

Supporting Information

Structural evolution and combustion energy of Al–B clusters

Elizaveta E. Vaneeva*,^{1,2} Anastasiia A. Mikhailova¹, Sergey V. Lepeshkin,^{1,2} Alexey P. Maltsev¹ and Artem R. Oganov¹

¹ Skolkovo Institute of Science and Technology, Bolshoy Boulevard 30, bld. 1, 121205 Moscow, Russian Federation

² Lebedev Physical Institute, Russian Academy of Sciences, Leninsky Ave. 53, 119991 Moscow, Russian Federation

*Elizaveta.Vaneeva@skoltech.ru

Section 1

Table S1. Values of Δ^2_{\min} , E_{frag} and fragmentation channels of Al_nB_m clusters ($0 \leq n, m \leq 15$).

Nanocluster	Δ^2_{\min} (eV)	E_{frag} (eV)	Fragment 1	Fragment 2
B2	-3.29971	2.57979	B1	B1
B3	0.52408	5.8795	B1	B2
B4	0.37515	5.35542	B1	B3
B5	0.51882	4.98028	B1	B4
B6	-1.47892	4.46145	B1	B5
B7	-0.14156	5.94037	B1	B6
B8	1.96302	6.08193	B1	B7
B9	-2.10124	4.11891	B1	B8
B10	0.96598	6.22015	B1	B9
B11	-0.40039	5.25417	B1	B10
B12	1.11977	5.65456	B1	B11
B13	-0.49198	4.53479	B1	B12
B14	0.14374	5.02677	B1	B13
B15	-0.38101	4.88304	B1	B14
Al1B1	-2.61161	1.82648	B1	Al1
Al1B2	-0.62785	3.68478	B2	Al1
Al1B3	-0.00583	2.87121	B3	Al1
Al1B4	-0.2551	2.57348	B4	Al1
Al1B5	-0.0315	2.7436	B5	Al1
Al1B6	-0.11495	3.46405	B6	Al1
Al1B7	-0.91552	2.82053	B7	Al1
Al1B8	0.27237	2.95097	B8	Al1

A11B9	0.1089	3.73166	B9	A11
A11B10	-1.15933	2.3022	B10	A11
A11B11	1.34406	2.99806	B11	A11
A11B12	-1.28766	1.55549	B12	A11
A11B13	0.29041	2.52035	B13	A11
A11B14	-0.37217	2.27968	B14	A11
A11B15	0.11623	2.55492	B15	A11
A12	-0.58092	1.30325	A11	A11
A12B1	-1.55048	2.65681	A11	A11B1
A12B2	-0.26321	2.94924	A11	A11B2
A12B3	-0.15711	2.87704	A11	A11B3
A12B4	0.2029	2.82858	A11	A11B4
A12B5	-0.7263	2.31485	A11	A11B5
A12B6	-0.54974	2.49591	A11	A11B6
A12B7	0.13351	3.11177	A11	A11B7
A12B8	0.98394	2.6786	A11	A11B8
A12B9	-1.32706	2.20745	A11	A11B9
A12B10	1.18319	3.17226	A11	A11B10
A12B11	-0.98099	1.654	A11	A11B11
A12B12	0.43139	2.8015	A11	A11B12
A12B13	-0.20625	2.22994	A11	A11B13
A12B14	-0.60032	2.26042	A11	A11B14
A12B15	-0.18562	2.43869	A11	A11B15
A13B0	0.14478	1.88416	A11	A12
A13B1	-0.43149	2.88257	A11	A12B1

