

Supplementary Material (ESI) for Dalton Transactions
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Supplementary material

(10,3)-a

TITLE 103a or Srsi2
CELL 6.0 6. 6. 90. 90. 90.
ATOM Si 0.125 0.125 0.125
SPGR I 41 3 2

63

C	-3.12500	0.62500	-0.62500
C	-4.37500	0.62500	0.62500
C	-5.62500	1.87500	0.62500
C	-6.87500	1.87500	-0.62500
C	-3.12500	-0.62500	-1.87500
C	-1.87500	-1.87500	-1.87500
C	-4.37500	-0.62500	-3.12500
C	-4.37500	-0.62500	1.87500
C	-3.12500	-0.62500	3.12500
C	-5.62500	-1.87500	1.87500
C	-5.62500	3.12500	1.87500
C	-6.87500	3.12500	-1.87500
C	-8.12500	0.62500	-0.62500
C	-9.37500	0.62500	0.62500
C	-8.12500	-0.62500	-1.87500
C	-1.87500	-1.87500	3.12500
C	-1.87500	-3.12500	-0.62500
C	-3.12500	0.62500	4.37500
C	-3.12500	-4.37500	-0.62500
C	-4.37500	0.62500	-4.37500
C	-5.62500	-1.87500	-3.12500
C	-6.87500	-1.87500	-1.87500
C	-6.87500	-1.87500	3.12500
C	-5.62500	-3.12500	0.62500
C	-8.12500	-0.62500	3.12500
C	-4.37500	-4.37500	0.62500
C	-6.87500	-3.12500	-0.62500
C	-8.12500	0.62500	4.37500
C	-9.37500	-0.62500	1.87500
C	-10.62500	1.87500	0.62500
C	-10.62500	-1.87500	1.87500
C	-11.87500	1.87500	-0.62500
C	-10.62500	3.12500	1.87500
C	-9.37500	-0.62500	-3.12500
C	-9.37500	0.62500	-4.37500
C	-10.62500	-1.87500	-3.12500
C	-8.12500	-4.37500	-0.62500
C	-9.37500	-4.37500	0.62500
C	-11.87500	3.12500	-1.87500
C	-11.87500	-1.87500	3.12500
C	-10.62500	-3.12500	0.62500
C	-13.12500	-0.62500	3.12500
C	-11.87500	-3.12500	-0.62500
C	-13.12500	0.62500	-0.62500
C	-14.37500	0.62500	0.62500
C	-13.12500	-0.62500	-1.87500
C	-11.87500	-1.87500	-1.87500
C	-1.87500	-3.12500	4.37500
C	-3.12500	-5.62500	-1.87500
C	-5.62500	-3.12500	-4.37500
C	-4.37500	-5.62500	1.87500
C	-10.62500	-3.12500	-4.37500
C	-8.12500	-5.62500	-1.87500
C	-14.37500	-0.62500	1.87500
C	-13.12500	0.62500	4.37500
C	-13.12500	-4.37500	-0.62500
C	-15.62500	1.87500	0.62500
C	-14.37500	-0.62500	-3.12500

C	-6.87500	-3.12500	4.37500
C	-11.87500	-3.12500	4.37500
C	-9.37500	-5.62500	1.87500
C	-15.62500	3.12500	1.87500
C	-13.12500	-5.62500	-1.87500

(10,3)-b

TITLE 103b or ThSi2
CELL 4.134 4.134 14.32 90. 90. 90.
ATOM Si 0. 0.25 0.2915
SPGR I 41/a m d

96

Si	0.00000	0.00000	5.97511
Si	-2.06300	0.00000	4.78439
Si	2.06300	0.00000	4.78439
Si	0.00000	0.00000	8.37089
Si	-2.06300	0.00000	2.38861
Si	4.12600	0.00000	5.97511
Si	2.06300	0.00000	2.38861
Si	0.00000	-2.06300	9.56161
Si	0.00000	2.06300	9.56161
Si	-2.06300	-2.06300	1.19789
Si	-2.06300	2.06300	1.19789
Si	-2.06300	-2.06300	-1.19789
Si	-2.06300	-4.12600	2.38861
Si	-2.06300	2.06300	-1.19789
Si	-2.06300	4.12600	2.38861
Si	6.18900	0.00000	4.78439
Si	4.12600	0.00000	8.37089
Si	8.25200	0.00000	5.97511
Si	6.18900	0.00000	2.38861
Si	4.12600	-2.06300	9.56161
Si	4.12600	2.06300	9.56161
Si	2.06300	-2.06300	1.19789
Si	2.06300	2.06300	1.19789
Si	2.06300	-2.06300	-1.19789
Si	2.06300	-4.12600	2.38861
Si	2.06300	2.06300	-1.19789
Si	2.06300	4.12600	2.38861
Si	0.00000	-4.12600	8.37089
Si	0.00000	-4.12600	5.97511
Si	0.00000	4.12600	8.37089
Si	0.00000	4.12600	5.97511
Si	-2.06300	-4.12600	4.78439
Si	-2.06300	4.12600	4.78439
Si	10.31500	0.00000	4.78439
Si	8.25200	0.00000	8.37089
Si	10.31500	0.00000	2.38861
Si	8.25200	-2.06300	9.56161
Si	8.25200	2.06300	9.56161
Si	6.18900	-2.06300	1.19789
Si	6.18900	2.06300	1.19789
Si	6.18900	-2.06300	-1.19789
Si	6.18900	-4.12600	2.38861
Si	6.18900	2.06300	-1.19789
Si	6.18900	4.12600	2.38861
Si	4.12600	-4.12600	5.97511
Si	4.12600	4.12600	8.37089
Si	4.12600	4.12600	5.97511
Si	2.06300	-4.12600	4.78439
Si	2.06300	4.12600	4.78439
Si	-2.06300	6.18900	1.19789
Si	-2.06300	6.18900	-1.19789
Si	2.06300	6.18900	1.19789
Si	2.06300	6.18900	-1.19789
Si	10.31500	-2.06300	1.19789
Si	10.31500	2.06300	1.19789
Si	10.31500	-2.06300	-1.19789
Si	10.31500	-4.12600	2.38861

