MIL-53_Cr_with1CO2uc-NP20MPa

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data_MIL-53(Cr)with1CO2uc-NP20MPa
_audit_creation_date              2011-10-21
_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P1'
_symmetry_Int_Tables_number       1
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loop_
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_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
O1     O     0.56672   0.34495   0.94960   0.04000  Uiso   1.00
C2     C     0.72497   0.29524   0.79078   0.04000  Uiso   1.00
H3     H     0.70666   0.32052   0.63562   0.04000  Uiso   1.00
O4     O     0.08243   0.11700   0.15910   0.04000  Uiso   1.00
C5     C     0.20350   0.26879   0.62276   0.04000  Uiso   1.00
H6     H     0.16911   0.29326   0.70880   0.04000  Uiso   1.00
C7     C     0.67814   0.28274   0.91495   0.04000  Uiso   1.00
C8     C     0.60837   0.36006   0.84584   0.04000  Uiso   1.00
O9     O     0.06672   0.84495   0.94960   0.04000  Uiso   1.00
C10    C     0.22497   0.79524   0.79078   0.04000  Uiso   1.00
H11    H     0.20666   0.82052   0.63562   0.04000  Uiso   1.00
O12    O     0.58243   0.61700   0.15910   0.04000  Uiso   1.00
C13    C     0.70350   0.76879   0.62276   0.04000  Uiso   1.00
H14    H     0.66911   0.79326   0.70880   0.04000  Uiso   1.00
C15    C     0.17814   0.78274   0.91495   0.04000  Uiso   1.00
C16    C     0.10837   0.86006   0.84584   0.04000  Uiso   1.00
O17    O     0.43328   0.34495   0.55040   0.04000  Uiso   1.00
C18    C     0.27503   0.29524   0.70922   0.04000  Uiso   1.00
H19    H     0.29334   0.32052   0.86438   0.04000  Uiso   1.00
O20    O     0.91757   0.11700   0.34090   0.04000  Uiso   1.00
C21    C     0.79650   0.26879   0.87724   0.04000  Uiso   1.00
H22    H     0.83089   0.29326   0.79120   0.04000  Uiso   1.00
C23    C     0.32186   0.28274   0.58505   0.04000  Uiso   1.00
C24    C     0.39163   0.36006   0.65416   0.04000  Uiso   1.00
O25    O     0.93328   0.84495   0.55040   0.04000  Uiso   1.00
C26    C     0.77503   0.79524   0.70922   0.04000  Uiso   1.00
H27    H     0.79334   0.82052   0.86438   0.04000  Uiso   1.00
O28    O     0.41757   0.61700   0.34090   0.04000  Uiso   1.00
C29    C     0.29650   0.76879   0.87724   0.04000  Uiso   1.00
H30    H     0.33089   0.79326   0.79120   0.04000  Uiso   1.00
C31    C     0.82186   0.78274   0.58505   0.04000  Uiso   1.00
C32    C     0.89163   0.86006   0.65416   0.04000  Uiso   1.00
O33    O     0.43328   0.65505   0.05040   0.04000  Uiso   1.00
C34    C     0.27503   0.70476   0.20922   0.04000  Uiso   1.00
H35    H     0.29334   0.67948   0.36438   0.04000  Uiso   1.00
O36    O     0.91757   0.88300   0.84090   0.04000  Uiso   1.00
C37    C     0.79650   0.73121   0.37724   0.04000  Uiso   1.00
H38    H     0.83089   0.70674   0.29120   0.04000  Uiso   1.00
C39    C     0.32186   0.71726   0.08505   0.04000  Uiso   1.00
C40    C     0.39163   0.63994   0.15416   0.04000  Uiso   1.00
O41    O     0.93328   0.15505   0.05040   0.04000  Uiso   1.00
C42    C     0.77503   0.20476   0.20922   0.04000  Uiso   1.00
H43    H     0.79334   0.17948   0.36438   0.04000  Uiso   1.00
O44    O     0.41757   0.38300   0.84090   0.04000  Uiso   1.00
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C45    C     0.29650   0.23121   0.37724   0.04000  Uiso   1.00
H46    H     0.33089   0.20674   0.29120   0.04000  Uiso   1.00
C47    C     0.82186   0.21726   0.08505   0.04000  Uiso   1.00
C48    C     0.89163   0.13994   0.15416   0.04000  Uiso   1.00
O49    O     0.56672   0.65505   0.44960   0.04000  Uiso   1.00
C50    C     0.72497   0.70476   0.29078   0.04000  Uiso   1.00
H51    H     0.70666   0.67948   0.13562   0.04000  Uiso   1.00
O52    O     0.08243   0.88300   0.65910   0.04000  Uiso   1.00
C53    C     0.20350   0.73121   0.12276   0.04000  Uiso   1.00
H54    H     0.16911   0.70674   0.20880   0.04000  Uiso   1.00
C55    C     0.67814   0.71726   0.41495   0.04000  Uiso   1.00
C56    C     0.60837   0.63994   0.34584   0.04000  Uiso   1.00
O57    O     0.06672   0.15505   0.44960   0.04000  Uiso   1.00