A13B2	-0.65595	2.76199	A11	A12B2
A13B3	0.54328	3.03414	A11	A12B3
A13B4	-0.44114	2.62568	A11	A12B4
A13B5	-0.30334	3.03093	A11	A12B5
A13B6	-0.05641	3.01322	A11	A12B6
A13B7	0.13834	2.50219	A11	A12B7
A13B8	-0.98209	1.69466	A11	A12B8
A13B9	0.62477	2.81778	A11	A12B9
A13B10	-0.15088	1.98907	A11	A12B10
A13B11	0.11048	2.63499	A11	A12B11
A13B12	-0.45225	2.24271	A11	A12B12
A13B13	-0.11957	2.43618	A11	A12B13
A13B14	0.14101	2.86074	A11	A12B14
A13B15	0.23264	2.62431	A11	A12B15
A14B0	-0.51777	1.73938	A11	A13
A14B1	-0.30831	2.416	A11	A13B1
A14B2	0.37606	2.96943	A11	A13B2
A14B3	0.04998	2.49086	A11	A13B3
A14B4	-0.159	2.62742	A11	A13B4
A14B5	-0.3069	2.48184	A11	A13B5
A14B6	-0.3803	2.33982	A11	A13B6
A14B7	-0.39016	2.36384	A11	A13B7
A14B8	0.43341	2.67674	A11	A13B8
A14B9	-0.79939	1.75502	A11	A13B9
A14B10	-0.17952	1.99854	A11	A13B10

A14B11	-0.31258	2.13522	A11	A13B11
A14B12	0.39256	2.69496	A11	A13B12
A14B13	-0.76905	2.37365	A11	A13B13
A14B14	0.65161	2.70183	A11	A13B14
A14B15	-0.67753	2.39168	A11	A13B15
A15B0	-0.03447	2.25715	A11	A14
A15B1	0.0436	2.41537	A11	A14B1
A15B2	-0.61347	2.04222	A11	A14B2
A15B3	-0.24945	2.22706	A11	A14B3
A15B4	-0.14346	2.4875	A11	A14B4
A15B5	-0.04972	2.7324	A11	A14B5
A15B6	-0.26862	2.72012	A11	A14B6
A15B7	0.48189	2.754	A11	A14B7
A15B8	-0.16701	2.24334	A11	A14B8
A15B9	0.14695	2.55441	A11	A14B9
A15B10	-0.53281	2.17806	A11	A14B10
A15B11	-0.42688	2.24585	A11	A14B11
A15B12	-0.37418	2.3024	A11	A14B12
A15B13	0.42196	2.77181	A11	A14B13
A15B14	-0.80807	2.05022	A11	A14B14
A15B15	0.98736	2.91603	A11	A14B15
A16B0	-0.58445	2.29162	A11	A15
A16B1	0.01928	2.37177	A11	A15B1
A16B2	0.28117	2.65569	A11	A15B2
A16B3	-0.35469	2.47651	A11	A15B3

A16B4	-0.02714	2.62641	A11	A15B4
A16B5	-0.36468	2.57392	A11	A15B5
A16B6	0.42343	2.76904	A11	A15B6
A16B7	0.05537	2.27212	A11	A15B7
A16B8	0.0857	2.4055	A11	A15B8
A16B9	-0.44822	2.28617	A11	A15B9
A16B10	-0.02536	2.71087	A11	A15B10
A16B11	-0.3433	2.67273	A11	A15B11
A16B12	0.75645	2.67657	A11	A15B12
A16B13	-1.18138	1.94868	A11	A15B13
A16B14	0.85025	2.82412	A11	A15B14
A16B15	-0.71464	1.85951	A11	A15B15
A17B0	0.933	2.87607	A11	A16
A17B1	-0.39391	2.30374	A11	A16B1
A17B2	-0.65312	2.1446	A11	A16B2
A17B3	-0.26904	2.4419	A11	A16B3
A17B4	-0.11218	2.65355	A11	A16B4
A17B5	0.86625	2.93859	A11	A16B5
A17B6	-0.38652	2.04764	A11	A16B6
A17B7	-0.47386	1.96663	A11	A16B7
A17B8	-0.66361	2.04104	A11	A16B8
A17B9	0.40095	2.73439	A11	A16B9
A17B10	-0.30708	2.6297	A11	A16B10
A17B11	0.72035	2.80674	A11	A16B11
A17B12	-0.85857	1.92012	A11	A16B12

