Electronic Supplementary Information.

Contents.

The following is a compilation of calculated tensor values for GIPAW refined x-ray powder, x-ray single crystal and neutron single crystal diffraction structures. The PBE functional was employed together with the ultrasoft pseudopotential for all calculated values. Tensor values computed using unrefined neutron diffraction coordinates are included for comparison.

I. **Acetaminophen**.

GIPAW refined neutron

Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1	218.97	136.78	35.51	130.42
C2	207.91	152.01	3.75	121.22
C3	195.96	129.31	13.20	112.82
C4	231.24	161.49	63.23	151.99
C5	194.29	128.30	16.70	113.10
C6	205.14	135.86	14.84	118.61
C7	236.70	171.01	88.31	165.34
C8	41.81	27.84	-4.69	21.65

GIPAW refined powder

Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1	219.20	135.68	35.56	130.15
C2	208.20	151.85	4.34	121.46
C3	196.37	129.48	13.82	113.22
C4	231.14	162.06	63.30	152.17
C5	195.22	129.84	16.29	113.78
C6	204.33	134.59	15.38	118.10
C7	238.41	169.27	87.95	165.21
C8	44.91	24.88	-9.89	19.97

	GIPAW refined X-ray single crystal			
Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1	218.96	136.91	35.70	130.52
C2	208.08	151.69	3.82	121.20
C3	195.98	129.41	13.25	112.88
C4	231.17	161.54	63.48	152.06
C5	194.45	128.56	16.72	113.24
C6	205.01	135.14	15.12	118.42
C7	237.05	170.76	88.66	165.49
C8	41.21	28.13	-4.78	21.52

I. **Acetaminophen** (continued).

	Neutron, no geometry optimization			
Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1	217.97	131.88	34.43	128.10
C2	206.08	150.45	0.13	118.89
C3	196.15	129.31	10.90	112.12
C4	226.55	154.34	61.47	147.45
C5	194.41	128.44	12.28	111.71
C6	207.07	134.14	10.18	117.13
C7	233.53	161.70	84.60	159.94
C8	30.60	14.33	-34.46	3.49

II. **Adenosine**.

	GIPAW refined neutron			
Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C2	232.68	164.33	58.83	151.95
C4	214.95	161.18	57.83	144.65
C5	159.43	153.85	45.71	119.67
C6	201.76	193.71	52.73	149.40
C8	212.82	135.00	60.72	136.18
C1’	110.56	100.51	74.11	95.06
C2’	107.29	74.55	34.56	72.14
C3’	89.54	80.94	59.13	76.54
C4’	115.29	97.47	45.13	85.96
C5’	90.58	66.79	31.69	63.02

GIPAW refined powder

Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C2	232.93	162.99	59.73	151.88
C4	215.16	161.29	58.28	144.91
C5	159.32	154.01	45.89	119.74
C6	201.39	194.53	53.21	149.71
C8	212.89	134.30	60.90	136.03
C1’	110.96	101.17	73.41	95.18
C2’	107.43	74.87	34.73	72.34
C3’	90.06	81.96	58.98	77.00
C4’	115.99	97.58	46.04	86.54
C5’	91.44	66.95	31.60	63.33

II. **Adenosine** (continued).

GIPAW refined X-ray single crystal

Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C2	232.97	163.14	59.23	151.78
C4	215.15	161.21	58.10	144.82
C5	159.39	153.92	45.72	119.67
C6	201.49	194.22	52.92	149.54
C8	212.75	134.63	60.67	136.02
C1’	110.73	100.89	73.81	95.15
C2’	107.40	74.67	34.38	72.15
C3’	90.04	81.15	58.91	76.70
C4’	115.50	97.44	45.25	86.06
C5’	90.87	67.26	31.43	63.18

Neutron, no geometry optimization

Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C2	233.17	162.39	59.59	151.71
C4	214.47	160.99	55.63	143.70
C5	156.95	152.91	45.46	118.44
C6	199.48	194.71	51.14	148.44
C8	209.93	132.70	60.16	134.26
C1’	109.67	98.17	74.24	94.02
C2’	105.25	74.40	33.05	70.90
C3’	89.53	78.99	58.66	75.73
C4’	115.09	96.52	44.73	85.45
C5’	89.57	67.45	31.96	62.99