C58    C     0.22497   0.20476   0.29078   0.04000  Uiso   1.00
H59    H     0.20666   0.17948   0.13562   0.04000  Uiso   1.00
O60    O     0.58243   0.38300   0.65910   0.04000  Uiso   1.00
C61    C     0.70350   0.23121   0.12276   0.04000  Uiso   1.00
H62    H     0.66911   0.20674   0.20880   0.04000  Uiso   1.00
C63    C     0.17814   0.21726   0.41495   0.04000  Uiso   1.00
C64    C     0.10837   0.13994   0.34584   0.04000  Uiso   1.00
Cr65   Cr    0.50000   0.50000   1.00000   0.04000  Uiso   1.00
Cr66   Cr    0.00000   1.00000   1.00000   0.04000  Uiso   1.00
Cr67   Cr    0.50000   0.50000   0.50000   0.04000  Uiso   1.00
Cr68   Cr    0.00000   1.00000   0.50000   0.04000  Uiso   1.00
O69    O     0.50000   0.63174   0.75000   0.04000  Uiso   1.00
O70    O     0.00000   0.13174   0.75000   0.04000  Uiso   1.00
O71    O     0.50000   0.36826   0.25000   0.04000  Uiso   1.00
O72    O     0.00000   0.86826   0.25000   0.04000  Uiso   1.00
H73    H     0.00000   0.22865   0.75000   0.04000  Uiso   1.00
H74    H     0.50000   0.72865   0.75000   0.04000  Uiso   1.00
H75    H     0.00000   0.77135   0.25000   0.04000  Uiso   1.00
H76    H     0.50000   0.27135   0.25000   0.04000  Uiso   1.00
C77    C     1.57466   2.97403   2.78110   0.04000  Uiso   1.00
O78    O     1.51549   2.98993   2.74654   0.04000  Uiso   1.00
O79    O     1.63375   2.96027   2.81923   0.04000  Uiso   1.00
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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
O1     C8      1.092   .      S
O1     Cr65    1.886   .      S
C2     H3      1.082   .      S
C2     C7      1.258   .      S
C2     C21     1.466   .      S
O4     C64     1.312   .      S
O4     Cr66    2.092   1_544  S
C5     H6      0.921   .      S
C5     C63     1.490   .      S
C5     C18     1.466   .      S
C7     C8      1.533   .      S
C7     C61     1.490   1_556  S
C8     O60     1.312   .      S
O9     C16     1.092   .      S
O9     Cr66    1.886   .      S
C10    H11     1.082   .      S
C10    C15     1.258   .      S
C10    C29     1.466   .      S
O12    C56     1.312   .      S
O12    Cr65    2.092   1_554  S
C13    H14     0.921   .      S
C13    C55     1.490   .      S
C13    C26     1.466   .      S
C15    C16     1.533   .      S
C15    C53     1.490   1_556  S
C16    O52     1.312   .      S
O17    C24     1.092   .      S
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O17	Cr67	1.886	.	S
C18	H19	1.082	.	S
C18	C23	1.258	.	S
O20	C48	1.312	.	S
O20	Cr68	2.092	1_645	S
C21	H22	0.921	.	S
C21	C47	1.490	1_556	S
C23	C45	1.490	.	S
C23	C24	1.533	.	S
C24	O44	1.312	.	S
O25	C32	1.092	.	S
O25	Cr68	1.886	1_655	S
C26	H27	1.082	.	S
C26	C31	1.258	.	S
O28	C40	1.312	.	S
O28	Cr67	2.092	.	S
C29	H30	0.921	.	S
C29	C39	1.490	1_556	S
C31	C37	1.490	.	S
C31	C32	1.533	.	S
C32	O36	1.312	.	S
O33	C40	1.092	.	S
O33	Cr65	1.886	1_554	S
C34	H35	1.082	.	S
C34	C39	1.258	.	S
C34	C53	1.466	.	S
O36	Cr66	2.092	1_655	S
C37	H38	0.921	.	S
C37	C50	1.466	.	S
C39	C40	1.533	.	S
C39	C29	1.490	1_554	S
O41	C48	1.092	.	S
O41	Cr66	1.886	1_644	S
C42	H43	1.082	.	S
C42	C47	1.258	.	S
C42	C61	1.466	.	S
O44	Cr65	2.092	.	S
C45	H46	0.921	.	S
C45	C58	1.466	.	S
C47	C48	1.533	.	S
C47	C21	1.490	1_554	S
O49	C56	1.092	.	S
O49	Cr67	1.886	.	S
C50	H51	1.082	.	S
C50	C55	1.258	.	S
O52	Cr68	2.092	.	S
C53	H54	0.921	.	S
C53	C15	1.490	1_554	S
C55	C56	1.533	.	S
O57	C64	1.092	.	S
O57	Cr68	1.886	1_545	S
C58	H59	1.082	.	S
C58	C63	1.258	.	S
O60	Cr67	2.092	.	S
C61	H62	0.921	.	S
C61	C7	1.490	1_554	S
C63	C64	1.533	.	S
Cr65	O69	1.997	.	S
Cr65	O12	2.092	1_556	S
Cr65	O33	1.886	1_556	S
Cr65	O71	1.997	1_556	S
Cr66	O4	2.092	1_566	S
Cr66	O36	2.092	1_455	S
Cr66	O41	1.886	1_466	S
Cr66	O72	1.997	1_556	S
Cr66	O70	1.997	1_565	S
Cr67	O71	1.997	.	S
Cr67	O69	1.997	.	S

MIL-53_Cr_with1CO2uc-NP20MPa

Cr68	O72	1.997	.	S
Cr68	O20	2.092	1_465	S
Cr68	O25	1.886	1_455	S
Cr68	O57	1.886	1_565	S
Cr68	O70	1.997	1_565	S
O69	H74	0.829	.	S
O70	H73	0.829	.	S
O70	Cr66	1.997	1_545	S
O70	Cr68	1.997	1_545	S
O71	H76	0.829	.	S
O71	Cr65	1.997	1_554	S
O72	H75	0.829	.	S
O72	Cr66	1.997	1_554	S
C77	O79	1.149	.	S
C77	O78	1.149	.	S