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Si	10.31500	2.06300	-1.19789	Al	7.00000	0.57735	4.62222
Si	10.31500	4.12600	2.38861	Al	4.00000	-1.15470	-2.31111
Si	8.25200	-4.12600	8.37089	Al	5.00000	-2.88675	4.62222
Si	8.25200	-4.12600	5.97511	Al	4.00000	-1.15470	8.08889
Si	8.25200	4.12600	8.37089	Al	2.00000	2.30940	8.08889
Si	8.25200	4.12600	5.97511	Al	-1.00000	-2.88675	1.15556
Si	6.18900	-4.12600	4.78439	Al	-4.00000	-1.15470	5.77778
Si	6.18900	4.12600	4.78439	Al	2.00000	-4.61880	5.77778
Si	6.18900	6.18900	1.19789	Al	1.00000	-2.88675	2.31111
Si	6.18900	6.18900	-1.19789	Al	-1.00000	-2.88675	9.24444
Si	0.00000	-2.06300	-2.38861	Al	1.00000	0.57735	9.24444
Si	0.00000	2.06300	-2.38861	Al	-3.00000	0.57735	9.24444
Si	4.12600	-2.06300	-2.38861	Al	9.00000	0.57735	-1.15556
Si	4.12600	2.06300	-2.38861	Al	8.00000	-1.15470	5.77778
Si	8.25200	-2.06300	-2.38861	Al	6.00000	2.30940	5.77778
Si	8.25200	2.06300	-2.38861	Al	3.00000	-2.88675	-1.15556
Si	0.00000	6.18900	-2.38861	Al	6.00000	-4.61880	5.77778
Si	4.12600	6.18900	-2.38861	Al	5.00000	-2.88675	2.31111
Si	10.31500	-4.12600	4.78439	Al	3.00000	-2.88675	9.24444
Si	10.31500	4.12600	4.78439	Al	5.00000	0.57735	9.24444
Si	10.31500	6.18900	1.19789	Al	-3.00000	-2.88675	2.31111
Si	8.25200	6.18900	-2.38861	Al	-3.00000	-2.88675	4.62222
Si	0.00000	-2.06300	-4.78439	Al	-4.00000	-1.15470	8.08889
Si	0.00000	2.06300	-4.78439	Al	2.00000	-4.61880	8.08889
Si	4.12600	-2.06300	-4.78439	Al	3.00000	-2.88675	1.15556
Si	4.12600	2.06300	-4.78439	Al	-2.00000	-4.61880	8.08889
Si	8.25200	-2.06300	-4.78439	Al	8.00000	-1.15470	8.08889
Si	8.25200	2.06300	-4.78439	Al	6.00000	2.30940	8.08889
Si	0.00000	6.18900	-4.78439	Al	6.00000	-4.61880	8.08889
Si	4.12600	6.18900	-4.78439	Al	7.00000	-2.88675	1.15556
Si	10.31500	6.18900	-1.19789	Al	-2.00000	-4.61880	5.77778
Si	8.25200	6.18900	-4.78439	Al	-2.00000	-4.61880	-2.31111
Si	0.00000	0.00000	-5.97511	Al	7.00000	-2.88675	9.24444
Si	0.00000	4.12600	-5.97511	Al	2.00000	-4.61880	-2.31111
Si	4.12600	0.00000	-5.97511	Al	9.00000	-2.88675	2.31111
Si	4.12600	4.12600	-5.97511	Al	7.00000	-2.88675	-1.15556
Si	8.25200	0.00000	-5.97511	Al	11.00000	0.57735	2.31111
Si	8.25200	4.12600	-5.97511	Al	8.00000	-1.15470	-2.31111
				Al	9.00000	-2.88675	4.62222
				Al	9.00000	0.57735	9.24444
(10,3) -c				Al	3.00000	-6.35085	4.62222
TITLE 103c or B2O3				Al	-1.00000	-2.88675	11.55556
CELL 3.46 3.46 9. 90. 90. 120.				Al	1.00000	0.57735	11.55556
ATOM Si 0.33333 0.166666				Al	-3.00000	0.57735	11.55556
0.111111				Al	7.00000	-6.35085	4.62222
SPGR P 31 1 2				Al	3.00000	-2.88675	11.55556
				Al	5.00000	0.57735	11.55556
105				Al	1.00000	-6.35085	9.24444
				Al	5.00000	-6.35085	9.24444
Al 1.00000	0.57735	1.15556		Al	-1.00000	-6.35085	4.62222
Al -1.00000	0.57735	2.31111		Al	7.00000	-2.88675	11.55556
Al 3.00000	0.57735	2.31111		Al	1.00000	-6.35085	-1.15556
Al 1.00000	0.57735	-1.15556		Al	6.00000	-4.61880	-2.31111
Al -3.00000	0.57735	1.15556		Al	11.00000	0.57735	4.62222
Al -1.00000	0.57735	4.62222		Al	9.00000	0.57735	11.55556
Al 5.00000	0.57735	1.15556		Al	10.00000	2.30940	8.08889
Al 3.00000	0.57735	4.62222		Al	4.00000	-8.08290	5.77778
Al 0.00000	-1.15470	-2.31111		Al	3.00000	-6.35085	2.31111
Al -5.00000	0.57735	2.31111		Al	-3.00000	-2.88675	12.71111
Al -3.00000	0.57735	-1.15556		Al	1.00000	-2.88675	12.71111
Al 0.00000	-1.15470	5.77778		Al	-1.00000	0.57735	12.71111
Al -2.00000	2.30940	5.77778		Al	3.00000	0.57735	12.71111
Al 7.00000	0.57735	2.31111		Al	-5.00000	0.57735	12.71111
Al 5.00000	0.57735	-1.15556		Al	7.00000	-6.35085	2.31111
Al 4.00000	-1.15470	5.77778		Al	5.00000	-2.88675	12.71111
Al 2.00000	2.30940	5.77778		Al	7.00000	0.57735	12.71111
Al -1.00000	-2.88675	-1.15556		Al	1.00000	-6.35085	11.55556
Al -5.00000	0.57735	4.62222		Al	0.00000	-8.08290	8.08889
Al -4.00000	-1.15470	-2.31111		Al	5.00000	-6.35085	11.55556
Al 1.00000	-2.88675	4.62222		Al	4.00000	-8.08290	8.08889
Al 0.00000	-1.15470	8.08889		Al	0.00000	-8.08290	5.77778
Al -2.00000	2.30940	8.08889		Al	-1.00000	-6.35085	2.31111
Al 9.00000	0.57735	1.15556					

