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Correction of the Space Group of {[Ni(bipy)$_2$(ONO$_2$)$_2$].-[2(pyrene)]}

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Synopsis.

Change of the space group of {[Ni(bipy)$_2$(ONO$_2$)$_2$].[2(pyrene)]} from *Pn* to *P*2$_1$/*n* leads to a revised description of the structure.

Abstract.

The crystal structure of {[Ni(bipy)$_2$(ONO$_2$)$_2$].[2(pyrene)]} was originally reported in space group *Pn* ((Biradha *et al*., *Chem. Commun*. 1327–1328, (1999)). Reasons are given for changing the space group to *P*2$_1$/*n.* Consequently, incorrect descriptions of the title compound in the literature must be altered. In particular, the structure is not polar. It is further contended that description in terms of "complementary, interpenetrating covalent and noncovalent 2D networks" is misleading as the "noncovalent network" (of pyrenes) has geometrical but not physical significance. The title compound is a typical host-guest inclusion complex.

Table A (to be deposited). The non-hydrogen coordinates of {[Ni(bipy)$_2$.(ONO$_2$)$_2$].-.2(pyrene)} in space group *P*2$_1$/*n.*

CELL 11.360 22.770 15.858 90.00 93.956 90.00

COORD Ni1 NI 0.243075 0.237795 0.254245

COORD O1 O 0.212350 0.244350 0.123250

COORD O2 O 0.249750 0.280500 0.005000

COORD O3 O 0.347150 0.207950 0.049950

COORD O4 O 0.244250 0.229250 0.386050

COORD O5 O 0.195550 0.267600 0.502200

COORD O6 O 0.374450 0.267200 0.474100

COORD N3 N 0.256900-0.168650 0.242000

COORD N4 N 0.244300 0.143750 0.251600

COORD N5 N 0.428700 0.240800 0.256050

COORD N6 N 1.054500 0.239950 0.253550

COORD N9 N 0.268250 0.245350 0.057150

COORD N10 N 0.265050 0.253650 0.454550

COORD C15 C 0.191400-0.137500 0.184250

COORD C14 C 0.187550-0.077150 0.182750

COORD C13 C 0.253100-0.045200 0.244400

COORD C12 C 0.321050-0.077250 0.303850

COORD C11 C 0.321250-0.137800 0.300250

COORD C16 C 0.250100 0.019950 0.246100

COORD C17 C 0.235450 0.053350 0.173300

COORD C18 C 0.234000 0.114050 0.178300

COORD C19 C 0.261650 0.050600 0.321900

COORD C20 C 0.257350 0.110950 0.322200

COORD C21 C 0.483150 0.269550 0.196050

COORD C22 C 0.604250 0.271800 0.192750

COORD C23 C 0.675900 0.244850 0.255350

COORD C24 C 0.619550 0.216750 0.319200

COORD C25 C 0.498200 0.215050 0.316600

COORD C26 C 0.806600 0.244600 0.255450

COORD C27 C 0.861450 0.226500 0.184250

COORD C28 C 0.983400 0.224500 0.186350

COORD C29 C 0.878950 0.261000 0.325700

COORD C30 C 1.000650 0.258550 0.321700

COORD C101 C 0.372250 0.512400 0.566700

COORD C102 C 0.340150 0.452300 0.581500

COORD C103 C 0.399550 0.408000 0.549400

COORD C104 C 0.499450 0.417400 0.499600

COORD C105 C 0.564450 0.371650 0.465900

COORD C106 C 0.656450 0.384500 0.417150

COORD C107 C 0.687800 0.441400 0.400900

COORD C116 C 0.468450 0.523800 0.516700

COORD C201 C 0.534400 0.512300 0.192650

COORD C202 C 0.549800 0.572300 0.194450

COORD C203 C 0.544100 0.604250 0.120550

COORD C204 C 0.523850 0.576450 0.041950

COORD C205 C 0.520900 0.607900-0.037200

COORD C206 C 0.504500 0.579750-0.111500

COORD C207 C 0.487500 0.517650-0.116700

COORD C215 C 0.508450 0.515000 0.039400

COORD C301 C 0.175450 0.578950-0.084850

COORD C302 C 0.120850 0.631050-0.066550

COORD C303 C 0.019550 0.632150-0.023600

COORD C304 C -0.030100 0.581050 0.003400

COORD C305 C -0.136750 0.580050 0.047100

COORD C306 C -0.180700 0.529850 0.073650

COORD C307 C -0.129200 0.474450 0.058700

COORD C315 C 0.025150 0.526400-0.013850

COORD C401 C 0.036950 0.491450 0.692950

COORD C402 C 0.050750 0.431500 0.697200

COORD C403 C 0.042500 0.397550 0.623700

COORD C404 C 0.022650 0.423850 0.545350

COORD C405 C 0.017500 0.391050 0.467350

COORD C406 C 0.001050 0.417700 0.391650

COORD C407 C -0.014500 0.479850 0.384000

COORD C415 C -0.009000 0.514100 0.459950