

MI L-53\_Cr\_-NP300MPa

data\_MIL-53(Cr)-NP300MPa  
\_audit\_creation\_date 2011-10-20  
\_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 19.3240  
\_cell\_length\_b 7.3970  
\_cell\_length\_c 6.5560  
\_cell\_angle\_alpha 90.0000  
\_cell\_angle\_beta 96.2300  
\_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 0.93756 0.68687 0.56798 0.04000 Uiso 1.00  
O2 O 0.08454 0.37420 0.14954 0.04000 Uiso 1.00  
C3 C 0.77164 0.70052 0.71042 0.04000 Uiso 1.00  
C4 C 0.20050 0.20839 0.61540 0.04000 Uiso 1.00  
C5 C 0.82180 0.73334 0.59301 0.04000 Uiso 1.00  
C6 C 0.89280 0.65477 0.66454 0.04000 Uiso 1.00  
H7 H 0.78723 0.67646 0.86935 0.04000 Uiso 1.00  
H8 H 0.16428 0.16884 0.69810 0.04000 Uiso 1.00  
O9 O 0.43756 0.18687 0.56798 0.04000 Uiso 1.00  
O10 O 0.58454 0.87420 0.14954 0.04000 Uiso 1.00  
C11 C 0.27164 0.20052 0.71042 0.04000 Uiso 1.00  
C12 C 0.70050 0.70839 0.61540 0.04000 Uiso 1.00  
C13 C 0.32180 0.23334 0.59301 0.04000 Uiso 1.00  
C14 C 0.39280 0.15477 0.66454 0.04000 Uiso 1.00  
H15 H 0.28723 0.17646 0.86935 0.04000 Uiso 1.00  
H16 H 0.66428 0.66884 0.69810 0.04000 Uiso 1.00  
O17 O 0.06244 0.68687 0.93202 0.04000 Uiso 1.00  
O18 O 0.91546 0.37420 0.35046 0.04000 Uiso 1.00  
C19 C 0.22836 0.70052 0.78958 0.04000 Uiso 1.00  
C20 C 0.79950 0.20839 0.88460 0.04000 Uiso 1.00  
C21 C 0.17820 0.73334 0.90699 0.04000 Uiso 1.00  
C22 C 0.10720 0.65477 0.83546 0.04000 Uiso 1.00  
H23 H 0.21277 0.67646 0.63065 0.04000 Uiso 1.00  
H24 H 0.83572 0.16884 0.80190 0.04000 Uiso 1.00  
O25 O 0.56244 0.18687 0.93202 0.04000 Uiso 1.00  
O26 O 0.41546 0.87420 0.35046 0.04000 Uiso 1.00  
C27 C 0.72836 0.20052 0.78958 0.04000 Uiso 1.00  
C28 C 0.29950 0.70839 0.88460 0.04000 Uiso 1.00  
C29 C 0.67820 0.23334 0.90699 0.04000 Uiso 1.00  
C30 C 0.60720 0.15477 0.83546 0.04000 Uiso 1.00  
H31 H 0.71277 0.17646 0.63065 0.04000 Uiso 1.00  
H32 H 0.33572 0.66884 0.80190 0.04000 Uiso 1.00  
O33 O 0.06244 0.31313 0.43202 0.04000 Uiso 1.00  
O34 O 0.91546 0.62580 0.85046 0.04000 Uiso 1.00  
C35 C 0.22836 0.29948 0.28958 0.04000 Uiso 1.00  
C36 C 0.79950 0.79161 0.38460 0.04000 Uiso 1.00  
C37 C 0.17820 0.26666 0.40699 0.04000 Uiso 1.00  
C38 C 0.10720 0.34523 0.33546 0.04000 Uiso 1.00  
H39 H 0.21277 0.32354 0.13065 0.04000 Uiso 1.00  
H40 H 0.83572 0.83116 0.30190 0.04000 Uiso 1.00  
O41 O 0.56244 0.81313 0.43202 0.04000 Uiso 1.00  
O42 O 0.41546 0.12580 0.85046 0.04000 Uiso 1.00  
C43 C 0.72836 0.79948 0.28958 0.04000 Uiso 1.00  
C44 C 0.29950 0.29161 0.38460 0.04000 Uiso 1.00

