MIL-53_Cr_with1CO2uc-NP300MPa

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data_MIL-53(Cr)with1CO2uc-NP300MPa-2
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_symmetry_Int_Tables_number       1
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_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
O1     O     0.58418   0.12032   0.15225   0.04000  Uiso   1.00
C2     C     0.70096   0.28383   0.61682   0.04000  Uiso   1.00
H3     H     0.66501   0.31913   0.69911   0.04000  Uiso   1.00
O4     O     0.06354   0.32630   0.93670   0.04000  Uiso   1.00
C5     C     0.22775   0.30001   0.79026   0.04000  Uiso   1.00
H6     H     0.21165   0.32670   0.63315   0.04000  Uiso   1.00
C7     C     0.67820   0.22602   0.40902   0.04000  Uiso   1.00
C8     C     0.60780   0.14740   0.33873   0.04000  Uiso   1.00
O9     O     0.08418   0.62032   0.15225   0.04000  Uiso   1.00
C10    C     0.20096   0.78383   0.61682   0.04000  Uiso   1.00
H11    H     0.16501   0.81913   0.69911   0.04000  Uiso   1.00
O12    O     0.56354   0.82630   0.93670   0.04000  Uiso   1.00
C13    C     0.72775   0.80001   0.79026   0.04000  Uiso   1.00
H14    H     0.71165   0.82670   0.63315   0.04000  Uiso   1.00
C15    C     0.17820   0.72602   0.40902   0.04000  Uiso   1.00
C16    C     0.10780   0.64740   0.33873   0.04000  Uiso   1.00
O17    O     0.41582   0.12032   0.34775   0.04000  Uiso   1.00
C18    C     0.29904   0.28383   0.88318   0.04000  Uiso   1.00
H19    H     0.33499   0.31913   0.80089   0.04000  Uiso   1.00
O20    O     0.93646   0.32630   0.56330   0.04000  Uiso   1.00
C21    C     0.77225   0.30001   0.70974   0.04000  Uiso   1.00
H22    H     0.78835   0.32670   0.86685   0.04000  Uiso   1.00
C23    C     0.32180   0.22602   0.09098   0.04000  Uiso   1.00
C24    C     0.39220   0.14740   0.16127   0.04000  Uiso   1.00
O25    O     0.91582   0.62032   0.34775   0.04000  Uiso   1.00
C26    C     0.79904   0.78383   0.88318   0.04000  Uiso   1.00
H27    H     0.83499   0.81913   0.80089   0.04000  Uiso   1.00
O28    O     0.43646   0.82630   0.56330   0.04000  Uiso   1.00
C29    C     0.27225   0.80001   0.70974   0.04000  Uiso   1.00
H30    H     0.28835   0.82670   0.86685   0.04000  Uiso   1.00
C31    C     0.82180   0.72602   0.09098   0.04000  Uiso   1.00
C32    C     0.89220   0.64740   0.16127   0.04000  Uiso   1.00
O33    O     0.41582   0.87968   0.84775   0.04000  Uiso   1.00
C34    C     0.29904   0.71617   0.38318   0.04000  Uiso   1.00
H35    H     0.33499   0.68087   0.30089   0.04000  Uiso   1.00
O36    O     0.93646   0.67370   0.06330   0.04000  Uiso   1.00
C37    C     0.77225   0.69999   0.20974   0.04000  Uiso   1.00
H38    H     0.78835   0.67330   0.36685   0.04000  Uiso   1.00
C39    C     0.32180   0.77398   0.59098   0.04000  Uiso   1.00
C40    C     0.39220   0.85260   0.66127   0.04000  Uiso   1.00
O41    O     0.91582   0.37968   0.84775   0.04000  Uiso   1.00
C42    C     0.79904   0.21617   0.38318   0.04000  Uiso   1.00
H43    H     0.83499   0.18087   0.30089   0.04000  Uiso   1.00
O44    O     0.43646   0.17370   0.06330   0.04000  Uiso   1.00
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MIL-53_Cr_with1CO2uc-NP300MPa

