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Supporting Information

Sorption of small molecule vapours by single crystals of [Pt{4'-(Ph)trpy}(NCS)]SbF_6 where trpy = 2,2':6',2''-terpyridine: a porous material with a structure stabilised by extended π-π interactions

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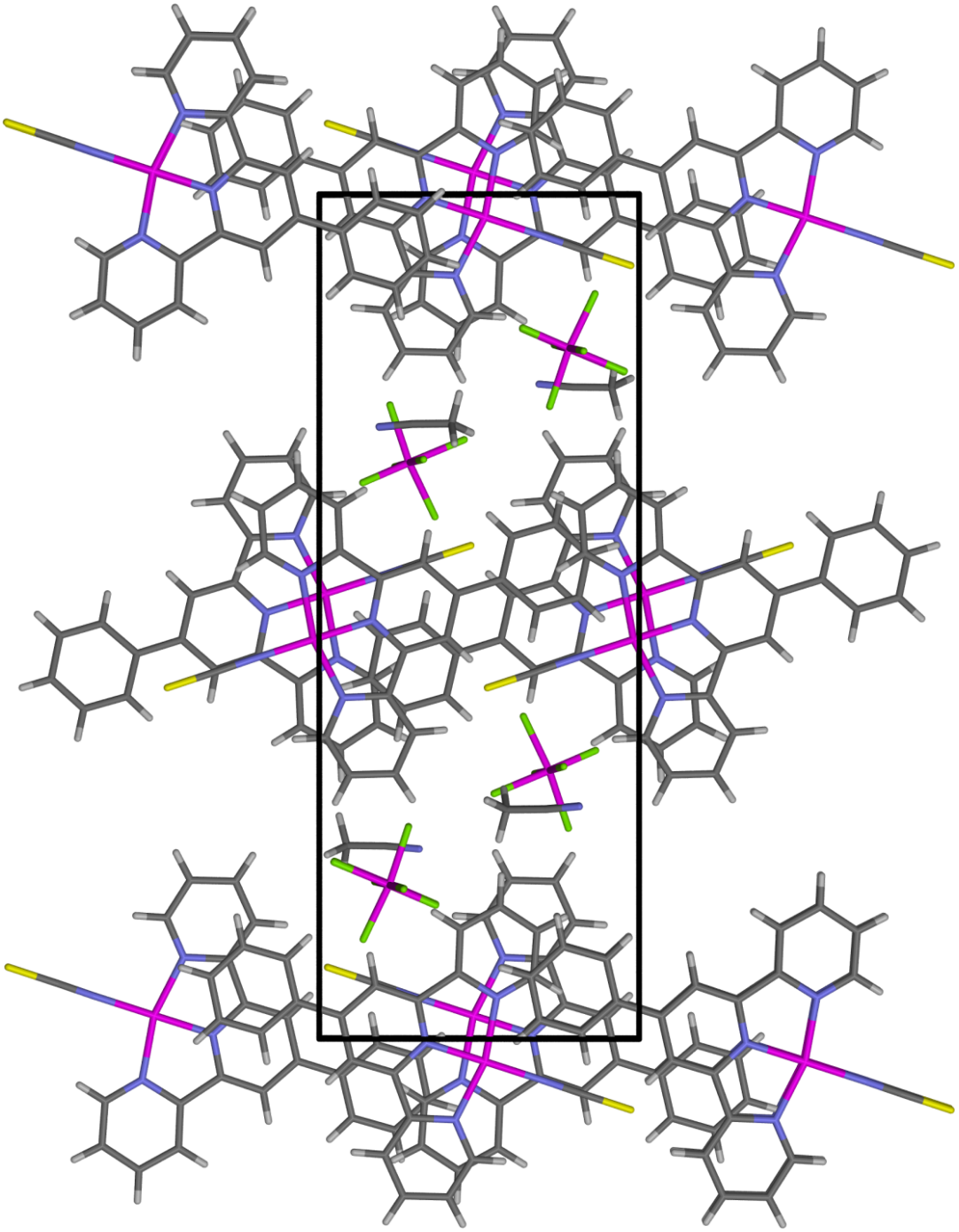

Figure S1 View down the [c]-axis showing the unit cell contents of **1·CH$_3$CN**. The [b]-axis points downwards.