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C45	C	0.67820	0.76666	0.40699	0.04000	Ui so	1.00
C46	C	0.60720	0.84523	0.33546	0.04000	Ui so	1.00
H47	H	0.71277	0.82354	0.13065	0.04000	Ui so	1.00
H48	H	0.33572	0.33116	0.30190	0.04000	Ui so	1.00
O49	O	0.93756	0.31313	0.06798	0.04000	Ui so	1.00
O50	O	0.08454	0.62580	0.64954	0.04000	Ui so	1.00
C51	C	0.77164	0.29948	0.21042	0.04000	Ui so	1.00
C52	C	0.20050	0.79161	0.11540	0.04000	Ui so	1.00
C53	C	0.82180	0.26666	0.09301	0.04000	Ui so	1.00
C54	C	0.89280	0.34523	0.16454	0.04000	Ui so	1.00
H55	H	0.78723	0.32354	0.36935	0.04000	Ui so	1.00
H56	H	0.16428	0.83116	0.19810	0.04000	Ui so	1.00
O57	O	0.43756	0.81313	0.06798	0.04000	Ui so	1.00
O58	O	0.58454	0.12580	0.64954	0.04000	Ui so	1.00
C59	C	0.27164	0.79948	0.21042	0.04000	Ui so	1.00
C60	C	0.70050	0.29161	0.11540	0.04000	Ui so	1.00
C61	C	0.32180	0.76666	0.09301	0.04000	Ui so	1.00
C62	C	0.39280	0.84523	0.16454	0.04000	Ui so	1.00
H63	H	0.28723	0.82354	0.36935	0.04000	Ui so	1.00
H64	H	0.66428	0.33116	0.19810	0.04000	Ui so	1.00
Cr65	Cr	0.00000	0.50000	0.50000	0.04000	Ui so	1.00
Cr66	Cr	0.50000	1.00000	0.50000	0.04000	Ui so	1.00
Cr67	Cr	0.00000	0.50000	1.00000	0.04000	Ui so	1.00
Cr68	Cr	0.50000	1.00000	1.00000	0.04000	Ui so	1.00
O69	O	0.00000	0.34554	0.75000	0.04000	Ui so	1.00
H70	H	0.00000	0.22962	0.75000	0.04000	Ui so	1.00
O71	O	0.50000	0.84554	0.75000	0.04000	Ui so	1.00
H72	H	0.50000	0.72962	0.75000	0.04000	Ui so	1.00
O73	O	0.00000	0.65446	0.25000	0.04000	Ui so	1.00
H74	H	0.00000	0.77038	0.25000	0.04000	Ui so	1.00
O75	O	0.50000	0.15446	0.25000	0.04000	Ui so	1.00
H76	H	0.50000	0.27038	0.25000	0.04000	Ui so	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

01	C6	1.151	.	S
01	Cr65	1.919	1_655	S
02	C38	1.268	.	S
02	Cr67	2.037	1_554	S
C3	H7	1.068	.	S
C3	C12	1.448	.	S
C3	C5	1.324	.	S
C4	C11	1.448	.	S
C4	C37	1.453	.	S
C4	H8	0.976	.	S
C5	C36	1.453	.	S
C5	C6	1.517	.	S
C6	O34	1.268	.	S
O9	C14	1.151	.	S
O9	Cr66	1.919	1_545	S
O10	C46	1.268	.	S
O10	Cr68	2.037	1_554	S
C11	H15	1.068	.	S
C11	C13	1.324	.	S
C12	C45	1.453	.	S
C12	H16	0.976	.	S
C13	C44	1.453	.	S
C13	C14	1.517	.	S
C14	O42	1.268	.	S
O17	C22	1.151	.	S
O17	Cr67	1.919	.	S
O18	C54	1.268	.	S
O18	Cr65	2.037	1_655	S
C19	H23	1.068	.	S
C19	C28	1.448	.	S

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C19	C21	1.324	.	S
C20	C27	1.448	.	S
C20	H24	0.976	.	S
C20	C53	1.453	1_556	S
C21	C22	1.517	.	S
C21	C52	1.453	1_556	S
C22	O50	1.268	.	S
O25	C30	1.151	.	S
O25	Cr68	1.919	1_545	S
O26	Cr66	2.037	.	S
O26	C62	1.268	.	S
C27	H31	1.068	.	S
C27	C29	1.324	.	S
C28	H32	0.976	.	S
C28	C61	1.453	1_556	S
C29	C30	1.517	.	S
C29	C60	1.453	1_556	S
C30	O58	1.268	.	S
O33	C38	1.151	.	S
O33	Cr65	1.919	.	S
O34	Cr67	2.037	1_655	S
C35	H39	1.068	.	S
C35	C44	1.448	.	S
C35	C37	1.324	.	S
C36	C43	1.448	.	S
C36	H40	0.976	.	S
C37	C38	1.517	.	S
O41	C46	1.151	.	S
O41	Cr66	1.919	.	S
O42	Cr68	2.037	1_545	S
C43	H47	1.068	.	S
C43	C45	1.324	.	S
C44	H48	0.976	.	S
C45	C46	1.517	.	S
O49	C54	1.151	.	S
O49	Cr67	1.919	1_654	S
O50	Cr65	2.037	.	S
C51	H55	1.068	.	S
C51	C60	1.448	.	S
C51	C53	1.324	.	S
C52	C59	1.448	.	S
C52	H56	0.976	.	S
C52	C21	1.453	1_554	S
C53	C54	1.517	.	S
C53	C20	1.453	1_554	S
O57	C62	1.151	.	S
O57	Cr68	1.919	1_554	S
O58	Cr66	2.037	1_545	S
C59	H63	1.068	.	S
C59	C61	1.324	.	S
C60	H64	0.976	.	S
C60	C29	1.453	1_554	S
C61	C62	1.517	.	S
C61	C28	1.453	1_554	S
Cr65	O69	1.998	.	S
Cr65	O73	1.998	.	S
Cr65	O1	1.919	1_455	S
Cr65	O18	2.037	1_455	S
Cr66	O71	1.998	.	S
Cr66	O9	1.919	1_565	S
Cr66	O58	2.037	1_565	S
Cr66	O75	1.998	1_565	S
Cr67	O69	1.998	.	S
Cr67	O2	2.037	1_556	S
Cr67	O34	2.037	1_455	S
Cr67	O49	1.919	1_456	S
Cr67	O73	1.998	1_556	S
Cr68	O71	1.998	.	S

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Cr68	010	2.037	1_556	S
Cr68	025	1.919	1_565	S
Cr68	042	2.037	1_565	S
Cr68	057	1.919	1_556	S
Cr68	075	1.998	1_566	S
069	H70	0.857	.	S
071	H72	0.857	.	S
073	H74	0.857	.	S
073	Cr67	1.998	1_554	S
075	H76	0.857	.	S
075	Cr66	1.998	1_545	S
075	Cr68	1.998	1_544	S