A17B13	0.79988	2.93762	A11	A16B13
A17B14	-0.53206	1.97387	A11	A16B14
A17B15	0.5065	2.57415	A11	A16B15
A18B0	-0.10982	1.94307	A11	A17
A18B1	-0.79187	2.17141	A11	A17B1
A18B2	0.74157	2.79772	A11	A17B2
A18B3	-0.81811	2.50719	A11	A17B3
A18B4	0.86991	2.76573	A11	A17B4
A18B5	-0.08751	2.07234	A11	A17B5
A18B6	-0.20912	2.34512	A11	A17B6
A18B7	-0.26882	2.44049	A11	A17B7
A18B8	0.21182	2.70465	A11	A17B8
A18B9	-0.27405	2.22373	A11	A17B9
A18B10	0.09891	2.3734	A11	A17B10
A18B11	-0.99199	1.95391	A11	A17B11
A18B12	0.32352	2.45094	A11	A17B12
A18B13	-0.60287	1.76588	A11	A17B13
A18B14	0.2203	2.32952	A11	A17B14
A18B15	-0.32403	2.05869	A11	A17B15
A19B0	-0.29326	2.05289	A11	A18
A19B1	-0.07972	2.32879	A11	A18B1
A19B2	-0.79142	1.89253	A11	A18B2
A19B3	0.74647	2.67646	A11	A18B3
A19B4	-0.34392	1.89582	A11	A18B4
A19B5	-0.12817	2.04595	A11	A18B5

A19B6	-0.78869	2.04418	A11	A18B6
A19B7	0.20053	2.54931	A11	A18B7
A19B8	-0.25052	2.35932	A11	A18B8
A19B9	0.13213	2.49778	A11	A18B9
A19B10	-0.63263	2.27449	A11	A18B10
A19B11	1.25727	2.9459	A11	A18B11
A19B12	-0.9188	2.03617	A11	A18B12
A19B13	0.14328	2.36875	A11	A18B13
A19B14	-0.43731	2.10922	A11	A18B14
A19B15	0.38196	2.38272	A11	A18B15
A110B0	0.08874	2.34614	A11	A19
A110B1	-0.59774	2.25604	A11	A19B1
A110B2	0.66712	2.68395	A11	A19B2
A110B3	-1.17746	1.73464	A11	A19B3
A110B4	0.12439	2.23974	A11	A19B4
A110B5	-0.65999	2.17412	A11	A19B5
A110B6	0.42682	2.83287	A11	A19B6
A110B7	-0.31887	2.34878	A11	A19B7
A110B8	0.36538	2.60985	A11	A19B8
A110B9	-0.60462	2.27322	A11	A19B9
A110B10	0.66956	2.67334	A11	A19B10
A110B11	-0.75574	1.68864	A11	A19B11
A110B12	0.40631	2.54905	A11	A19B12
A110B13	-0.78359	2.08435	A11	A19B13
A110B14	0.6445	2.54653	A11	A19B14

A110B15	-0.7216	2.00075	A11	A19B15
A111B0	-0.26842	2.2574	A11	A110
A111B1	-0.26947	2.54103	A11	A110B1
A111B2	-1.23505	2.01683	A11	A110B2
A111B3	0.74881	2.91209	A11	A110B3
A111B4	-0.45165	2.11535	A11	A110B4
A111B5	-0.39331	2.30154	A11	A110B5
A111B6	-0.25043	2.22105	A11	A110B6
A111B7	0.27528	2.58798	A11	A110B7
A111B8	-0.60689	2.24446	A11	A110B8
A111B9	0.48868	2.68554	A11	A110B9
A111B10	-0.41798	2.00378	A11	A110B10
A111B11	0.30285	2.44437	A11	A110B11
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A111B13	-0.17691	2.16605	A11	A110B13
A111B14	-0.86607	1.90203	A11	A110B14
A111B15	-0.09712	2.72236	A11	A110B15
A112B0	-0.0928	2.52582	A11	A111
A112B1	0.0534	2.8105	A11	A111B1
A112B2	1.00911	3.25188	A11	A111B2
A112B3	-0.50827	2.16328	A11	A111B3
A112B4	0.10833	2.567	A11	A111B4
A112B5	-0.51798	2.4569	A11	A111B5
A112B6	-0.09799	2.47147	A11	A111B6
A112B7	-0.55836	2.3127	A11	A111B7