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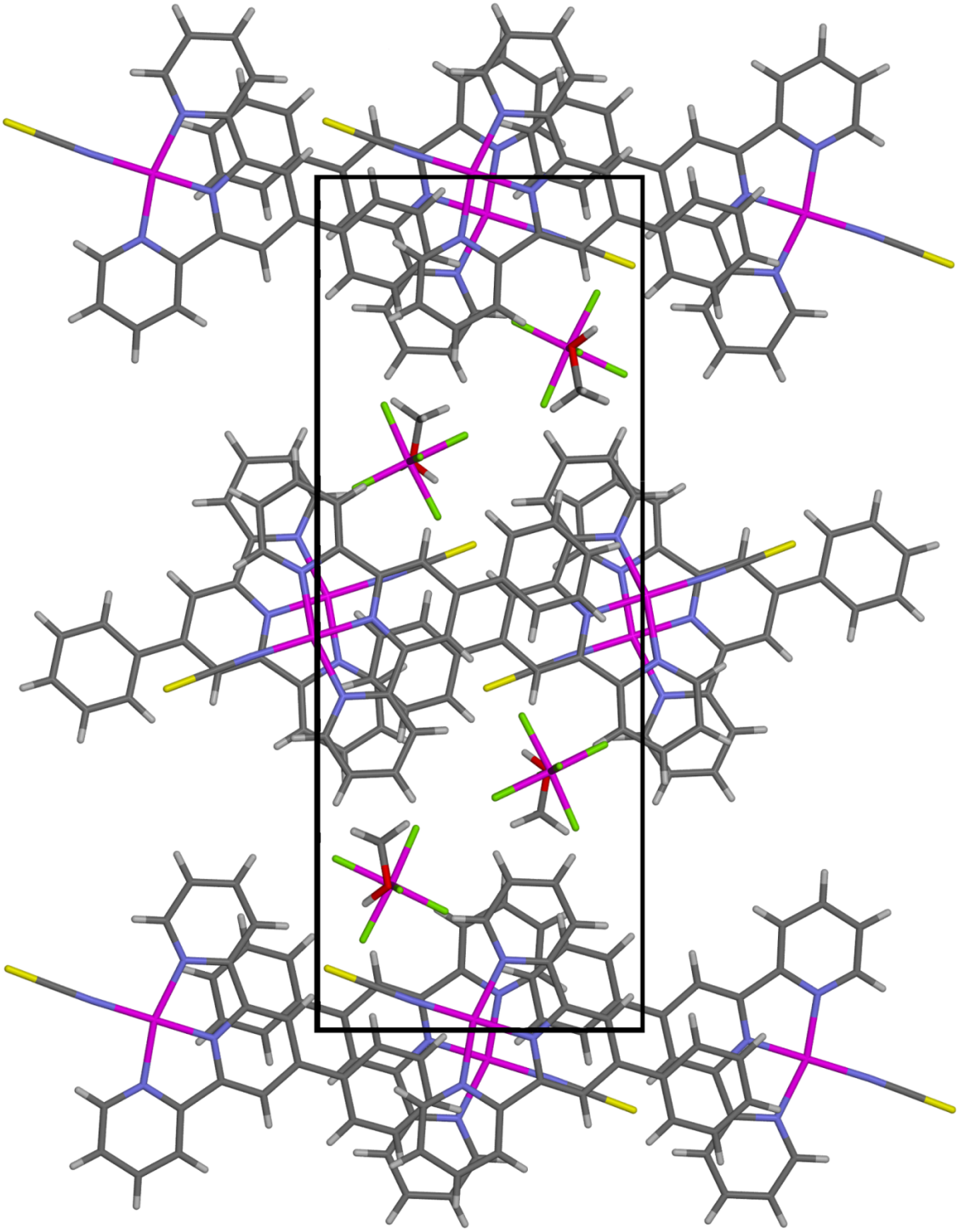

Figure S2 View down the [c]-axis showing the unit cell contents of **1·CH$_3$OH**. The [b]-axis points downwards.