III. **Naphthalene**.

	GIPAW refined neutron			
Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1, C5	224.04	143.53	17.37	128.32
C2, C6	226.82	139.74	3.98	123.51
C3, C7	226.49	139.71	3.53	123.24
C4, C8	222.72	149.10	14.28	128.70
C4a, C8a	205.39	201.99	-12.52	131.62

III. **Naphthalene** (continued).

	GIPAW refined powder			
Position	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1, C5	224.20	143.29	17.50	128.33
C2, C6	226.97	139.66	4.06	123.56
C3, C7	226.77	139.33	3.82	123.31
C4, C8	222.73	148.50	14.55	128.59
C4a, C8a	205.28	201.88	-12.33	131.61

	GIPAW refined X-ray single crystal			
Positions	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1, C5	224.06	143.29	17.35	128.23
C2, C6	226.76	139.94	3.94	123.55
C3, C7	226.38	139.75	3.44	123.19
C4, C8	222.70	148.77	14.31	128.59
C4a, C8a	205.25	201.77	-12.53	131.50

	Neutron, no geometry optimization			
Positions	δ_{11} (ppm)	δ_{22} (ppm)	δ_{33} (ppm)	δ_{iso} (ppm)
C1, C5	223.84	142.23	15.58	127.22
C2, C6	225.71	138.21	0.39	121.44
C3, C7	224.93	138.17	0.41	121.17
C4, C8	221.54	146.68	11.28	126.50
C4a, C8a	203.50	200.46	-14.84	129.71

Force, RMDS, SSNMR and bond length data before and after GIPAW refinement.

The following is a compilation of calculated forces upon the atoms, the RMSD deviation of atomic positions and the agreement between calculated and experimental SSNMR ^{13}C shift tensor principal values before and after GIPAW refinement of the x-ray powder, x-ray single crystal and neutron single crystal diffraction structures. A comparison of the changes in bond lengths from refinement in also included as Table 9. All calculated values use the PBE functional together with the ultrasoft pseudopotential.

Powder data.

Table 1. Comparison of the forces on the atoms in the unrefined powder (P) and the GIPAW refined powder (rP) structures.

	Forces (eV Å^{-1})			
	P	rP (PBE)	rP (PW91)	rP (LDA)
Naphthalene	0.2515	0.0020	0.0030	0.0031
Acetaminophen	1.7435	0.0028	0.0029	0.0081
Adenosine	0.5361	0.0032	0.0047	0.0087

Table 2. Comparison between experimental and computed ^{13}C tensor principal values for the unrefined powder (P) and GIPAW refined powder (rP) structures.

	SSNMR error (ppm)[a]			
	P	rP (PBE)	rP (PW91)	rP (LDA)
Naphthalene	4.25	3.01[b]	3.13	2.82
Acetaminophen	10.99	4.78[b]	4.80	4.95
Adenosine	4.50	4.16[b]	4.31	5.49

[a]All RMS error values are calculated by comparing experimental principal values to computed principal values obtained using the diffraction coordinates both before and after GIPAW refinement. All values were computed using Alderman's icosahedral representation (D. W. Alderman, G. McGeorge, J. Z. Hu, R. J. Pugmire and D. M. Grant, *Mol. Phys.*, 1998, **95**, 1113-1126).
[b]The SSNMR error for these refined structures differ statistically from errors computed using the original diffraction coordinates at statistical confidence levels of 90.00%, 99.99%, and 67.00%, respectively, for naphthalene, acetaminophen and adenosine.

X-ray single crystal data.

Table 3. A comparison of the average forces on the atoms in the unrefined single crystal x-ray (SC) and the GIPAW refinement coordinates (rSC).

	Forces (eV Å^{-1})	
Structure	SC	rSC (PBE)
Naphthalene	1.3461	0.0045
Acetaminophen	3.8630	0.0021
Adenosine	3.2600	0.0027

Table 4. Errors computed SSNMR ^{13}C tensor principal values for x-ray single crystal structures (SC) and the structures after GIPAW refinement (rSC).