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Al	9.00000	-2.88675	12.71111	B	3.60000	-0.30016	3.13040
Al	1.00000	-6.35085	1.15556	B	5.60000	-0.30016	0.44720
Al	10.00000	2.30940	5.77778	B	4.40000	1.29984	1.34160
Al	5.00000	-6.35085	-1.15556	B	4.40000	-1.90016	-2.23600
Al	11.00000	0.57735	12.71111	B	2.40000	-1.90016	-1.34160
Al	5.00000	-6.35085	1.15556	B	1.60000	2.89984	-3.13040
Al	-1.00000	-6.35085	12.71111	B	0.40000	1.29984	-2.23600
Al	3.00000	-6.35085	12.71111	B	4.40000	1.29984	-2.23600
Al	7.00000	-6.35085	12.71111	B	3.60000	2.89984	-0.44720
				B	0.40000	4.49984	1.34160
				B	-0.40000	2.89984	-0.44720
(10,3)-d				B	2.40000	4.49984	-1.34160
TITLE (10,3)-d or 3/10/o1				B	1.60000	-0.30016	4.02480
CELL 4. 3.2 3.5776 90.000 90.000				B	3.60000	2.89984	3.13040
90.000				B	1.60000	2.89984	4.02480
ATOM C .100 0.0938 0.125				B	0.40000	4.49984	4.91920
SPGR P n n a				B	-2.40000	2.89984	4.02480
				B	-1.60000	4.49984	2.23600
				B	-2.40000	2.89984	0.44720
140				B	-3.60000	1.29984	1.34160
B	0.40000	0.30016	0.44720	B	-2.40000	-0.30016	4.02480
B	1.60000	-0.30016	0.44720	B	-4.40000	-0.30016	-0.44720
B	0.40000	1.29984	1.34160	B	-3.60000	-1.90016	1.34160
B	-0.40000	-0.30016	-0.44720	B	-2.40000	2.89984	-3.13040
B	1.60000	-1.29984	1.34160	B	-3.60000	1.29984	-2.23600
B	2.40000	0.30016	-0.44720	B	1.60000	-3.50016	-3.13040
B	1.60000	1.90016	1.34160	B	-0.40000	-3.50016	-4.02480
B	-0.40000	1.90016	2.23600	B	1.60000	-0.30016	-3.13040
B	-1.60000	0.30016	-0.44720	B	-2.40000	-0.30016	-3.13040
B	-0.40000	-1.29984	-1.34160	B	-3.60000	-1.90016	-2.23600
B	0.40000	-1.90016	1.34160	B	-2.40000	-3.50016	0.44720
B	2.40000	-1.90016	2.23600	B	1.60000	-4.49984	1.34160
B	3.60000	-0.30016	-0.44720	B	2.40000	-2.89984	-0.44720
B	2.40000	1.29984	-1.34160	B	-0.40000	-4.49984	-1.34160
B	1.60000	2.89984	0.44720	B	0.40000	0.30016	4.02480
B	2.40000	1.29984	2.23600	B	-1.60000	-2.89984	3.13040
B	-0.40000	2.89984	3.13040	B	0.40000	-2.89984	4.02480
B	-1.60000	1.29984	2.23600	B	1.60000	-4.49984	4.91920
B	-2.40000	-0.30016	0.44720	B	4.40000	-2.89984	4.02480
B	-1.60000	1.29984	-1.34160	B	3.60000	-4.49984	2.23600
B	0.40000	-1.90016	-2.23600	B	4.40000	-2.89984	0.44720
B	-1.60000	-1.90016	-1.34160	B	5.60000	-1.29984	1.34160
B	0.40000	-2.89984	0.44720	B	4.40000	0.30016	4.02480
B	-0.40000	-1.29984	2.23600	B	6.40000	0.30016	-0.44720
B	2.40000	-2.89984	3.13040	B	5.60000	1.90016	1.34160
B	3.60000	-1.29984	2.23600	B	4.40000	-2.89984	-3.13040
B	4.40000	0.30016	0.44720	B	5.60000	-1.29984	-2.23600
B	3.60000	-1.29984	-1.34160	B	0.40000	3.50016	-3.13040
B	1.60000	1.90016	-2.23600	B	2.40000	3.50016	-4.02480
B	3.60000	1.90016	-1.34160	B	0.40000	0.30016	-3.13040
B	0.40000	3.50016	0.44720	B	4.40000	0.30016	-3.13040
B	2.40000	3.50016	-0.44720	B	5.60000	1.90016	-2.23600
B	2.40000	0.30016	3.13040	B	4.40000	3.50016	0.44720
B	3.60000	1.90016	2.23600	B	1.60000	5.10016	1.34160
B	0.40000	3.50016	4.02480	B	-0.40000	5.10016	2.23600
B	-1.60000	3.50016	3.13040	B	-1.60000	3.50016	-0.44720
B	-2.40000	1.90016	1.34160	B	1.60000	5.10016	-2.23600
B	-1.60000	0.30016	3.13040	B	3.60000	5.10016	-1.34160
B	-3.60000	0.30016	0.44720	B	1.60000	-1.29984	4.91920
B	-2.40000	-1.29984	1.34160	B	4.40000	3.50016	4.02480
B	-2.40000	1.90016	-2.23600	B	2.40000	3.50016	3.13040
B	-0.40000	1.90016	-1.34160	B	1.60000	1.90016	4.91920
B	0.40000	-2.89984	-3.13040	B	1.60000	5.10016	4.91920
B	1.60000	-1.29984	-2.23600	B	-0.40000	5.10016	5.81360
B	-2.40000	-1.29984	-2.23600	B	3.60000	3.50016	4.02480
B	-1.60000	-2.89984	-0.44720	B	-2.40000	1.90016	4.91920
B	1.60000	-3.50016	0.44720	B	-2.40000	5.10016	1.34160
B	-0.40000	-3.50016	-0.44720	B	-3.60000	3.50016	0.44720
B	-0.40000	-0.30016	3.13040	B	-4.40000	1.90016	2.23600
B	-1.60000	-1.90016	2.23600	B	-3.60000	0.30016	4.02480
B	1.60000	-3.50016	4.02480	B	-2.40000	-1.29984	4.91920
B	3.60000	-3.50016	3.13040	B	-5.60000	0.30016	-0.44720
B	4.40000	-1.90016	1.34160				

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B	-4.40000	-1.29984	-1.34160	Al	-2.70833	-2.81458	-3.00000
B	-3.60000	-2.89984	0.44720	Al	3.79167	-2.81458	-3.00000
B	-4.40000	-1.29984	2.23600	Al	0.54167	2.81458	-3.00000
B	-3.60000	3.50016	-3.13040	Al	-2.70833	-2.81458	0.00000
B	-1.60000	3.50016	-4.02480	Al	3.79167	-2.81458	0.00000
B	-3.60000	0.30016	-3.13040	Al	-2.70833	-2.81458	3.00000
B	-4.40000	1.90016	-1.34160	Al	3.79167	-2.81458	3.00000
B	1.60000	-4.49984	-2.23600	Al	-2.16667	-3.75278	-2.50000
B	2.40000	-2.89984	-4.02480	Al	4.33333	-3.75278	-2.50000
B	-1.60000	-2.89984	-4.02480	Al	1.08333	1.87639	-2.50000
B	-0.40000	-4.49984	-4.91920	Al	-2.16667	-3.75278	0.50000
B	2.40000	0.30016	-4.02480	Al	4.33333	-3.75278	0.50000
B	-1.60000	0.30016	-4.02480	Al	-1.08333	-3.75278	-2.00000
B	-3.60000	-2.89984	-3.13040	Al	5.41667	-3.75278	-2.00000
B	-2.40000	-4.49984	1.34160	Al	2.16667	1.87639	-2.00000
				Al	-1.08333	-3.75278	1.00000
(10,3)-e				Al	5.41667	-3.75278	1.00000
				Al	-0.54167	-2.81458	-1.50000
TITLE	103e			Al	5.95833	-2.81458	-1.50000
CELL	7.5 7.5 3 90. 90. 120.			Al	-0.54167	-2.81458	1.50000
ATOM	C1	0.33333	0.50000	Al	5.95833	-2.81458	1.50000
		0.00000		Al	-1.08333	-1.87639	-1.00000
ATOM	C2	0.33333	0.33333	Al	5.41667	-1.87639	-1.00000
		0.16667		Al	-1.08333	-1.87639	2.00000
ATOM	C3	0.50000	0.33333	Al	5.41667	-1.87639	2.00000
		0.33333		Al	-2.16667	-1.87639	-0.50000
ATOM	C4	0.66667	0.50000	Al	4.33333	-1.87639	-0.50000
		0.50000		Al	-2.16667	-1.87639	2.50000
ATOM	C5	0.66667	0.66667	Al	4.33333	-1.87639	2.50000
		0.66667		Al	-2.92500	-0.56292	-0.50000
ATOM	C6	0.50000	0.66667	Al	3.57500	-0.56292	-0.50000
		0.83333		Al	-2.92500	-0.56292	2.50000
ATOM	C7	0.50000	0.90000	Al	3.57500	-0.56292	2.50000
		0.83333		Al	-0.32500	-0.56292	-1.00000
ATOM	C8	0.90000	0.90000	Al	6.17500	-0.56292	-1.00000
		0.66667		Al	-0.32500	-0.56292	2.00000
ATOM	C9	0.90000	0.50000	Al	6.17500	-0.56292	2.00000
		0.50000		Al	0.97500	-2.81458	-1.50000
ATOM	C10	0.50000	0.10000	Al	7.47500	-2.81458	-1.50000
		0.33333		Al	-2.27500	2.81458	-1.50000
ATOM	C11	0.10000	0.10000	Al	4.22500	2.81458	-1.50000
		0.16667		Al	0.97500	-2.81458	1.50000
ATOM	C12	0.10000	0.50000	Al	7.47500	-2.81458	1.50000
		0.00000		Al	-2.27500	2.81458	1.50000
SPGR	P 1			Al	-0.32500	-5.06625	-2.00000
				Al	6.17500	-5.06625	-2.00000
151				Al	-3.57500	0.56292	-2.00000
				Al	2.92500	0.56292	-2.00000
Al	0.54167	2.81458	0.00000	Al	-0.32500	-5.06625	1.00000
Al	1.08333	1.87639	0.50000	Al	6.17500	-5.06625	1.00000
Al	2.16667	1.87639	1.00000	Al	-3.57500	0.56292	1.00000
Al	2.70833	2.81458	1.50000	Al	-2.92500	-5.06625	-2.50000
Al	2.16667	3.75278	2.00000	Al	3.57500	-5.06625	-2.50000
Al	1.08333	3.75278	2.50000	Al	0.32500	0.56292	-2.50000
Al	0.54167	2.81458	3.00000	Al	-2.92500	-5.06625	0.50000
Al	0.32500	5.06625	2.50000	Al	3.57500	-5.06625	0.50000
Al	2.92500	5.06625	2.00000	Al	-4.22500	-2.81458	-3.00000
Al	4.22500	2.81458	1.50000	Al	2.27500	-2.81458	-3.00000
Al	2.92500	0.56292	1.00000	Al	-0.97500	2.81458	-3.00000
Al	0.32500	0.56292	0.50000	Al	-4.22500	-2.81458	0.00000
Al	-0.97500	2.81458	0.00000	Al	2.27500	-2.81458	0.00000
Al	-0.97500	2.81458	3.00000	Al	-4.22500	-2.81458	3.00000
Al	1.08333	3.75278	-0.50000	Al	2.27500	-2.81458	3.00000
Al	1.08333	1.87639	3.50000	Al	2.16667	3.75278	5.00000
Al	2.16667	3.75278	-1.00000	Al	-2.16667	-1.87639	-3.50000
Al	0.32500	5.06625	-0.50000	Al	4.33333	-1.87639	-3.50000
Al	2.16667	1.87639	4.00000	Al	1.08333	3.75278	-3.50000
Al	0.32500	0.56292	3.50000	Al	-2.16667	-3.75278	3.50000
Al	2.70833	2.81458	-1.50000	Al	4.33333	-3.75278	3.50000
Al	2.92500	5.06625	-1.00000	Al	2.16667	3.75278	-4.00000
Al	2.70833	2.81458	4.50000	Al	-1.08333	-3.75278	4.00000
Al	2.92500	0.56292	4.00000	Al	5.41667	-3.75278	4.00000