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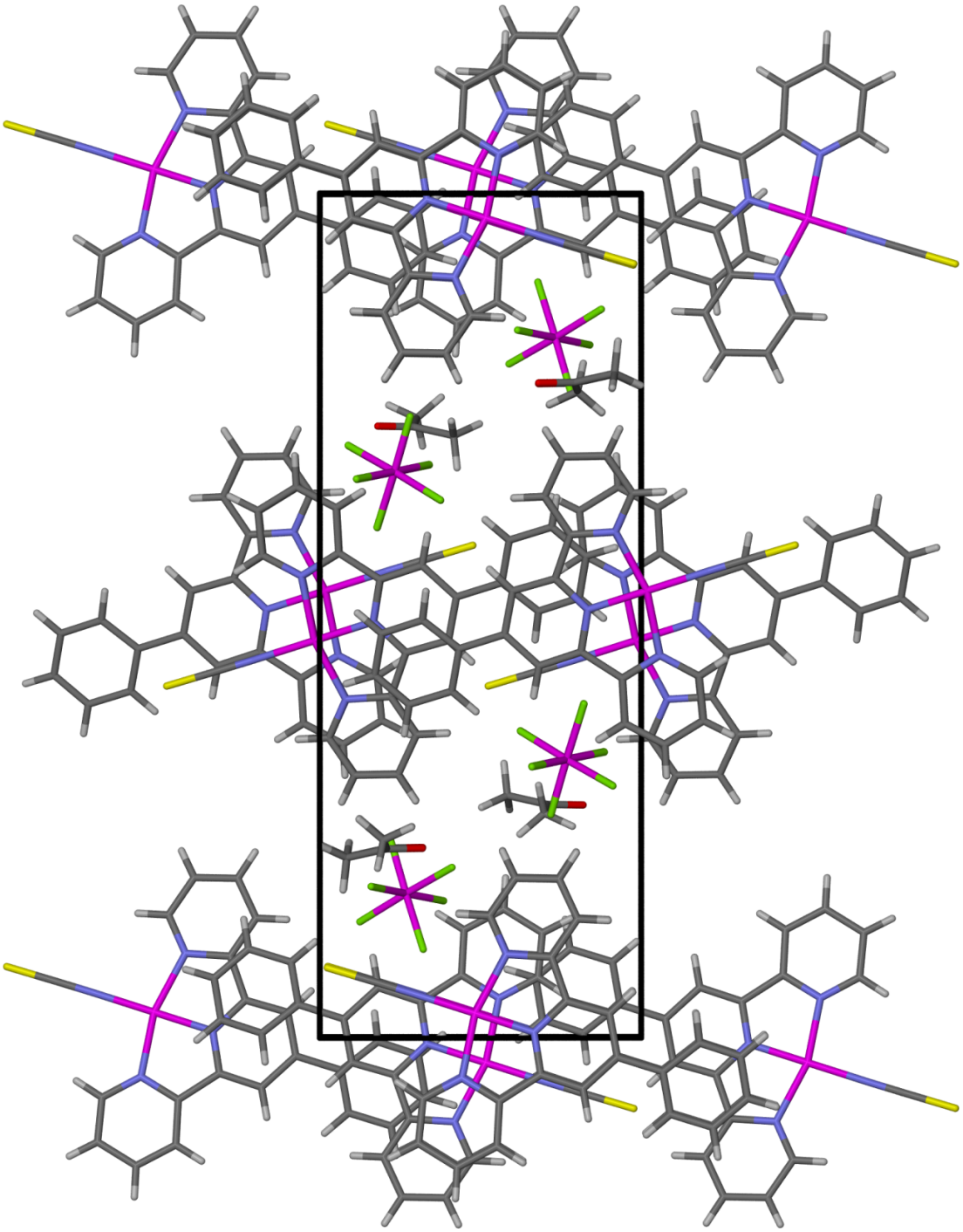

Figure S3 View down the [c]-axis showing the unit cell contents of **1·(CH$_3$)$_2$CO**. The [b]-axis points downwards.