C45	C	0.27225	0.19999	0.20974	0.04000	Uiso	1.00
H46	H	0.28835	0.17330	0.36685	0.04000	Uiso	1.00
C47	C	0.82180	0.27398	0.59098	0.04000	Uiso	1.00
C48	C	0.89220	0.35260	0.66127	0.04000	Uiso	1.00
O49	O	0.58418	0.87968	0.65225	0.04000	Uiso	1.00
C50	C	0.70096	0.71617	0.11682	0.04000	Uiso	1.00
H51	H	0.66501	0.68087	0.19911	0.04000	Uiso	1.00
O52	O	0.06354	0.67370	0.43670	0.04000	Uiso	1.00
C53	C	0.22775	0.69999	0.29026	0.04000	Uiso	1.00
H54	H	0.21165	0.67330	0.13315	0.04000	Uiso	1.00
C55	C	0.67820	0.77398	0.90902	0.04000	Uiso	1.00
C56	C	0.60780	0.85260	0.83873	0.04000	Uiso	1.00
O57	O	0.08418	0.37968	0.65225	0.04000	Uiso	1.00
C58	C	0.20096	0.21617	0.11682	0.04000	Uiso	1.00
H59	H	0.16501	0.18087	0.19911	0.04000	Uiso	1.00
O60	O	0.56354	0.17370	0.43670	0.04000	Uiso	1.00
C61	C	0.72775	0.19999	0.29026	0.04000	Uiso	1.00
H62	H	0.71165	0.17330	0.13315	0.04000	Uiso	1.00
C63	C	0.17820	0.27398	0.90902	0.04000	Uiso	1.00
C64	C	0.10780	0.35260	0.83873	0.04000	Uiso	1.00
Cr65	Cr	0.50000	1.00000	1.00000	0.04000	Uiso	1.00
Cr66	Cr	-0.00000	0.50000	1.00000	0.04000	Uiso	1.00
Cr67	Cr	0.50000	1.00000	0.50000	0.04000	Uiso	1.00
Cr68	Cr	-0.00000	0.50000	0.50000	0.04000	Uiso	1.00
O69	O	0.50000	0.85499	0.25000	0.04000	Uiso	1.00
O70	O	0.00000	0.35499	0.25000	0.04000	Uiso	1.00
O71	O	0.50000	0.14501	0.75000	0.04000	Uiso	1.00
O72	O	0.00000	0.64501	0.75000	0.04000	Uiso	1.00
H73	H	0.00000	0.24869	0.25000	0.04000	Uiso	1.00
H74	H	0.50000	0.74869	0.25000	0.04000	Uiso	1.00
H75	H	0.00000	0.75131	0.75000	0.04000	Uiso	1.00
H76	H	0.50000	0.25131	0.75000	0.04000	Uiso	1.00
C77	C	1.46353	1.53804	4.84723	0.04000	Uiso	1.00
O78	O	1.42216	1.57527	4.95476	0.04000	Uiso	1.00
O79	O	1.50562	1.50570	4.74000	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
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O1	C8	1.279	.	S
O1	Cr65	2.051	1_544	S
C2	H3	0.958	.	S
C2	C7	1.461	.	S
C2	C21	1.452	.	S
O4	Cr66	1.907	.	S
O4	C64	1.133	.	S
C5	C18	1.452	.	S
C5	C63	1.303	.	S
C5	H6	1.066	.	S
C7	C61	1.303	.	S
C7	C8	1.521	.	S
C8	O60	1.133	.	S
O9	C16	1.279	.	S
O9	Cr66	2.051	1_554	S
C10	H11	0.958	.	S
C10	C15	1.461	.	S
C10	C29	1.452	.	S
O12	Cr65	1.907	.	S
O12	C56	1.133	.	S
C13	C26	1.452	.	S
C13	C55	1.303	.	S
C13	H14	1.066	.	S
C15	C53	1.303	.	S
C15	C16	1.521	.	S
C16	O52	1.133	.	S
O17	C24	1.279	.	S

O17	Cr67	2.051	1_545	S
C18	H19	0.958	.	S
C18	C23	1.461	1_556	S
O20	C48	1.133	.	S
O20	Cr68	1.907	1_655	S
C21	C47	1.303	.	S
C21	H22	1.066	.	S
C23	C45	1.303	.	S
C23	C24	1.521	.	S
C23	C18	1.461	1_554	S
C24	O44	1.133	.	S
O25	C32	1.279	.	S
O25	Cr68	2.051	1_655	S
C26	H27	0.958	.	S
C26	C31	1.461	1_556	S
O28	Cr67	1.907	.	S
O28	C40	1.133	.	S
C29	C39	1.303	.	S
C29	H30	1.066	.	S
C31	C37	1.303	.	S
C31	C32	1.521	.	S
C31	C26	1.461	1_554	S
C32	O36	1.133	.	S
O33	Cr65	2.051	.	S
O33	C40	1.279	.	S
C34	H35	0.958	.	S
C34	C39	1.461	.	S
C34	C53	1.452	.	S
O36	Cr66	1.907	1_654	S
C37	C50	1.452	.	S
C37	H38	1.066	.	S
C39	C40	1.521	.	S
O41	C48	1.279	.	S
O41	Cr66	2.051	1_655	S
C42	H43	0.958	.	S
C42	C47	1.461	.	S
C42	C61	1.452	.	S
O44	Cr65	1.907	1_544	S
C45	C58	1.452	.	S
C45	H46	1.066	.	S
C47	C48	1.521	.	S
O49	Cr67	2.051	.	S
O49	C56	1.279	.	S
C50	H51	0.958	.	S
C50	C55	1.461	1_554	S
O52	Cr68	1.907	.	S
C53	H54	1.066	.	S
C55	C56	1.521	.	S
C55	C50	1.461	1_556	S
O57	Cr68	2.051	.	S
O57	C64	1.279	.	S
C58	H59	0.958	.	S
C58	C63	1.461	1_554	S
O60	Cr67	1.907	1_545	S
C61	H62	1.066	.	S
C63	C64	1.521	.	S
C63	C58	1.461	1_556	S
Cr65	O1	2.051	1_566	S
Cr65	O44	1.907	1_566	S
Cr65	O71	1.996	1_565	S
Cr65	O69	1.996	1_556	S
Cr66	O72	1.996	.	S
Cr66	O9	2.051	1_556	S
Cr66	O36	1.907	1_456	S
Cr66	O41	2.051	1_455	S
Cr66	O70	1.996	1_556	S
Cr67	O69	1.996	.	S
Cr67	O17	2.051	1_565	S

MIL-53_Cr_with1CO2uc-NP300MPa

Cr67	O60	1.907	1_565	S
Cr67	O71	1.996	1_565	S
Cr68	O72	1.996	.	S
Cr68	O70	1.996	.	S
Cr68	O20	1.907	1_455	S
Cr68	O25	2.051	1_455	S
O69	H74	0.837	.	S
O69	Cr65	1.996	1_554	S
O70	H73	0.837	.	S
O70	Cr66	1.996	1_554	S
O71	H76	0.837	.	S
O71	Cr65	1.996	1_545	S
O71	Cr67	1.996	1_545	S
O72	H75	0.837	.	S
C77	O78	1.150	.	S
C77	O79	1.150	.	S