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Al	4.22500	2.81458	4.50000	ATOM	C7	0.00000	0.25000
Al	2.92500	5.06625	5.00000			0.87500	
Al	-2.92500	-0.56292	-3.50000	ATOM	C8	0.25000	0.37500
Al	3.57500	-0.56292	-3.50000			0.75000	
Al	0.32500	5.06625	-3.50000	ATOM	C9	0.00000	0.62500
Al	-2.92500	-5.06625	3.50000			0.75000	
Al	3.57500	-5.06625	3.50000	ATOM	C10	0.25000	0.75000
Al	-0.32500	-0.56292	-4.00000			0.62500	
Al	6.17500	-0.56292	-4.00000	ATOM	C11	0.50000	0.87500
Al	2.92500	5.06625	-4.00000			0.75000	
Al	-0.54167	-2.81458	4.50000	ATOM	C12	0.75000	0.75000
Al	-0.32500	-2.81458	4.00000			0.87500	
Al	5.95833	-2.81458	4.50000	ATOM	C13	0.00000	0.75000
Al	6.17500	-5.06625	4.00000			0.37500	
Al	-3.57500	0.56292	4.00000	ATOM	C14	0.25000	0.62500
Al	-0.32500	6.19208	1.00000			0.25000	
Al	-0.32500	6.19208	4.00000	ATOM	C15	0.50000	0.75000
Al	3.57500	6.19208	0.50000			0.12500	
Al	3.57500	6.19208	3.50000	ATOM	C16	0.75000	0.87500
Al	5.52500	2.81458	0.00000			0.25000	
Al	5.52500	2.81458	3.00000	SPGR	P 1		
Al	-2.27500	2.81458	4.50000				
Al	-0.32500	6.19208	-2.00000	56			
Al	-0.32500	-0.56292	5.00000				
Al	3.57500	6.19208	-2.50000	B	0.00000	2.06250	1.37500
Al	6.82500	0.56292	-2.50000	B	0.75000	1.37500	0.68750
Al	6.82500	0.56292	0.50000	B	1.50000	0.68750	1.37500
Al	6.82500	0.56292	3.50000	B	1.50000	1.37500	3.43750
Al	8.77500	-2.81458	-3.00000	B	2.25000	1.37500	2.06250
Al	8.77500	-2.81458	0.00000	B	2.25000	0.68750	4.12500
Al	5.52500	2.81458	-3.00000	B	0.00000	1.37500	4.81250
Al	8.77500	-2.81458	3.00000	B	0.00000	3.43750	4.12500
Al	0.32500	-6.19208	-3.50000	B	0.75000	2.06250	4.12500
Al	0.32500	-6.19208	-0.50000	B	0.75000	4.12500	3.43750
Al	6.82500	-6.19208	-3.50000	B	1.50000	4.81250	4.12500
Al	6.82500	-6.19208	-0.50000	B	2.25000	4.12500	4.81250
Al	0.32500	-6.19208	2.50000	B	0.00000	4.12500	2.06250
Al	6.82500	-6.19208	2.50000	B	0.75000	3.43750	1.37500
Al	-3.57500	-6.19208	-4.00000	B	1.50000	4.12500	0.68750
Al	-3.57500	-6.19208	-1.00000	B	2.25000	4.81250	1.37500
Al	2.92500	-6.19208	-4.00000	B	-0.75000	1.37500	2.06250
Al	2.92500	-6.19208	-1.00000	B	0.00000	1.37500	-0.68750
Al	-3.57500	-6.19208	2.00000	B	2.25000	-0.68750	1.37500
Al	2.92500	-6.19208	2.00000	B	3.00000	2.06250	1.37500
Al	-5.52500	-2.81458	-1.50000	B	3.00000	1.37500	4.81250
Al	-5.52500	-2.81458	1.50000	B	1.50000	-0.68750	4.12500
Al	-5.52500	-2.81458	4.50000	B	0.75000	1.37500	6.18750
Al	0.97500	-2.81458	4.50000	B	-0.75000	0.68750	4.12500
Al	-3.57500	-6.19208	5.00000	B	-0.75000	4.12500	4.81250
Al	2.92500	-6.19208	5.00000	B	2.25000	6.18750	4.12500
Al	-1.08333	-1.87639	5.00000	B	3.00000	3.43750	4.12500
Al	0.32500	-6.19208	5.50000	B	1.50000	4.12500	6.18750
Al	5.41667	-1.87639	5.00000	B	-0.75000	4.81250	1.37500
Al	7.47500	-2.81458	4.50000	B	2.25000	4.12500	-0.68750
Al	6.82500	-6.19208	5.50000	B	1.50000	6.18750	1.37500
				B	3.00000	4.12500	2.06250
(10,3)-f				B	-1.50000	0.68750	1.37500
				B	-1.50000	1.37500	3.43750
TITLE	103f			B	3.75000	1.37500	0.68750
CELL	5. 5.5 5.5 90. 90. 90.			B	3.75000	3.43750	1.37500
ATOM	C1	0.00000	0.37500	B	3.75000	1.37500	6.18750
				B	3.75000	2.06250	4.12500
ATOM	C2	0.25000	0.25000	B	-1.50000	-0.68750	4.12500
				B	-1.50000	4.81250	4.12500
ATOM	C3	0.50000	0.12500	B	-1.50000	4.12500	6.18750
				B	3.75000	4.12500	3.43750
ATOM	C4	0.75000	0.25000	B	-1.50000	6.18750	1.37500
				B	-1.50000	4.12500	0.68750
ATOM	C5	0.50000	0.25000	B	-2.25000	1.37500	0.68750
				B	-0.75000	-0.68750	1.37500
ATOM	C6	0.75000	0.12500	B	-2.25000	2.06250	4.12500
				B	4.50000	0.68750	1.37500