	SSNMR error (ppm)[a]		
	SC	rSC (all atoms)	rSC (H only)
Naphthalene	5.34	3.11[b]	5.19
Acetaminophen	13.06	4.73[b]	5.81
Adenosine	9.65	4.13[b]	4.68

[a]All error values are obtained by comparing experimental principal values to computed principal values obtained using the diffraction coordinates both before and after GIPAW refinement. All values were computed using Alderman's icosahedral representation (D. W. Alderman, G. McGeorge, J. Z. Hu, R. J. Pugmire and D. M. Grant, *Mol. Phys.*, 1998, **95**, 1113-1126). The PBE functional was used for all calculations.
[b]The SSNMR error for these refined structures differ from errors computed using the original diffraction coordinates at a statistical confidence of 98%, 99.999% and 99.999%, respectively, for the naphthalene, acetaminophen and adenosine structures.

Tables 5. A comparison of RMSDs (Å) in atom positions for powder (P) and single crystal x-ray coordinates (SC) relative to the neutron diffraction values after refinement of all atoms and after refinement of only H atoms.

	RMSD (Å)					
	SC	rSC (all atoms)	rSC (H only)	P	rP (all atoms)	rP (H only)
Naphthalene	0.012	0.019[a]	-	0.013	0.019	0.013
Acetaminophen	0.067	0.053	0.053	0.163	0.046	0.039
Adenosine	0.093	0.086	0.035	0.354	0.109	0.064

[a]No hydrogen positions were reported in this structure, thus only carbon positions are compared.

Neutron single crystal data.

Table 6. A comparison of the average forces on the atoms in the unrefined single crystal neutron diffraction structures (N) and these structures after GIPAW refinement (rN).

	Forces (eV Å^{-1})	
Structure	N	rN
Naphthalene	0.2210	0.0052
Acetaminophen	1.9608	0.0036
Adenosine	0.0753	0.0031

Table 7. A comparison of experimental and computed SSNMR ^{13}C tensor principal values for the unrefined neutron single crystal (N) and GIPAW refined (rN) structures.

	SSNMR error (ppm)[a]	
	N	rN
Naphthalene	4.77	3.09[b]
Acetaminophen	10.05	4.75[b]
Adenosine	4.39	4.11[b]

[a]All error values are obtained by comparing experimental principal values to the corresponding computed principal values calculated using the diffraction coordinates both before and after GIPAW refinement. All values were computed using Alderman's icosahedral representation (D. W. Alderman, G. McGeorge, J. Z. Hu, R. J. Pugmire and D. M. Grant, *Mol. Phys.*, 1998, **95**, 1113-1126). The PBE functional was used for all calculations.
[b]The SSNMR error for these refined structures can be said to differ from the pre-GIPAW structures at a statistical confidence level of 95.0%, 99.98% and 64.0%, respectively, for the naphthalene, acetaminophen and adenosine structures.

Table 8. A comparison of the RMSDs (Å) in atomic positions of the unrefined single crystal neutron coordinates (N) versus GIPAW refined neutron (rN) and unrefined x-ray single crystal (SC) positions.

	RMSD (Å)[a]	
	N vs rN	N vs SC
Naphthalene	0.019	0.012
Acetaminophen	0.050	0.067
Adenosine	0.067	0.093

[a]These RMSDs compare all atoms in the structures.

A comparison of bond lengths from GIPAW refinement.

Table 9. A comparison of differences (Å) in bond lengths for structures obtained from powder (P) or x-ray single crystal (SC) data versus neutron diffraction values (N) and the influence of GIPAW refinement on bond lengths.

Compound	Bond	P vs N[a]	rP vs N[a]	SC vs N	rSC vs N
Naphthalene	C – C	0.0059	0.0093	0.0119	0.0093
	C – H	H positions not reported in SC or P data			
Acetaminophen	C – C	0.0149	0.0209	0.0154	0.0213
	C – N	0.0184	0.0206	0.0032	0.0206
	C – O	0.0396	0.0282	0.0150	0.0300
	C – H	0.0639	0.0921	0.0986	0.0927
	N – H	0.0220	0.0520	0.0740	0.0510
	O – H	0.0360	0.0430	0.0790	0.0420
Adenosine	C – C	0.0112	0.0127	0.0076	0.0061
	C – N	0.0102	0.0072	0.0050	0.0059
	C – O	0.0151	0.0097	0.0049	0.0057
	C – H	NA	0.0101	0.1456	0.0041
	N – H	NA	0.0028	0.1643	0.0107
	O – H	NA	0.0135	0.1177	0.0173
Overall RMSD[b]	C – C	0.0109	0.0146	0.0116	0.0136
	C – N	0.0108	0.0072	0.0046	0.0059
	C – O	0.0203	0.0097	0.0073	0.0057
	C – H	0.0639	0.0101	0.1215	0.0036
	N – H	0.0220	0.0368	0.1274	0.0389
	O – H	0.0360	0.0135	0.1063	0.0233