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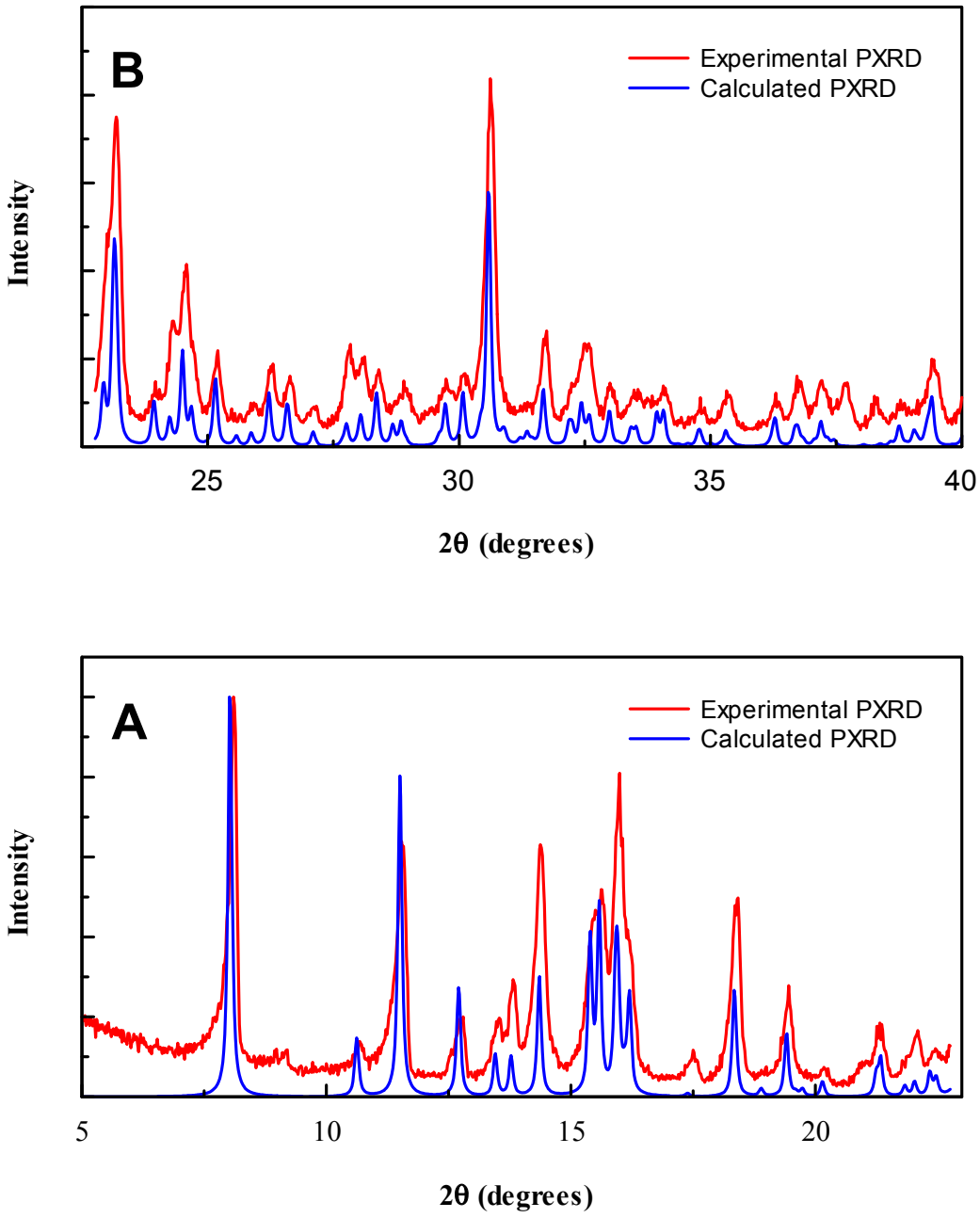

Figure S4 Comparison of the experimentally measured 295 K powder XRD spectrum of **1** (where the powder was obtained by crushing single crystals of **1**) with the spectrum calculated from a single crystal structure determination of **1** also at 295 K: see **1_295K.cif** in the Supplementary Data. The 2θ ranges are 5-23° in (A) and 23-40° in (B).