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B	3.00000	1.37500	-0.68750	Al	10.20000	8.50000	11.90000
B	4.50000	4.12500	0.68750	Al	3.40000	1.70000	0.00000
B	4.50000	1.37500	3.43750	Al	3.40000	1.70000	17.00000
B	-0.75000	6.18750	4.12500	Al	11.90000	10.20000	8.50000
B	-2.25000	4.12500	3.43750	Al	0.00000	3.40000	1.70000
B	4.50000	4.81250	4.12500	Al	17.00000	3.40000	1.70000
B	-0.75000	4.12500	-0.68750	Al	8.50000	11.90000	10.20000
B	-2.25000	3.43750	1.37500	Al	0.00000	5.10000	1.70000
				Al	17.00000	5.10000	1.70000
				Al	8.50000	13.60000	10.20000
(10,3)-g				Al	3.40000	15.30000	8.50000
				Al	11.90000	6.80000	0.00000
TITLE 103g				Al	11.90000	6.80000	17.00000
CELL 10. 10. 10. 90. 90. 90.				Al	8.50000	3.40000	15.30000
ATOM C1 0.125 0.125 0.125				Al	0.00000	11.90000	6.80000
ATOM C2 0.125 0.125 0.375				Al	17.00000	11.90000	6.80000
ATOM C3 0.100 0.000 0.200				Al	13.60000	6.80000	0.00000
ATOM C4 0.350 0.050 0.250				Al	13.60000	6.80000	17.00000
SPGR I a -3				Al	5.10000	15.30000	8.50000
				Al	5.10000	1.70000	0.00000
184				Al	5.10000	1.70000	17.00000
				Al	13.60000	10.20000	8.50000
Ag 2.12500 2.12500 6.37500				Al	0.00000	13.60000	6.80000
Ag 10.62500 10.62500 14.87500				Al	17.00000	13.60000	6.80000
Ag 6.37500 2.12500 2.12500				Al	8.50000	5.10000	15.30000
Ag 14.87500 10.62500 10.62500				Al	15.30000	8.50000	3.40000
Ag 2.12500 6.37500 2.12500				Al	6.80000	0.00000	11.90000
Ag 10.62500 14.87500 10.62500				Al	6.80000	17.00000	11.90000
Ag 14.87500 2.12500 2.12500				Al	1.70000	0.00000	5.10000
Ag 6.37500 10.62500 10.62500				Al	1.70000	17.00000	5.10000
Ag 6.37500 14.87500 6.37500				Al	10.20000	8.50000	13.60000
Ag 14.87500 6.37500 14.87500				Al	6.80000	0.00000	13.60000
Ag 6.37500 6.37500 14.87500				Al	6.80000	17.00000	13.60000
Ag 14.87500 14.87500 6.37500				Al	15.30000	8.50000	5.10000
Ag 10.62500 6.37500 2.12500				Al	15.30000	0.00000	13.60000
Ag 2.12500 14.87500 10.62500				Al	15.30000	17.00000	13.60000
Ag 2.12500 2.12500 14.87500				Al	6.80000	8.50000	5.10000
Ag 10.62500 10.62500 6.37500				Al	13.60000	15.30000	0.00000
Ag 2.12500 10.62500 6.37500				Al	13.60000	15.30000	17.00000
Ag 10.62500 2.12500 14.87500				Al	5.10000	6.80000	8.50000
Ag 14.87500 6.37500 6.37500				Al	0.00000	13.60000	15.30000
Ag 6.37500 14.87500 14.87500				Al	17.00000	13.60000	15.30000
Ag 2.12500 14.87500 2.12500				Al	8.50000	5.10000	6.80000
Ag 10.62500 6.37500 10.62500				Al	0.00000	11.90000	15.30000
Ag 6.37500 2.12500 10.62500				Al	17.00000	11.90000	15.30000
Ag 14.87500 10.62500 2.12500				Al	8.50000	3.40000	6.80000
Ag 14.87500 14.87500 10.62500				Al	13.60000	1.70000	8.50000
Ag 6.37500 6.37500 2.12500				Al	5.10000	10.20000	0.00000
Ag 10.62500 14.87500 14.87500				Al	5.10000	10.20000	17.00000
Ag 2.12500 6.37500 6.37500				Al	8.50000	13.60000	1.70000
Ag 14.87500 10.62500 14.87500				Al	0.00000	5.10000	10.20000
Ag 6.37500 2.12500 6.37500				Al	17.00000	5.10000	10.20000
Ag 2.12500 14.87500 14.87500				Al	3.40000	10.20000	0.00000
Ag 10.62500 6.37500 6.37500				Al	3.40000	10.20000	17.00000
Ag 10.62500 2.12500 10.62500				Al	11.90000	1.70000	8.50000
Ag 2.12500 10.62500 2.12500				Al	11.90000	15.30000	0.00000
Ag 10.62500 10.62500 2.12500				Al	11.90000	15.30000	17.00000
Ag 2.12500 2.12500 10.62500				Al	3.40000	6.80000	8.50000
Ag 6.37500 10.62500 14.87500				Al	0.00000	3.40000	10.20000
Ag 14.87500 2.12500 6.37500				Al	17.00000	3.40000	10.20000
Ag 14.87500 14.87500 2.12500				Al	8.50000	11.90000	1.70000
Ag 6.37500 6.37500 10.62500				Al	1.70000	8.50000	13.60000
Ag 14.87500 6.37500 10.62500				Al	10.20000	0.00000	5.10000
Ag 6.37500 14.87500 2.12500				Al	10.20000	17.00000	5.10000
Ag 2.12500 10.62500 10.62500				Al	15.30000	0.00000	11.90000
Ag 10.62500 2.12500 2.12500				Al	15.30000	17.00000	11.90000
Ag 14.87500 2.12500 14.87500				Al	6.80000	8.50000	3.40000
Ag 6.37500 10.62500 6.37500				Al	10.20000	0.00000	3.40000
Ag 10.62500 14.87500 6.37500				Al	10.20000	17.00000	3.40000
Ag 2.12500 6.37500 14.87500				Al	1.70000	8.50000	11.90000
Al 1.70000 0.00000 3.40000				Al	5.95000	8.50000	4.25000
Al 1.70000 17.00000 3.40000				Al	14.45000	9.35000	12.75000