[a]Differences in bond lengths for corresponding positions both before and after GIPAW refinement of the original diffraction data.
[b]The number of C–C, C–N, C–O bond included in this analysis was, respectively, 19, 12 and 7. The number of C–H, N–H, and O–H bonds evaluated was, respectively, 15, 3 and 4.

GIPAW refined crystal structure coordinates.

This file contains a total of nine sets of refined diffraction coordinates in CIF format. The structures include the refined x-ray powder, x-ray single crystal and neutron single crystal coordinates for adenosine, acetaminophen and naphthalene. All structures were refined at the GGA-PBE level of theory using parameters summarized in the Experimental section of the manuscript. In all cases, the reported diffraction coordinates were used as an initial starting point.

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N3     N    -0.36334   0.02503   0.30052   0.00000  Uiso   1.00
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```
N4     N    -0.30637   0.22832   0.05788   0.00000  Uiso   1.00
N5     N    -0.51578   0.23494   0.21487   0.00000  Uiso   1.00
O1     O    -0.83823   0.39126   0.26043   0.00000  Uiso   1.00
O2     O    -0.63997   0.29520   0.50711   0.00000  Uiso   1.00
O3     O    -0.37332   0.53541   0.50079   0.00000  Uiso   1.00
O4     O    -0.99817   0.64405   0.18409   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C3      1.539   .     S
C1     H9      1.101   .     S
C1     N5      1.469   .     S
C1     O1      1.412   .     S
C2     H1      1.088   .     S
C2     N1      1.340   .     S
C2     N3      1.340   .     S
C3     C4      1.533   .     S
C3     H10     1.102   .     S
C3     O2      1.411   .     S
C4     C6      1.536   .     S
C4     H12     1.101   .     S
C4     O3      1.413   .     S
C5     C7      1.403   .     S
C5     N3      1.350   .     S
C5     N5      1.377   .     S
C6     C8      1.515   .     S
C6     H2      1.104   .     S
C6     O1      1.454   .     S
C7     C9      1.419   .     S
C7     N4      1.385   .     S
C8     H3      1.104   .     S
C8     H4      1.107   .     S
C8     O4      1.425   .     S
C9     N1      1.364   .     S
C9     N2      1.336   .     S
C10    H6      1.084   .     S
C10    N4      1.323   .     S
C10    N5      1.374   .     S
H5     O4      1.010   .     S
H7     N2      1.028   .     S
H8     N2      1.037   .     S
H11    O2      1.000   .     S
H13    O3      1.005   .     S
#===END


data_ADENOS11_powder_H_added
_audit_creation_date              2012-05-17
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P21'
_symmetry_Int_Tables_number       4
```