A112B8	0.88961	2.85135	A11	A111B8
A112B9	-0.36115	2.19686	A11	A111B9
A112B10	-0.04147	2.42176	A11	A111B10
A112B11	0.12982	2.14153	A11	A111B11
A112B12	-0.41516	2.32439	A11	A111B12
A112B13	-0.57242	2.34296	A11	A111B13
A112B14	0.06677	2.7681	A11	A111B14
A112B15	0.7115	2.81947	A11	A111B15
A113B0	0.09885	2.61863	A11	A112
A113B1	1.04108	2.72384	A11	A112B1
A113B2	-0.56377	1.84137	A11	A112B2
A113B3	0.334	2.43102	A11	A112B3
A113B4	-0.74522	2.16374	A11	A112B4
A113B5	0.24884	2.75002	A11	A112B5
A113B6	-0.3294	2.56946	A11	A112B6
A113B7	0.97939	2.87105	A11	A112B7
A113B8	-0.66961	1.88741	A11	A112B8
A113B9	0.04501	2.46299	A11	A112B9
A113B10	0.11241	2.46323	A11	A112B10
A113B11	-0.71363	2.01171	A11	A112B11
A113B12	0.08656	2.42323	A11	A112B12
A113B13	0.00509	2.33305	A11	A112B13
A113B14	-1.56766	1.43856	A11	A112B14
A113B15	-0.56711	1.53774	A11	A112B15
A114B0	0.45787	2.51978	A11	A113

A114B1	-0.67185	1.64784	A11	A113B1
A114B2	0.24921	2.40513	A11	A113B2
A114B3	-0.70014	2.09701	A11	A113B3
A114B4	0.11659	2.57091	A11	A113B4
A114B5	-0.46089	2.18298	A11	A113B5
A114B6	0.52975	2.50479	A11	A113B6
A114B7	-0.25749	1.84822	A11	A113B7
A114B8	-0.52854	2.20363	A11	A113B8
A114B9	0.24685	2.41797	A11	A113B9
A114B10	0.44922	2.35082	A11	A113B10
A114B11	-0.50902	2.42115	A11	A113B11
A114B12	-0.13891	2.28687	A11	A113B12
A114B13	-0.50384	2.32795	A11	A113B13
A114B14	0.65275	3.00622	A11	A113B14
A114B15	-0.4912	2.10485	A11	A113B15
A115B0	-0.31112	2.06192	A11	A114
A115B1	-0.1666	2.31969	A11	A114B1
A115B2	-0.5301	2.15593	A11	A114B2
A115B3	0.79895	2.79716	A11	A114B3
A115B4	-0.81389	2.01186	A11	A114B4
A115B5	-0.13369	2.15705	A11	A114B5
A115B6	-0.31543	1.97504	A11	A114B6
A115B7	0.01893	2.10571	A11	A114B7
A115B8	-0.43568	2.18485	A11	A114B8
A115B9	0.00836	2.17112	A11	A114B9

Al15B10	-0.71706	1.72635	Al1	Al14B10
Al15B11	0.23455	2.44786	Al1	Al14B11
Al15B12	-0.51688	2.42579	Al1	Al14B12
Al15B13	0.80708	2.83179	Al1	Al14B13
Al15B14	-0.49897	2.02541	Al1	Al14B14
Al15B15	0.20716	2.37075	Al1	Al14B15