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Al	4.25000	5.95000	0.85000	128			
Al	12.75000	14.45000	9.35000				
Al	0.85000	4.25000	5.95000	Al	0.64000	1.44250	2.37362
Al	9.35000	12.75000	14.45000	Al	1.86000	-1.05750	2.37362
Al	16.15000	4.25000	5.95000	Al	-0.64000	1.44250	2.88163
Al	7.65000	12.75000	14.45000	Al	1.86000	1.05750	2.88163
Al	4.25000	11.05000	7.65000	Al	0.64000	-1.44250	2.88163
Al	12.75000	2.55000	16.15000	Al	3.14000	-1.05750	2.88163
Al	7.65000	4.25000	11.05000	Al	1.86000	3.94250	2.37362
Al	16.15000	12.75000	2.55000	Al	-1.86000	1.05750	2.37362
Al	12.75000	2.55000	0.85000	Al	-1.05750	1.86000	4.12537
Al	4.25000	11.05000	9.35000	Al	1.44250	0.64000	4.12537
Al	4.25000	5.95000	16.15000	Al	3.14000	1.05750	2.37362
Al	12.75000	14.45000	7.65000	Al	1.05750	-1.86000	4.12537
Al	0.85000	12.75000	2.55000	Al	-0.64000	-1.44250	2.37362
Al	9.35000	4.25000	11.05000	Al	3.55750	-0.64000	4.12537
Al	11.05000	7.65000	4.25000	Al	4.36000	-1.44250	2.37362
Al	2.55000	16.15000	12.75000	Al	0.64000	-3.55750	2.37362
Al	5.95000	16.15000	4.25000	Al	0.64000	3.55750	2.88163
Al	14.45000	7.65000	12.75000	Al	3.14000	3.94250	2.88163
Al	2.55000	0.85000	12.75000	Al	-3.14000	1.05750	2.88163
Al	11.05000	9.35000	4.25000	Al	-1.44250	0.64000	4.63338
Al	11.05000	16.15000	12.75000	Al	-1.05750	3.14000	4.63338
Al	2.55000	7.65000	4.25000	Al	1.05750	1.86000	4.63338
Al	12.75000	11.05000	16.15000	Al	1.44250	-0.64000	4.63338
Al	4.25000	2.55000	7.65000	Al	4.36000	1.44250	2.88163
Al	16.15000	12.75000	11.05000	Al	1.05750	-3.14000	4.63338
Al	7.65000	4.25000	2.55000	Al	-1.86000	-1.05750	2.88163
Al	0.85000	12.75000	11.05000	Al	3.55750	0.64000	4.63338
Al	9.35000	4.25000	2.55000	Al	3.94250	-1.86000	4.63338
Al	12.75000	5.95000	9.35000	Al	-0.64000	-3.55750	2.88163
Al	4.25000	14.45000	0.85000	Al	1.86000	-3.94250	2.88163
Al	9.35000	12.75000	5.95000	Al	1.05750	3.14000	4.12537
Al	0.85000	4.25000	14.45000	Al	-0.64000	3.55750	2.37362
Al	4.25000	14.45000	16.15000	Al	3.55750	4.36000	4.12537
Al	12.75000	5.95000	7.65000	Al	4.36000	3.55750	2.37362
Al	12.75000	11.05000	0.85000	Al	-3.55750	0.64000	4.12537
Al	4.25000	2.55000	9.35000	Al	-1.44250	-0.64000	4.12537
Al	16.15000	4.25000	14.45000	Al	-1.44250	4.36000	4.12537
Al	7.65000	12.75000	5.95000	Al	3.94250	1.86000	4.12537
Al	5.95000	9.35000	12.75000	Al	1.44250	-4.36000	4.12537
Al	14.45000	0.85000	4.25000	Al	-3.14000	-1.05750	2.37362
Al	11.05000	0.85000	12.75000	Al	3.94250	-3.14000	4.12537
Al	2.55000	9.35000	4.25000	Al	-1.86000	-3.94250	2.37362
Al	14.45000	16.15000	4.25000	Al	-1.05750	-3.14000	4.12537
Al	5.95000	7.65000	12.75000	Al	3.14000	-3.94250	2.37362
Ag	2.12500	2.12500	2.12500	Al	-1.86000	1.05750	5.87712
Ag	10.62500	10.62500	10.62500	Al	-0.64000	3.55750	5.87712
Ag	14.87500	6.37500	2.12500	Al	0.64000	1.44250	5.87712
Ag	6.37500	14.87500	10.62500	Al	1.86000	-1.05750	5.87712
Ag	2.12500	14.87500	6.37500	Al	0.64000	-3.55750	5.87712
Ag	10.62500	6.37500	14.87500	Al	3.14000	1.05750	5.87712
Ag	6.37500	2.12500	14.87500	Al	4.36000	-1.44250	5.87712
Ag	14.87500	10.62500	6.37500	Al	1.44250	4.36000	4.63338
Ag	14.87500	14.87500	14.87500	Al	-1.86000	3.94250	2.88163
Ag	6.37500	6.37500	6.37500	Al	3.94250	3.14000	4.63338
Ag	2.12500	10.62500	14.87500	Al	-3.94250	1.86000	4.63338
Ag	10.62500	2.12500	6.37500	Al	-3.55750	-0.64000	4.63338
Ag	14.87500	2.12500	10.62500	Al	-1.05750	-1.86000	4.63338
Ag	6.37500	10.62500	2.12500	Al	-4.36000	-1.44250	2.88163
Ag	10.62500	14.87500	2.12500	Al	4.36000	-3.55750	2.88163
Ag	2.12500	6.37500	10.62500	Al	3.55750	-4.36000	4.63338
				Al	-3.14000	-3.94250	2.88163
				Al	-1.44250	-4.36000	4.63338
				Al	-0.64000	1.44250	6.38513
				Al	-3.14000	1.05750	6.38513
				Al	0.64000	3.55750	6.38513
				Al	-1.86000	3.94250	6.38513
				Al	1.86000	1.05750	6.38513
				Al	0.64000	-1.44250	6.38513
				Al	3.14000	-1.05750	6.38513
				Al	-0.64000	-3.55750	6.38513