```
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x,y+1/2,-z
_cell_length_a                    4.8392
_cell_length_b                    10.2908
_cell_length_c                    11.8569
_cell_angle_alpha                 90.0000
_cell_angle_beta                  99.3090
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
N1     N     0.90054  -0.10255   0.18321   0.00000  Uiso   1.00
C2     C     0.77575  -0.08455   0.27499   0.00000  Uiso   1.00
N3     N     0.63252   0.01959   0.30113   0.00000  Uiso   1.00
C4     C     0.62394   0.11268   0.22040   0.00000  Uiso   1.00
C5     C     0.75201   0.10913   0.12238   0.00000  Uiso   1.00
C6     C     0.89803  -0.00651   0.10378   0.00000  Uiso   1.00
N7     N     0.69662   0.22254   0.05986   0.00000  Uiso   1.00
C8     C     0.53822   0.29150   0.11869   0.00000  Uiso   1.00
N9     N     0.48783   0.23043   0.21635   0.00000  Uiso   1.00
N10    N     1.02780  -0.02699   0.01406   0.00000  Uiso   1.00
C11    C     0.32532   0.27669   0.30275   0.00000  Uiso   1.00
C12    C     0.51322   0.31652   0.41482   0.00000  Uiso   1.00
C13    C     0.54249   0.46325   0.39759   0.00000  Uiso   1.00
C14    C     0.25760   0.50112   0.32835   0.00000  Uiso   1.00
C15    C     0.26804   0.61537   0.24849   0.00000  Uiso   1.00
O16    O     0.16500   0.38628   0.26130   0.00000  Uiso   1.00
O17    O     0.37196   0.29402   0.50807   0.00000  Uiso   1.00
O18    O     0.62597   0.53482   0.49914   0.00000  Uiso   1.00
O19    O    -0.00064   0.63720   0.18211   0.00000  Uiso   1.00
H20    H     0.79151  -0.16421   0.33602   0.00000  Uiso   1.00
H21    H     0.45044   0.38646   0.09523   0.00000  Uiso   1.00
H22    H     1.02257   0.04065  -0.05102   0.00000  Uiso   1.00
H23    H     1.11076  -0.11740   0.00385   0.00000  Uiso   1.00
H24    H     0.18574   0.19650   0.31845   0.00000  Uiso   1.00
H25    H     0.71757   0.26671   0.42569   0.00000  Uiso   1.00
H26    H     0.70405   0.47883   0.34345   0.00000  Uiso   1.00
H27    H     0.10819   0.52087   0.38739   0.00000  Uiso   1.00
H28    H     0.42652   0.59660   0.19284   0.00000  Uiso   1.00
H29    H     0.33761   0.70184   0.30050   0.00000  Uiso   1.00
H30    H     0.36116   0.19734   0.51447   0.00000  Uiso   1.00
H31    H     0.51567   0.51179   0.56123   0.00000  Uiso   1.00
H32    H    -0.02771   0.73420   0.17290   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
```

```
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
N1      C2      1.340   .      S
N1      C6      1.364   .      S
C2      N3      1.340   .      S
C2      H20     1.088   .      S
N3      C4      1.350   .      S
C4      C5      1.403   .      S
C4      N9      1.376   .      S
C5      C6      1.419   .      S
C5      N7      1.385   .      S
C6      N10     1.337   .      S
N7      C8      1.323   .      S
C8      N9      1.374   .      S
C8      H21     1.084   .      S
N9      C11     1.468   .      S
N10     H22     1.036   .      S
N10     H23     1.028   .      S
C11     C12     1.539   .      S
C11     O16     1.411   .      S
C11     H24     1.101   .      S
C12     C13     1.533   .      S
C12     O17     1.410   .      S
C12     H25     1.103   .      S
C13     C14     1.536   .      S
C13     O18     1.414   .      S
C13     H26     1.101   .      S
C14     C15     1.516   .      S
C14     O16     1.454   .      S
C14     H27     1.104   .      S
C15     O19     1.425   .      S
C15     H28     1.107   .      S
C15     H29     1.104   .      S
O17     H30     1.000   .      S
O18     H31     1.005   .      S
O19     H32     1.010   .      S
#===END


data_HXACAN01_x-ray
_audit_creation_date              2012-05-23
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P21/A'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,y+1/2,-z
  -x,-y,-z
  x+1/2,-y+1/2,z
_cell_length_a                    12.9300
```