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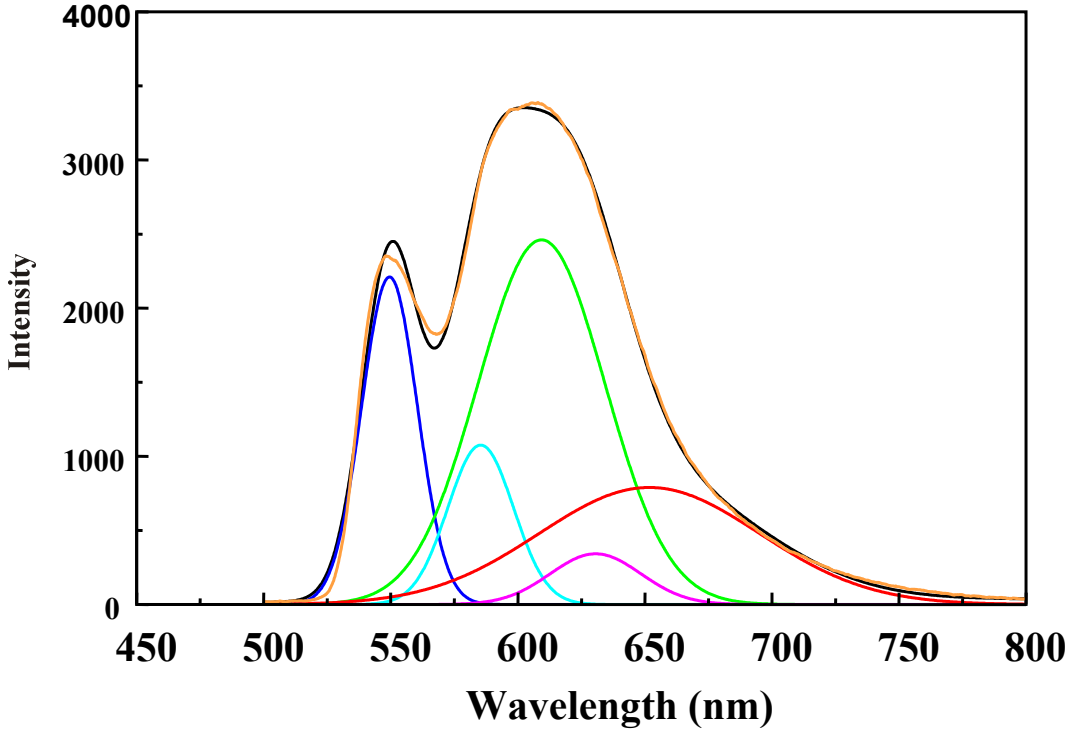

Figure S5 Solid state emission spectrum recorded at 77 K of **1·CH$_3$OH,** deconvoluted into five constituent Gaussian bands (r^2 = 0.9990; fit std error = 35.29). Components due to ^{3}MLCT emission are shown in blue, light-blue and pink, to ^{3}MMLCT emission in green and to excimeric π-π* emission in red. The observed spectrum is shown by the orange line and the calculated spectrum by the black line.

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checkCIF/PLATON report (basic structural check)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: 1Me2CO_exp

Bond precision: C-C = 0.0326 A Wavelength=0.71073

Cell: a=9.8258(11) b=25.4680(3) c=10.9263(12)
alpha=90 beta=98.527(9) gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	2704.0(4)	2704.0(4)
Space group	P 21/n	P2(1)/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C22 H15 N4 Pt S, C3 H6 O, F6 Sb	C22 H15 N4 Pt S, C3 H6 O, F6 Sb
Sum formula	C25 H21 F6 N4 O Pt S Sb	C25 H21 F6 N4 O Pt S Sb
Mr	856.37	856.36
Dx,g cm-3	2.104	2.104
Z	4	4
Mu (mm-1)	6.313	6.312
F000	1624.0	1624.0
F000'	1616.35	
h,k,lmax	12,31,13	11,31,13
Nref	5393	5158
Tmin,Tmax	0.240,0.388	0.161,0.388
Tmin'	0.073	

Correction method= AbsCorr=MULTI-SCAN

Data completeness= Ratio = 0.956 Theta(max)= 26.130

R(reflections)= 0.1002(3484) wR2(reflections)= 0.2037(5158)

S = 1.608 Npar= 352

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

PLAT211 ALERT 2 A ADP of Atom C17 is NPD .....
?

Alert level B

SHFSU01 ALERT 2 B The absolute value of parameter shift to su ratio > 0.10

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```
            Absolute value of the parameter shift to su ratio given
0.182
            Additional refinement cycles may be required.
PLAT080_ALERT_2_B Maximum Shift/Error ..........................
0.18
PLAT213_ALERT_2_B Atom N2      has ADP max/min Ratio .............
4.20 oblat
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds (x 1000) Ang ...
33
```

Alert level C