3/10/t2

TITLE 3/10/t2

CELL 4. 4. 2.8 90.000 90.000

90.000

ATOM C .0385 .3780 -0.0725

SPGR P 42/n b c

Supplementary Material (ESI) for Dalton Transactions
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Al	1.86000	-3.94250	6.38513	Al	-0.53040	2.34720	4.97403
Al	4.36000	1.44250	6.38513	Al	2.34720	4.53040	6.18863
Al	1.86000	3.94250	5.87712	Al	2.34720	3.46960	8.61783
Al	-3.14000	3.94250	2.37362	Al	-0.53040	2.34720	9.83243
Al	4.36000	3.55750	5.87712	Al	-1.65280	3.46960	4.74277
Al	-3.94250	3.14000	4.12537	Al	1.65280	4.53040	4.74277
Al	-4.36000	1.44250	5.87712	Al	1.65280	4.53040	9.60117
Al	-3.14000	-1.05750	5.87712	Al	0.53040	1.65280	10.81577
Al	-3.94250	-1.86000	4.12537	Al	-1.65280	3.46960	9.60117
Al	-0.64000	-1.44250	5.87712	Al	-2.34720	3.46960	6.18863
Al	3.14000	-3.94250	5.87712	Al	0.53040	5.65280	4.97403
Al	-3.55750	-4.36000	4.12537	Al	2.34720	4.53040	11.04703
Al	-1.86000	-3.94250	5.87712	Al	0.53040	5.65280	9.83243
Al	-1.05750	1.86000	7.62887	Al	0.53040	2.34720	12.26163
Al	-3.55750	0.64000	7.62887	Al	-2.34720	3.46960	11.04703
Al	1.05750	3.14000	7.62887	Al	-2.34720	4.53040	8.61783
Al	-3.14000	3.94250	5.87712	Al	-1.65280	4.53040	7.17197
Al	-1.44250	4.36000	7.62887	Al	-0.53040	6.34720	5.95737
Al	1.44250	0.64000	7.62887	Al	1.65280	3.46960	12.03037
Al	1.05750	-1.86000	7.62887	Al	-0.53040	6.34720	10.81577
Al	3.55750	-0.64000	7.62887	Al	0.53040	6.34720	8.38657
Al	-1.05750	-3.14000	7.62887	Al	-0.53040	1.65280	13.24497
Al	1.44250	-4.36000	7.62887	Al	-1.65280	4.53040	12.03037
Al	3.94250	1.86000	7.62887	Al	2.34720	3.46960	13.47623
Al	3.14000	3.94250	6.38513	Al	-0.53040	5.65280	7.40323
Al	-4.36000	3.55750	2.88163	Al	-0.53040	5.65280	12.26163
Al	-3.55750	4.36000	4.63338	Al	0.53040	6.34720	13.24497
Al	-4.36000	-1.44250	6.38513	Al	1.65280	0.53040	6.18863
Al	-1.86000	-1.05750	6.38513	Al	-1.65280	0.53040	8.61783
Al	-3.94250	-3.14000	4.63338	Al	3.46960	5.65280	5.95737
Al	4.36000	-3.55750	6.38513	Al	3.46960	2.34720	8.38657
Al	-3.14000	-3.94250	6.38513	Al	1.65280	0.53040	11.04703
Al	-1.44250	0.64000	8.13688	Al	-3.46960	2.34720	5.95737
Al	-1.05750	3.14000	8.13688	Al	3.46960	5.65280	10.81577
Al	-3.94250	1.86000	8.13688	Al	-3.46960	2.34720	10.81577
Al	-3.55750	-0.64000	8.13688	Al	-3.46960	5.65280	8.38657
Al	1.05750	1.86000	8.13688	Al	-1.65280	7.46960	11.04703
Al	-4.36000	3.55750	6.38513	Al	1.65280	7.46960	8.61783
Al	1.44250	-0.64000	8.13688	Al	-1.65280	0.53040	13.47623
Al	1.05750	-3.14000	8.13688	Al	3.46960	2.34720	13.24497
Al	3.55750	0.64000	8.13688	Al	1.65280	7.46960	13.47623
Al	3.94250	-1.86000	8.13688	Al	2.34720	0.53040	4.74277
Al	-1.05750	-1.86000	8.13688	Al	-2.34720	0.53040	7.17197
Al	3.94250	3.14000	8.13688	Al	3.46960	6.34720	7.40323
Al	3.55750	4.36000	7.62887	Al	4.53040	6.34720	4.97403
Al	-3.94250	-1.86000	7.62887	Al	3.46960	1.65280	9.83243
Al	-1.44250	-0.64000	7.62887	Al	4.53040	1.65280	7.40323
Al	-4.36000	-3.55750	5.87712	Al	2.34720	0.53040	9.60117
Al	3.94250	-3.14000	7.62887	Al	-3.46960	1.65280	7.40323
Al	-3.55750	-4.36000	7.62887	Al	3.46960	1.65280	4.97403
Al	-3.94250	3.14000	7.62887	Al	3.46960	6.34720	12.26163
Al	-3.94250	-3.14000	8.13688	Al	4.53040	6.34720	9.83243
Al	-4.36000	1.44250	2.37362	Al	-3.46960	1.65280	12.26163
Al	-4.36000	-3.55750	2.37362	Al	-3.46960	6.34720	9.83243
Al	1.44250	4.36000	8.13688	Al	-2.34720	7.46960	9.60117
Al	-1.44250	-4.36000	8.13688	Al	2.34720	7.46960	7.17197
Al	3.55750	-4.36000	8.13688	Al	-2.34720	0.53040	12.03037
Al	-3.55750	4.36000	8.13688	Al	4.53040	1.65280	12.26163
				Al	2.34720	7.46960	12.03037
				Al	4.53040	5.65280	8.38657
				Al	5.65280	7.46960	4.74277
				Al	4.53040	2.34720	10.81577
				Al	4.53040	2.34720	5.95737
				Al	5.65280	0.53040	7.17197
				Al	4.53040	5.65280	13.24497
				Al	5.65280	7.46960	9.60117
				Al	5.65280	4.53040	8.61783
				Al	6.34720	7.46960	6.18863
				Al	5.65280	3.46960	11.04703
				Al	5.65280	3.46960	6.18863
				Al	6.34720	0.53040	8.61783
				Al	5.65280	4.53040	13.47623

3/10/t5

TITLE 3/10/t5

CELL 8. 8. 4.8584 90. 90. 90.

ATOM C 0.06630 0.20660 0.22620

SPGR I 41/a c d

86

Al	0.53040	2.34720	7.40323
Al	0.53040	1.65280	5.95737
Al	1.65280	3.46960	7.17197
Al	-0.53040	1.65280	8.38657

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Al	6.34720	7.46960	11.04703	B	-3.92540	2.80345	0.38862
Al	6.34720	4.53040	7.17197	B	-1.94655	8.67540	1.36033
Al	6.34720	3.46960	9.60117	B	1.94655	8.67540	-0.38862
Al	7.46960	6.34720	5.95737	B	-1.94655	8.67540	-2.13757
Al	6.34720	4.53040	12.03037	B	-1.94655	0.82460	-3.88652
Al	7.46960	1.65280	8.38657	B	-3.92540	6.69655	2.13757
Al	7.46960	6.34720	10.81577	B	3.92540	2.80345	2.13757
Al	7.46960	5.65280	7.40323	B	-1.94655	8.67540	-5.63547
Al	7.46960	2.34720	9.83243	B	1.94655	8.67540	-3.88652
Al	7.46960	5.65280	12.26163	B	1.94655	0.82460	-5.63547