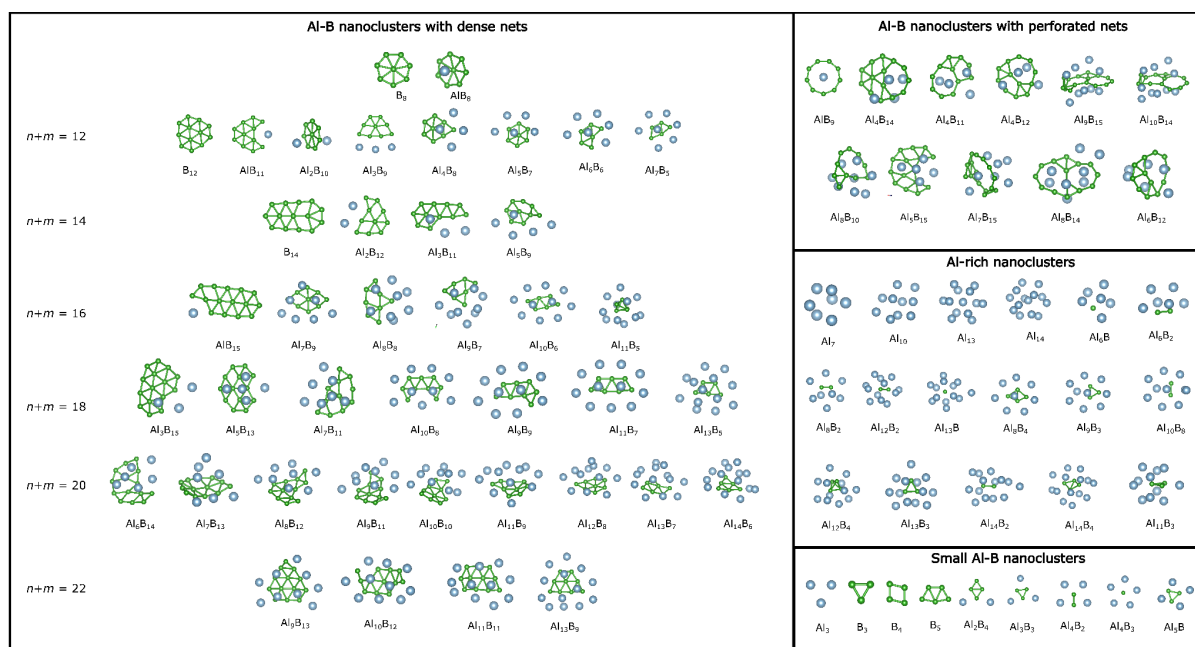


Figure S1. Al_nB_m molecules with $\Delta^2_{\min} > 0$ classified by their structural topology. Blue spheres are aluminum atoms and green ones are boron atoms, respectively.

Section 2. Ground-state structures of Al_nB_m

Atomic coordinates of all calculated ground-state structures of Al_nB_m molecules ($0 \leq n, m \leq 16$) in the XYZ format.