```
RFACG01_ALERT_3_C  The value of the R factor is > 0.10
            R factor given   0.100
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low .......
0.97
PLAT213_ALERT_2_C Atom C15     has ADP max/min Ratio .............
3.30 prola
PLAT214_ALERT_2_C Atom C25     (Anion/Solvent) ADP max/min Ratio
5.00 prola
PLAT362_ALERT_2_C Short  C(sp3)-C(sp2) Bond  C23    -   C25    ...
1.41 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact  F6     ..  C1      ..
2.89 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for
C23
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors for
Sb
```

```
   1 ALERT level A = In general: serious problem
   4 ALERT level B = Potentially serious problem
   8 ALERT level C = Check and explain
   0 ALERT level G = General alerts; check

   0 ALERT type 1 CIF construction/syntax error, inconsistent or
missing data
   8 ALERT type 2 Indicator that the structure model may be wrong or
deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for p
IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiati*
you intend to submit to *Acta Crystallographica Section C* or *E*, you should make sure that full publication ch
the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submi

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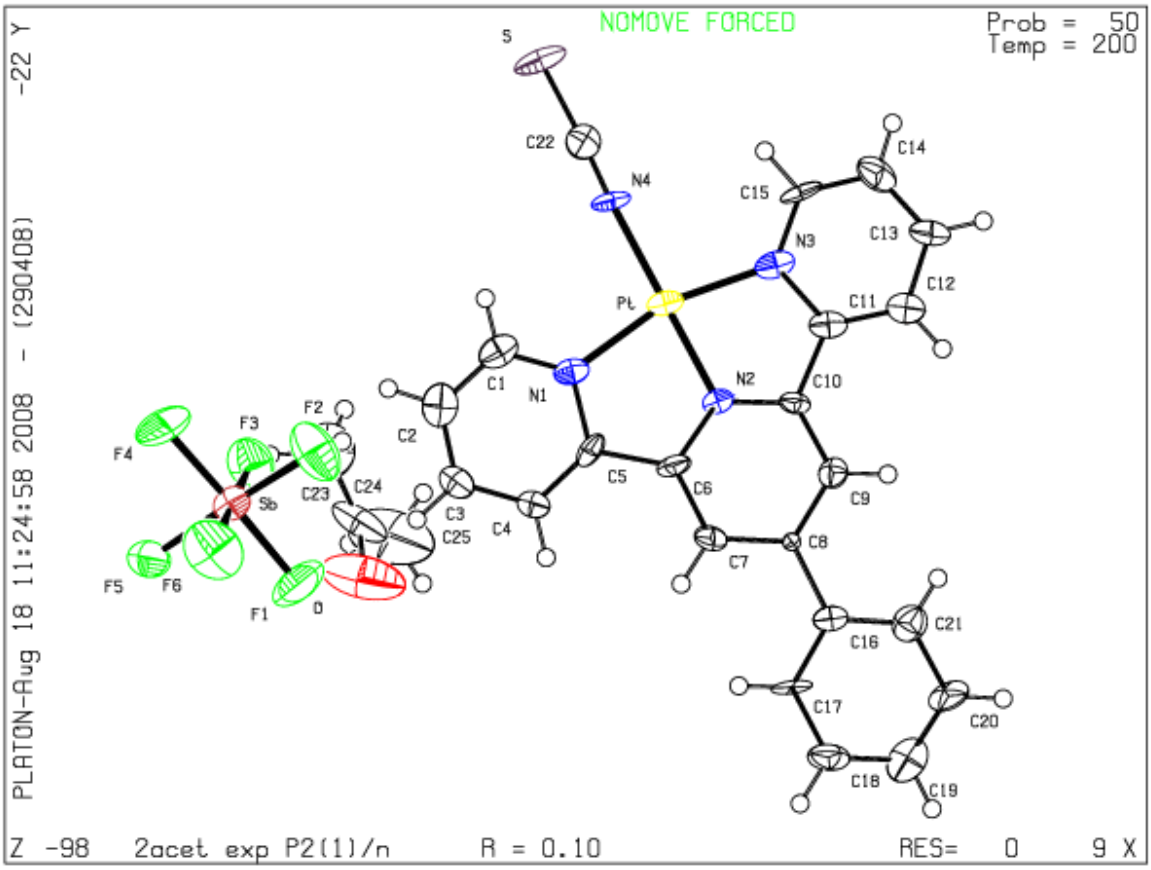
PLATON version of 29/04/2008; check.def file version of 22/04/2008

Datablock 1Me2CO_exp - ellipsoid plot



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