MIL-53_Cr_-NP53.5MPa

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data_MIL-53(Cr)-NP53.5MPa
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_audit_creation_method            'Materials Studio'
_symmetry_space_group_name_H-M    'P1'
_symmetry_Int_Tables_number       1
_symmetry_cell_setting            triclinic
loop_
_symmetry_equiv_pos_as_xyz
  x,y,z
_cell_length_a                    19.2730
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_cell_length_c                    6.5830
_cell_angle_alpha                 90.0000
_cell_angle_beta                  95.0000
_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
O1     O     0.91658   0.37828   0.84551   0.04000  Uiso   1.00
O2     O     0.06458   0.67099   0.44100   0.04000  Uiso   1.00
C3     C     0.79817   0.21753   0.38226   0.04000  Uiso   1.00
C4     C     0.22677   0.70150   0.29072   0.04000  Uiso   1.00
C5     C     0.82192   0.27388   0.58963   0.04000  Uiso   1.00
C6     C     0.89230   0.35218   0.65945   0.04000  Uiso   1.00
H7     H     0.83349   0.18320   0.29927   0.04000  Uiso   1.00
H8     H     0.20994   0.67552   0.13403   0.04000  Uiso   1.00
O9     O     0.41658   0.87828   0.84551   0.04000  Uiso   1.00
O10    O     0.56458   0.17099   0.44100   0.04000  Uiso   1.00
C11    C     0.29817   0.71753   0.38226   0.04000  Uiso   1.00
C12    C     0.72677   0.20150   0.29072   0.04000  Uiso   1.00
C13    C     0.32192   0.77388   0.58963   0.04000  Uiso   1.00
C14    C     0.39230   0.85218   0.65945   0.04000  Uiso   1.00
H15    H     0.33349   0.68320   0.29927   0.04000  Uiso   1.00
H16    H     0.70994   0.17552   0.13403   0.04000  Uiso   1.00
O17    O     0.08342   0.37828   0.65449   0.04000  Uiso   1.00
O18    O     0.93542   0.67099   0.05900   0.04000  Uiso   1.00
C19    C     0.20183   0.21753   0.11774   0.04000  Uiso   1.00
C20    C     0.77323   0.70150   0.20928   0.04000  Uiso   1.00
C21    C     0.17808   0.27388   0.91037   0.04000  Uiso   1.00
C22    C     0.10770   0.35218   0.84055   0.04000  Uiso   1.00
H23    H     0.16651   0.18320   0.20073   0.04000  Uiso   1.00
H24    H     0.79006   0.67552   0.36597   0.04000  Uiso   1.00
O25    O     0.58342   0.87828   0.65449   0.04000  Uiso   1.00
O26    O     0.43542   0.17099   0.05900   0.04000  Uiso   1.00
C27    C     0.70183   0.71753   0.11774   0.04000  Uiso   1.00
C28    C     0.27323   0.20150   0.20928   0.04000  Uiso   1.00
C29    C     0.67808   0.77388   0.91037   0.04000  Uiso   1.00
C30    C     0.60770   0.85218   0.84055   0.04000  Uiso   1.00
H31    H     0.66651   0.68320   0.20073   0.04000  Uiso   1.00
H32    H     0.29006   0.17552   0.36597   0.04000  Uiso   1.00
O33    O     0.08342   0.62172   0.15449   0.04000  Uiso   1.00
O34    O     0.93542   0.32901   0.55900   0.04000  Uiso   1.00
C35    C     0.20183   0.78247   0.61774   0.04000  Uiso   1.00
C36    C     0.77323   0.29850   0.70928   0.04000  Uiso   1.00
C37    C     0.17808   0.72612   0.41037   0.04000  Uiso   1.00
C38    C     0.10770   0.64782   0.34055   0.04000  Uiso   1.00
H39    H     0.16651   0.81680   0.70073   0.04000  Uiso   1.00
H40    H     0.79006   0.32448   0.86597   0.04000  Uiso   1.00
O41    O     0.58342   0.12172   0.15449   0.04000  Uiso   1.00
O42    O     0.43542   0.82901   0.55900   0.04000  Uiso   1.00
C43    C     0.70183   0.28247   0.61774   0.04000  Uiso   1.00
C44    C     0.27323   0.79850   0.70928   0.04000  Uiso   1.00
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MIL-53_Cr_-NP53.5MPa