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10
energy
Al 0.6718930000 -0.0482290000 1.4460520000
Al -0.4595880000 -2.4254550000 -0.0002120000
Al 2.0750280000 -2.1050600000 0.0012610000
Al -1.7906890000 -0.5735070000 -1.5060390000
Al -1.7889920000 -0.5705540000 1.5078510000
Al -3.2142100000 0.9101100000 0.0006230000
Al 2.8755410000 0.3349810000 -0.0016420000
Al 0.6707170000 -0.0493990000 -1.4459850000
Al -0.7538180000 1.8342360000 -0.0025220000
Al 1.7141190000 2.6928770000 0.0006120000
11
energy
Al -2.7722670000 1.4824700000 0.0004750000
Al -0.2941580000 2.5012830000 -0.0005330000
Al -0.9864760000 -0.0075480000 1.3924500000
Al -0.9866620000 -0.0072190000 -1.3917640000
Al 2.2787710000 1.8465130000 -0.0009140000
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Al -0.5743980000 -2.3744630000 -0.0002140000
Al 3.5602700000 -0.4813060000 0.0000970000
Al 1.4055970000 -1.0089570000 -1.4186110000
Al -3.2678460000 -1.1305370000 -0.0004870000
B 0.6015400000 0.4856340000 -0.0001490000
20
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Al -2.0088330000 -0.8949740000 1.2087330000
Al 0.2384520000 -2.4383140000 0.3898880000
Al 0.4941670000 0.5282080000 1.1150740000
Al 2.7278380000 -1.5935800000 -1.2808050000
Al 0.0328710000 -1.5074910000 2.8368050000
Al 0.0865480000 3.2991400000 -0.2758870000
Al -1.9046210000 1.8317920000 0.3191870000
Al 2.4534080000 2.3543660000 0.2308310000
Al 3.8314190000 -0.0972250000 0.7097550000
Al -4.1522900000 0.7509500000 -0.1764230000
B -3.2414830000 -0.9869900000 -0.6505350000
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B 0.8948270000 -0.2134050000 -1.5614820000
B 0.8654630000 1.4469230000 -1.1129900000
B -0.5992540000 0.7398440000 -1.3918760000
B 0.7117640000 -1.9471750000 -1.8193200000
B -0.6637800000 -0.9243760000 -1.6941110000
B -2.0797260000 -1.9085410000 -1.2016660000
B -0.7257730000 -2.5845820000 -1.6653490000
B 2.2070320000 0.5309230000 -0.8812330000
21
energy
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Al 1.3240670000 -0.3700780000 -1.5964220000
Al -1.3076730000 -0.0489660000 -1.4823720000
Al 3.2098530000 1.3971000000 -0.1956820000
Al 2.8494080000 -1.2986250000 0.7300280000
Al 0.2149810000 -2.1299120000 0.1660980000
Al -2.5732960000 -2.7443690000 -0.5920480000
Al 4.0337640000 -0.6604820000 -1.6583400000
Al -3.9101210000 0.2821900000 -0.9106520000
Al -2.3661020000 2.6717380000 -0.5784780000
B 1.6015570000 0.5829960000 1.6548620000
B -1.0821090000 1.4665930000 1.5329380000
B 0.4561550000 1.8940110000 1.8382120000
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B	0.039040000	0.268284000	2.224777000
B	1.167503000	-0.994031000	1.995494000
B	-0.414533000	-1.365725000	2.256076000
B	-2.606556000	-0.746991000	0.523500000
B	-1.655435000	-1.839054000	1.348423000
B	-1.504657000	-0.179302000	1.683228000
B	-2.393436000	0.908762000	0.758444000
B	1.862909000	2.130513000	1.135126000

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energy

Al	-0.700319000	2.326827000	-0.543121000
Al	-1.276214000	-0.474516000	-1.568503000
Al	1.190177000	0.327039000	-1.397957000
Al	-3.301505000	1.737635000	-0.967242000
Al	-2.365170000	-2.101994000	0.800234000
Al	0.242714000	-2.114860000	0.072026000
Al	2.670516000	-2.053206000	-0.724727000
Al	-3.832624000	-0.998188000	-1.248191000
Al	1.774923000	2.540243000	0.582378000
Al	4.247283000	-0.071939000	-1.473591000
B	-1.513290000	-0.054501000	1.599014000
B	-2.056680000	1.442777000	1.020429000
B	-2.603576000	0.100941000	0.315019000
B	0.789802000	1.589739000	2.249111000
B	-0.769307000	1.538482000	1.975280000
B	0.032358000	0.098236000	2.374526000
B	2.924692000	1.279302000	-0.610605000
B	0.884090000	-1.343837000	2.179017000
B	2.639780000	0.081501000	0.452151000
B	2.225094000	-1.228934000	1.291161000
B	1.654899000	0.234457000	1.893174000
B	-0.697293000	-1.442470000	2.080328000

23

energy

Al	-2.161103000	-0.210700000	1.180305000
Al	0.117534000	-1.610009000	1.432862000
Al	2.143819000	0.183570000	1.467107000
Al	0.966373000	2.485790000	0.565847000
Al	-1.529731000	2.697384000	0.113003000
Al	-3.815189000	1.600042000	-0.084719000
Al	3.327102000	2.013363000	-0.375779000
Al	-4.940101000	-0.829589000	0.163422000
Al	3.142814000	-1.993339000	-0.102804000
Al	4.875586000	-0.090418000	-0.152085000
B	1.149868000	-2.694934000	-0.480385000
B	-0.284524000	-3.220309000	-0.091016000
B	-1.728677000	-2.623708000	-0.325206000
B	-3.037950000	-0.138150000	-1.113197000
B	-3.035248000	-1.661182000	-0.477033000
B	-1.630520000	-0.994641000	-1.203817000
B	-0.172544000	-1.799377000	-1.084864000
B	1.297446000	-0.966745000	-0.857906000
B	2.667811000	-0.002768000	-0.939376000
B	-0.180037000	1.516925000	-1.285297000
B	-1.636978000	0.796393000	-1.191317000
B	-0.202305000	-0.100481000	-0.771139000
B	1.263190000	0.849133000	-1.118063000