```
_cell_length_b                          9.4000
_cell_length_c                          7.1000
_cell_angle_alpha                       90.0000
_cell_angle_beta                        115.9000
_cell_angle_gamma                       90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C    -0.06411   0.35155  -0.15085   0.00000  Uiso   1.00
C2     C     0.00863   0.34873  -0.25040   0.00000  Uiso   1.00
C3     C     0.10399   0.25909  -0.17703   0.00000  Uiso   1.00
C4     C     0.12882   0.17090  -0.00355   0.00000  Uiso   1.00
C5     C     0.05727   0.17571   0.09828   0.00000  Uiso   1.00
C6     C    -0.03781   0.26520   0.02531   0.00000  Uiso   1.00
C7     C    -0.22220   0.50524  -0.39935   0.00000  Uiso   1.00
C8     C    -0.32404   0.59084  -0.41443   0.00000  Uiso   1.00
H1     H    -0.00915   0.41624  -0.38510   0.00000  Uiso   1.00
H2     H     0.16055   0.25967  -0.25449   0.00000  Uiso   1.00
H3     H     0.07579   0.10846   0.23413   0.00000  Uiso   1.00
H4     H    -0.09310   0.26841   0.10537   0.00000  Uiso   1.00
H5     H     0.24275   0.04200   0.20291   0.00000  Uiso   1.00
H6     H    -0.19661   0.44554  -0.10771   0.00000  Uiso   1.00
H7     H    -0.39822   0.57090  -0.56505   0.00000  Uiso   1.00
H8     H    -0.34716   0.56898  -0.28595   0.00000  Uiso   1.00
H9     H    -0.30394   0.70461  -0.41211   0.00000  Uiso   1.00
N1     N    -0.16249   0.43862  -0.21400   0.00000  Uiso   1.00
O1     O     0.22201   0.08291   0.06000   0.00000  Uiso   1.00
O2     O    -0.19471   0.49883  -0.54792   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.402   .     S
C1     C6      1.403   .     S
C1     N1      1.411   .     S
C2     C3      1.393   .     S
C2     H1      1.085   .     S
C3     C4      1.401   .     S
C3     H2      1.090   .     S
C4     C5      1.402   .     S
C4     O1      1.366   .     S
C5     C6      1.390   .     S
C5     H3      1.089   .     S
C6     H4      1.091   .     S
C7     C8      1.507   .     S
C7     N1      1.354   .     S
```

```
C7     O2      1.253   .     S
C8     H7      1.097   .     S
C8     H8      1.096   .     S
C8     H9      1.099   .     S
H5     O1      1.006   .     S
H6     N1      1.029   .     S
#===END


data_HXACAN19_neutron
_audit_creation_date              2012-05-17
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P21/A'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,y+1/2,-z
  -x,-y,-z
  x+1/2,-y+1/2,z
_cell_length_a                    12.8720
_cell_length_b                    9.3700
_cell_length_c                    7.0850
_cell_angle_alpha                 90.0000
_cell_angle_beta                  115.6200
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C    -0.06547   0.35300  -0.15123   0.00000  Uiso   1.00
C2     C     0.00815   0.34995  -0.25012   0.00000  Uiso   1.00
C3     C     0.10346   0.25968  -0.17684   0.00000  Uiso   1.00
C4     C     0.12752   0.17099  -0.00364   0.00000  Uiso   1.00
C5     C     0.05536   0.17643   0.09822   0.00000  Uiso   1.00
C6     C    -0.03977   0.26647   0.02495   0.00000  Uiso   1.00
C7     C    -0.22388   0.50611  -0.40072   0.00000  Uiso   1.00
C8     C    -0.32647   0.59154  -0.41639   0.00000  Uiso   1.00
N1     N    -0.16423   0.44015  -0.21497   0.00000  Uiso   1.00
O1     O     0.22040   0.08204   0.05939   0.00000  Uiso   1.00
O2     O    -0.19584   0.49928  -0.54913   0.00000  Uiso   1.00
H1     H    -0.00911   0.41771  -0.38458   0.00000  Uiso   1.00
H2     H     0.16062   0.26006  -0.25395   0.00000  Uiso   1.00
H3     H     0.07343   0.10906   0.23410   0.00000  Uiso   1.00
H4     H    -0.09562   0.27000   0.10484   0.00000  Uiso   1.00
H5     H     0.24103   0.04110   0.20256   0.00000  Uiso   1.00
H6     H    -0.19880   0.44722  -0.10878   0.00000  Uiso   1.00
H7     H    -0.39937   0.57448  -0.56937   0.00000  Uiso   1.00
```