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C45    C     0.67808   0.22612   0.41037   0.04000  Uiso   1.00
C46    C     0.60770   0.14782   0.34055   0.04000  Uiso   1.00
H47    H     0.66651   0.31680   0.70073   0.04000  Uiso   1.00
H48    H     0.29006   0.82448   0.86597   0.04000  Uiso   1.00
O49    O     0.91658   0.62172   0.34551   0.04000  Uiso   1.00
O50    O     0.06458   0.32901   0.94100   0.04000  Uiso   1.00
C51    C     0.79817   0.78247   0.88226   0.04000  Uiso   1.00
C52    C     0.22677   0.29850   0.79072   0.04000  Uiso   1.00
C53    C     0.82192   0.72612   0.08963   0.04000  Uiso   1.00
C54    C     0.89230   0.64782   0.15945   0.04000  Uiso   1.00
H55    H     0.83349   0.81680   0.79927   0.04000  Uiso   1.00
H56    H     0.20994   0.32448   0.63403   0.04000  Uiso   1.00
O57    O     0.41658   0.12172   0.34551   0.04000  Uiso   1.00
O58    O     0.56458   0.82901   0.94100   0.04000  Uiso   1.00
C59    C     0.29817   0.28247   0.88226   0.04000  Uiso   1.00
C60    C     0.72677   0.79850   0.79072   0.04000  Uiso   1.00
C61    C     0.32192   0.22612   0.08963   0.04000  Uiso   1.00
C62    C     0.39230   0.14782   0.15945   0.04000  Uiso   1.00
H63    H     0.33349   0.31680   0.79927   0.04000  Uiso   1.00
H64    H     0.70994   0.82448   0.63403   0.04000  Uiso   1.00
Cr65   Cr   -0.00000   0.50000   1.00000   0.04000  Uiso   1.00
Cr66   Cr    0.50000   1.00000   1.00000   0.04000  Uiso   1.00
Cr67   Cr   -0.00000   0.50000   0.50000   0.04000  Uiso   1.00
Cr68   Cr    0.50000   1.00000   0.50000   0.04000  Uiso   1.00
O69    O     0.00000   0.64306   0.75000   0.04000  Uiso   1.00
H70    H     0.00000   0.75023   0.75000   0.04000  Uiso   1.00
O71    O     0.50000   0.14306   0.75000   0.04000  Uiso   1.00
H72    H     0.50000   0.25023   0.75000   0.04000  Uiso   1.00
O73    O     0.00000   0.35694   0.25000   0.04000  Uiso   1.00
H74    H     0.00000   0.24977   0.25000   0.04000  Uiso   1.00
O75    O     0.50000   0.85694   0.25000   0.04000  Uiso   1.00
H76    H     0.50000   0.74977   0.25000   0.04000  Uiso   1.00
loop_
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_geom_bond_atom_site_label_2
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_geom_bond_site_symmetry_2
_ccdc_geom_bond_type
O1     C6      1.289   .      S
O1     Cr65    2.064   1_655  S
O2     Cr67    1.901   .      S
O2     C38     1.121   .      S
C3     C5      1.471   .      S
C3     H7      0.949   .      S
C3     C12     1.459   .      S
C4     C11     1.459   .      S
C4     C37     1.291   .      S
C4     H8      1.074   .      S
C5     C36     1.291   .      S
C5     C6      1.525   .      S
C6     O34     1.121   .      S
O9     Cr66    2.064   .      S
O9     C14     1.289   .      S
O10    C46     1.121   .      S
O10    Cr68    1.901   1_545  S
C11    C13     1.471   .      S
C11    H15     0.949   .      S
C12    C45     1.291   .      S
C12    H16     1.074   .      S
C13    C44     1.291   .      S
C13    C14     1.525   .      S
C14    O42     1.121   .      S
O17    Cr67    2.064   .      S
O17    C22     1.289   .      S
O18    C54     1.121   .      S
O18    Cr65    1.901   1_654  S
C19    H23     0.949   .      S
C19    C28     1.459   .      S
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C19	C21	1.471	1_554	S
C20	C27	1.459	.	S
C20	C53	1.291	.	S
C20	H24	1.074	.	S
C21	C52	1.291	.	S
C21	C22	1.525	.	S
C21	C19	1.471	1_556	S
C22	O50	1.121	.	S
O25	Cr68	2.064	.	S
O25	C30	1.289	.	S
O26	C62	1.121	.	S
O26	Cr66	1.901	1_544	S
C27	H31	0.949	.	S
C27	C29	1.471	1_554	S
C28	C61	1.291	.	S
C28	H32	1.074	.	S
C29	C60	1.291	.	S
C29	C30	1.525	.	S
C29	C27	1.471	1_556	S
C30	O58	1.121	.	S
O33	C38	1.289	.	S
O33	Cr65	2.064	1_554	S
O34	Cr67	1.901	1_655	S
C35	C37	1.471	.	S
C35	H39	0.949	.	S
C35	C44	1.459	.	S
C36	C43	1.459	.	S
C36	H40	1.074	.	S
C37	C38	1.525	.	S
O41	C46	1.289	.	S
O41	Cr66	2.064	1_544	S
O42	Cr68	1.901	.	S
C43	C45	1.471	.	S
C43	H47	0.949	.	S
C44	H48	1.074	.	S
C45	C46	1.525	.	S
O49	C54	1.289	.	S
O49	Cr67	2.064	1_655	S
O50	Cr65	1.901	.	S
C51	H55	0.949	.	S
C51	C60	1.459	.	S
C51	C53	1.471	1_556	S
C52	C59	1.459	.	S
C52	H56	1.074	.	S
C53	C54	1.525	.	S
C53	C51	1.471	1_554	S
O57	C62	1.289	.	S
O57	Cr68	2.064	1_545	S
O58	Cr66	1.901	.	S
C59	H63	0.949	.	S
C59	C61	1.471	1_556	S
C60	H64	1.074	.	S
C61	C62	1.525	.	S
C61	C59	1.471	1_554	S
Cr65	O69	1.998	.	S
Cr65	O1	2.064	1_455	S
Cr65	O18	1.901	1_456	S
Cr65	O33	2.064	1_556	S
Cr65	O73	1.998	1_556	S
Cr66	O26	1.901	1_566	S
Cr66	O41	2.064	1_566	S
Cr66	O71	1.998	1_565	S
Cr66	O75	1.998	1_556	S
Cr67	O69	1.998	.	S
Cr67	O73	1.998	.	S
Cr67	O34	1.901	1_455	S
Cr67	O49	2.064	1_455	S
Cr68	O75	1.998	.	S

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Cr68	O10	1.901	1_565	S
Cr68	O57	2.064	1_565	S
Cr68	O71	1.998	1_565	S
O69	H70	0.848	.	S
O71	H72	0.848	.	S
O71	Cr66	1.998	1_545	S
O71	Cr68	1.998	1_545	S
O73	H74	0.848	.	S
O73	Cr65	1.998	1_554	S
O75	H76	0.848	.	S
O75	Cr66	1.998	1_554	S