0.107994	0.105503
Band Gap	/ eV	3.003	2.939	2.871
Calculated absorption	/ nm	413	422	432
Measured excitation	/ nm	n/a	n/a	420
Measured emission	/ nm	545	538	527

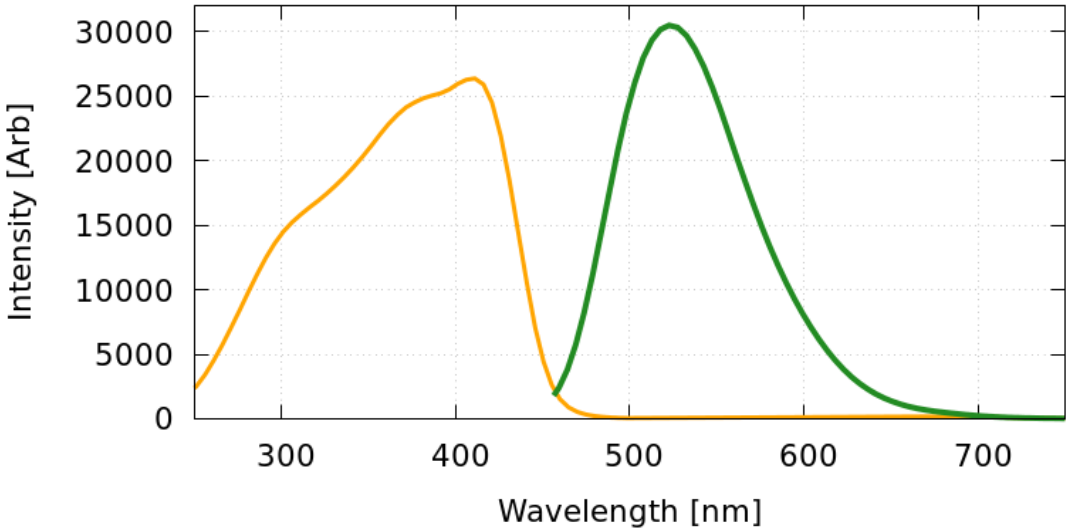

Figure 4.1: *Excitation (orange) and emission (green) spectra of crystalline 1AP-γ (excitation spectra recorded for emission maximum at 532 nm).*

Chapter 5

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