```
H8     H    -0.35212   0.56655  -0.29123   0.00000  Uiso   1.00
H9     H    -0.30532   0.70578  -0.40789   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.401   .     S
C1     C6      1.403   .     S
C1     N1      1.411   .     S
C2     C3      1.393   .     S
C2     H1      1.085   .     S
C3     C4      1.401   .     S
C3     H2      1.090   .     S
C4     C5      1.402   .     S
C4     O1      1.364   .     S
C5     C6      1.390   .     S
C5     H3      1.089   .     S
C6     H4      1.091   .     S
C7     C8      1.507   .     S
C7     N1      1.353   .     S
C7     O2      1.252   .     S
C8     H7      1.096   .     S
C8     H8      1.097   .     S
C8     H9      1.100   .     S
N1     H6      1.029   .     S
O1     H5      1.007   .     S
#===END


data_HXACAN26_powder
_audit_creation_date              2012-05-29
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P21/A'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,y+1/2,-z
  -x,-y,-z
  x+1/2,-y+1/2,z
_cell_length_a                    12.8856
_cell_length_b                    9.3801
_cell_length_c                    7.1010
_cell_angle_alpha                 90.0000
_cell_angle_beta                  115.7002
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
```

```
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.44111   0.35006  -0.14759   0.00000  Uiso   1.00
C2     C     0.51567   0.34905  -0.24418   0.00000  Uiso   1.00
C3     C     0.61093   0.25879  -0.17085   0.00000  Uiso   1.00
C4     C     0.63380   0.16801  -0.00078   0.00000  Uiso   1.00
C5     C     0.55994   0.17013   0.09723   0.00000  Uiso   1.00
C6     C     0.46516   0.26058   0.02478   0.00000  Uiso   1.00
C7     C     0.28233   0.50163  -0.39830   0.00000  Uiso   1.00
C8     C     0.17398   0.57618  -0.41948   0.00000  Uiso   1.00
N1     N     0.34266   0.43758  -0.21130   0.00000  Uiso   1.00
O1     O     0.72742   0.08032   0.06326   0.00000  Uiso   1.00
O2     O     0.31219   0.49756  -0.54401   0.00000  Uiso   1.00
H1     H     0.74879   0.04092   0.20721   0.00000  Uiso   1.00
H2     H     0.49988   0.41887  -0.37568   0.00000  Uiso   1.00
H3     H     0.66924   0.26136  -0.24525   0.00000  Uiso   1.00
H4     H     0.57595   0.09928   0.22844   0.00000  Uiso   1.00
H5     H     0.40813   0.26184   0.10192   0.00000  Uiso   1.00
H6     H     0.14212   0.64609  -0.55615   0.00000  Uiso   1.00
H7     H     0.10720   0.49683  -0.43834   0.00000  Uiso   1.00
H8     H     0.18906   0.63899  -0.27965   0.00000  Uiso   1.00
H9     H     0.30771   0.44477  -0.10583   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.402   .     S
C1     C6      1.403   .     S
C1     N1      1.411   .     S
C2     C3      1.393   .     S
C2     H2      1.085   .     S
C3     C4      1.401   .     S
C3     H3      1.090   .     S
C4     C5      1.402   .     S
C4     O1      1.365   .     S
C5     C6      1.390   .     S
C5     H4      1.089   .     S
C6     H5      1.091   .     S
C7     C8      1.510   .     S
C7     N1      1.354   .     S
C7     O2      1.251   .     S
C8     H6      1.093   .     S
C8     H7      1.101   .     S
C8     H8      1.097   .     S
N1     H9      1.030   .     S
O1     H1      1.007   .     S
#===END


data_NAPHTA11_x-ray_H_added
```

```
_audit_creation_date              2012-05-17
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P21/A'
_symmetry_Int_Tables_number       14
_symmetry_cell_setting            monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,y+1/2,-z
  -x,-y,-z
  x+1/2,-y+1/2,z
_cell_length_a                    8.2350
_cell_length_b                    6.0030
_cell_length_c                    8.6580
_cell_angle_alpha                 90.0000
_cell_angle_beta                  122.9200
_cell_angle_gamma                 90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.08740   0.01708   0.32901   0.00000  Uiso   1.00
C2     C     0.11545   0.16019   0.22091   0.00000  Uiso   1.00
C3     C     0.04843   0.10443   0.03628   0.00000  Uiso   1.00
C4     C     0.07447   0.24835  -0.07854   0.00000  Uiso   1.00
C5     C    -0.00842  -0.18889   0.25730   0.00000  Uiso   1.00
H6     H     0.13920   0.06349   0.47052   0.00000  Uiso   1.00
H7     H     0.18877   0.31952   0.27531   0.00000  Uiso   1.00
H8     H     0.14860   0.40691  -0.02263   0.00000  Uiso   1.00
H9     H    -0.03090  -0.30104   0.34339   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.379   .     S
C1     C5      1.416   .     S
C1     H6      1.092   .     S
C2     C3      1.419   .     S
C2     H7      1.092   .     S
C3     C4      1.419   .     S
C3     C3      1.435   3     S
C4     H8      1.092   .     S
C4     C5      1.380   3     S
C5     H9      1.092   .     S
C5     C4      1.380   3     S
#===END
```