3/10/t6

TITLE 3/10/t6
CELL 10. 10. 3.682 90. 90. 90.
ATOM C 0.0868 0.4549 -0.0139
SPGR I41/acd

89

B	0.82460	1.94655	0.38862
B	-0.82460	2.80345	0.48586
B	0.82460	2.80345	-1.26309
B	-0.82460	1.94655	2.13757
B	-1.94655	3.92540	-0.48586
B	1.94655	3.92540	-2.23481
B	-0.82460	1.94655	-1.36033
B	0.82460	2.80345	2.23481
B	-2.80345	3.92540	-2.13757
B	-2.80345	5.57460	-0.38862
B	2.80345	5.57460	-2.13757
B	2.80345	3.92540	-3.88652
B	-0.82460	2.80345	-3.01204
B	1.94655	3.92540	1.26309
B	-1.94655	5.57460	-2.23481
B	-1.94655	5.57460	1.26309
B	1.94655	5.57460	-0.48586
B	1.94655	5.57460	-3.98376
B	0.82460	1.94655	-3.10928
B	-1.94655	3.92540	-3.98376
B	2.80345	5.57460	1.36033
B	2.80345	3.92540	-0.38862
B	-0.82460	6.69655	-1.26309
B	-2.80345	5.57460	-3.88652
B	-2.80345	3.92540	1.36033
B	-0.82460	6.69655	2.23481
B	0.82460	6.69655	0.48586
B	2.80345	5.57460	-5.63547
B	0.82460	6.69655	-3.01204
B	0.82460	2.80345	-4.76099
B	-2.80345	3.92540	-5.63547
B	-1.94655	3.92540	3.01204
B	1.94655	5.57460	3.01204
B	-0.82460	7.55345	0.38862
B	0.82460	7.55345	-1.36033
B	1.94655	3.92540	2.13757
B	-0.82460	7.55345	-3.10928
B	-0.82460	1.94655	-4.85823
B	-1.94655	5.57460	-5.73271
B	-2.80345	5.57460	3.10928
B	2.80345	3.92540	3.10928
B	-0.82460	6.69655	-4.76099
B	0.82460	7.55345	-4.85823
B	-1.94655	0.82460	-0.38862
B	-3.92540	6.69655	-1.36033
B	3.92540	6.69655	-3.10928
B	3.92540	2.80345	-4.85823
B	1.94655	0.82460	-2.13757
B	3.92540	6.69655	0.38862
B	3.92540	2.80345	-1.36033
B	-3.92540	6.69655	-4.85823

3/10/t7

TITLE 3/10/t7
CELL 6. 6. 8.3088 90. 90. 90.
ATOM C 0.1227 0.5342 -0.0377
SPGR I 41/a c d

120

Al	1.51060	2.64110	-0.84625
Al	1.51060	0.85890	-1.57715
Al	1.98940	4.35890	-1.57715
Al	1.98940	-0.85890	-0.84625
Al	0.85890	1.51060	-3.26965
Al	2.64110	5.01060	-3.26965
Al	1.98940	6.14110	-0.84625
Al	1.98940	-2.64110	-1.57715
Al	2.64110	1.51060	-4.00055
Al	-0.85890	1.98940	-4.00055
Al	4.35890	5.48940	-4.00055
Al	0.85890	5.01060	-4.00055
Al	-1.98940	0.85890	-0.84625
Al	5.01060	0.85890	-0.84625
Al	2.64110	-1.98940	-3.26965
Al	1.98940	0.85890	-5.69305
Al	4.35890	1.98940	-3.26965
Al	-1.51060	2.64110	-5.69305
Al	-2.64110	1.98940	-3.26965
Al	6.14110	5.48940	-3.26965
Al	5.01060	6.14110	-5.69305
Al	1.51060	4.35890	-5.69305
Al	-0.85890	5.48940	-3.26965
Al	-1.51060	-0.85890	-1.57715
Al	-1.98940	2.64110	-1.57715

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Al	5.48940	-0.85890	-1.57715	Al	5.01060	-2.64110	3.26965
Al	5.01060	2.64110	-1.57715	Al	1.51060	-0.85890	3.26965
Al	4.35890	-1.51060	-4.00055	Al	-1.98940	4.35890	3.26965
Al	0.85890	-1.98940	-4.00055	Al	5.01060	4.35890	3.26965
Al	1.98940	2.64110	-6.42395	Al	1.51060	6.14110	3.26965
Al	1.51060	-0.85890	-6.42395	Al	-5.48940	6.14110	3.26965
Al	6.14110	1.98940	-4.00055	Al	5.48940	0.85890	3.26965
Al	-1.98940	4.35890	-6.42395	Al	1.98940	2.64110	3.26965
Al	-1.51060	0.85890	-6.42395	Al	-1.51060	0.85890	3.26965
Al	-4.35890	1.51060	-4.00055	Al	-5.01060	2.64110	3.26965
Al	5.48940	6.14110	-1.57715	Al	-5.48940	-0.85890	3.26965
Al	5.01060	4.35890	-6.42395	Al	1.51060	-2.64110	4.00055
Al	1.51060	6.14110	-6.42395	Al	1.98940	0.85890	4.00055
Al	-2.64110	5.48940	-4.00055	Al	5.01060	-0.85890	4.00055
Al	-1.51060	6.14110	-1.57715	Al	-5.48940	-2.64110	4.00055
Al	-0.85890	-1.51060	-3.26965	Al	-5.48940	4.35890	4.00055
Al	-1.51060	-2.64110	-0.84625	Al	-5.01060	0.85890	4.00055
Al	-1.51060	4.35890	-0.84625	Al	-1.51060	2.64110	4.00055
Al	-5.48940	2.64110	-0.84625	Al	-1.98940	-0.85890	4.00055
Al	6.14110	-1.51060	-3.26965	Al	1.51060	4.35890	4.00055
Al	5.48940	-2.64110	-0.84625	Al	5.48940	2.64110	4.00055
Al	5.48940	4.35890	-0.84625	Al	-1.98940	6.14110	4.00055
Al	5.01060	-0.85890	-5.69305	Al	5.01060	6.14110	4.00055
Al	1.51060	-2.64110	-5.69305				
Al	5.48940	2.64110	-5.69305				
Al	-1.98940	6.14110	-5.69305				
Al	-1.98940	-0.85890	-5.69305				
Al	-6.14110	1.51060	-3.26965				
Al	-5.01060	0.85890	-5.69305				
Al	-4.35890	5.01060	-3.26965				
Al	-2.64110	-1.51060	-4.00055				
Al	-5.48940	0.85890	-1.57715				
Al	-5.01060	4.35890	-1.57715				
Al	5.01060	-2.64110	-6.42395				
Al	5.48940	0.85890	-6.42395				
Al	-1.98940	-2.64110	-6.42395				
Al	-5.01060	2.64110	-6.42395				
Al	-5.48940	-0.85890	-6.42395				
Al	-6.14110	5.01060	-4.00055				
Al	-4.35890	-1.98940	-3.26965				
Al	-5.01060	-0.85890	-0.84625				
Al	-5.01060	6.14110	-0.84625				
Al	-5.48940	4.35890	-5.69305				
Al	-5.48940	-2.64110	-5.69305				
Al	-6.14110	-1.98940	-4.00055				
Al	-5.01060	-2.64110	-1.57715				
Al	-5.48940	6.14110	-6.42395				
Al	0.85890	1.98940	0.84625				
Al	2.64110	-1.51060	0.84625				
Al	4.35890	1.51060	0.84625				
Al	2.64110	5.48940	0.84625				
Al	-2.64110	1.51060	0.84625				
Al	-6.14110	1.98940	0.84625				
Al	-0.85890	-1.98940	0.84625				
Al	6.14110	-1.98940	0.84625				
Al	6.14110	5.01060	0.84625				
Al	-4.35890	-1.51060	0.84625				
Al	-0.85890	5.01060	0.84625				
Al	-4.35890	5.48940	0.84625				
Al	-2.64110	-1.98940	1.57715				
Al	0.85890	-1.51060	1.57715				
Al	4.35890	-1.98940	1.57715				
Al	4.35890	5.01060	1.57715				
Al	6.14110	1.51060	1.57715				
Al	-6.14110	-1.51060	1.57715				
Al	-2.64110	5.01060	1.57715				
Al	0.85890	5.48940	1.57715				
Al	-6.14110	5.48940	1.57715				
Al	-4.35890	1.98940	1.57715				
Al	-0.85890	1.51060	1.57715				
Al	2.64110	1.98940	1.57715				
Al	-1.98940	-2.64110	3.26965				