```
data_NAPHTA36_neutron
_audit_creation_date                2012-05-17
_audit_creation_method              'Materials Studio'
_symmetry_space_group_name_H-M      'P21/A'
_symmetry_Int_Tables_number         14
_symmetry_cell_setting              monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x+1/2,y+1/2,-z
  -x,-y,-z
  x+1/2,-y+1/2,z
_cell_length_a                      8.2560
_cell_length_b                      5.9830
_cell_length_c                      8.6770
_cell_angle_alpha                   90.0000
_cell_angle_beta                    122.7290
_cell_angle_gamma                   90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.08653   0.01746   0.32788   0.00000  Uiso   1.00
C2     C     0.11573   0.16022   0.22027   0.00000  Uiso   1.00
C3     C     0.04881   0.10440   0.03619   0.00000  Uiso   1.00
C4     C     0.07582   0.24811  -0.07815   0.00000  Uiso   1.00
C5     C    -0.01018  -0.18841   0.25625   0.00000  Uiso   1.00
H1     H     0.13833   0.06388   0.46899   0.00000  Uiso   1.00
H2     H     0.19013   0.31928   0.27453   0.00000  Uiso   1.00
H3     H     0.15024   0.40679  -0.02236   0.00000  Uiso   1.00
H4     H    -0.03364  -0.30034   0.34189   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.379   .     S
C1     C5      1.416   .     S
C1     H1      1.092   .     S
C2     C3      1.419   .     S
C2     H2      1.092   .     S
C3     C4      1.419   .     S
C3     C3      1.434   3     S
C4     H3      1.092   .     S
C4     C5      1.380   3     S
C5     H4      1.093   .     S
C5     C4      1.380   3     S
```

```
#===END


data_NAPHTHA37_power_H_added
_audit_creation_date                2012-05-17
_audit_creation_method              'Materials Studio'
_symmetry_space_group_name_H-M      'P21/C'
_symmetry_Int_Tables_number         14
_symmetry_cell_setting              monoclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
  -x,y+1/2,-z+1/2
  -x,-y,-z
  x,-y+1/2,z+1/2
_cell_length_a                      8.6869
_cell_length_b                      6.0123
_cell_length_c                      8.2938
_cell_angle_alpha                   90.0000
_cell_angle_beta                    122.5971
_cell_angle_gamma                   90.0000
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
C1     C     0.03510   0.10438   0.04808   0.00000  Uiso   1.00
C2     C     0.21833   0.16248   0.11448   0.00000  Uiso   1.00
C3     C     0.32727   0.02184   0.08635   0.00000  Uiso   1.00
C4     C    -0.25785   0.18392   0.00886   0.00000  Uiso   1.00
C5     C    -0.08061   0.24576   0.07410   0.00000  Uiso   1.00
H6     H     0.27102   0.32149   0.18768   0.00000  Uiso   1.00
H7     H     0.46773   0.06977   0.13784   0.00000  Uiso   1.00
H8     H    -0.34463   0.29413   0.03133   0.00000  Uiso   1.00
H9     H    -0.02673   0.40437   0.14753   0.00000  Uiso   1.00
loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
C1     C2      1.419   .     S
C1     C5      1.419   .     S
C1     C1      1.435   3     S
C2     C3      1.379   .     S
C2     H6      1.092   .     S
C3     H7      1.092   .     S
C3     C4      1.416   3     S
C4     C5      1.380   .     S
C4     H8      1.092   .     S
```

```
C4      C3      1.416   3       S
C5      H9      1.092   .       S
#===END
```