24

energy

Al	2.391711000	-1.611111000	-2.049473000
Al	-0.319462000	-1.482481000	-1.922031000
Al	2.048255000	-1.877729000	0.603575000
Al	2.510744000	2.647829000	-0.335100000
Al	1.652330000	0.839765000	1.900486000
Al	-1.748514000	-1.422889000	1.680614000
Al	-0.153409000	2.243304000	-0.176640000
Al	-2.645278000	2.242887000	0.692436000

Al	-2.8644830000	-1.8550940000	-0.9230680000
Al	-3.8482560000	-0.0845420000	1.1692040000
B	2.4982480000	0.6616570000	-1.6941570000
B	3.1345360000	0.3362960000	-0.2805430000
B	1.3457530000	0.2441400000	-0.4272710000
B	3.1367860000	-0.9100670000	2.3971230000
B	-1.9306750000	-0.1085870000	-1.8919290000
B	0.9642540000	0.9482470000	-1.9646050000
B	-0.6496880000	0.9188840000	-2.1369210000
B	0.0819090000	-0.3441220000	0.5545460000
B	0.2768080000	-1.2205560000	2.0337540000
B	1.6863390000	-1.3131230000	2.7315680000
B	-1.9410750000	1.5058130000	-1.2902090000
B	-3.0442380000	0.3963150000	-0.7216190000
B	-1.4560110000	0.0518050000	-0.0955720000
B	3.6355960000	-0.2305460000	1.1218210000

25

energy

Al	-2.5983350000	0.5454630000	1.4396090000
Al	-0.7002150000	2.3818410000	0.9773710000
Al	1.8064620000	1.7922220000	1.3081000000
Al	0.0870340000	-0.3936710000	0.8036870000
Al	-0.6487680000	-2.9500110000	0.0516780000
Al	-3.0362710000	-2.0994530000	0.3941670000
Al	3.0252600000	-0.4868120000	1.7018970000
Al	1.8113560000	-2.4437790000	-0.0690320000
Al	-4.9110470000	-0.1593410000	0.1123560000
Al	4.1195270000	-1.4352760000	-0.8231660000
B	2.2578130000	2.4088990000	-0.8188020000
B	0.7297110000	2.8740180000	-1.1144770000
B	-2.0794460000	2.2744630000	-1.0623860000
B	-2.8815900000	-0.4850810000	-0.9822330000
B	-3.2001490000	1.1058960000	-0.8129280000
B	-1.6906030000	0.5809810000	-1.3168870000
B	-0.4339820000	1.6848110000	-1.6361400000
B	2.7279230000	0.5496170000	-0.8364270000
B	0.2918170000	-1.4852190000	-1.4170710000
B	-1.2951840000	-1.0991300000	-1.1967060000
B	-0.1051670000	0.0922590000	-1.6992480000
B	1.4514540000	-0.3857970000	-1.1999340000
B	3.5707080000	1.8805940000	-0.1906730000
B	4.1606930000	0.4255880000	0.0438860000
B	-0.7870030000	3.2250270000	-1.0913080000

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energy

Al	-1.9972500000	0.8294850000	-1.3450920000
Al	0.0137890000	-1.2511620000	-2.0932360000
Al	-1.9249550000	-0.0709350000	2.0867380000
Al	-0.0895980000	-2.1324950000	1.3588440000
Al	-3.1902800000	-2.5721160000	-0.5126380000
Al	-0.7920140000	3.1363350000	-1.4373990000
Al	1.3883740000	1.5890950000	-1.1918790000
Al	1.2509990000	0.9352050000	1.9441030000
Al	2.8376760000	-0.6525990000	-2.1897880000
Al	2.3433400000	-1.5119840000	2.1346000000
B	1.7828560000	-2.2809130000	-0.4872890000
B	-3.3105110000	0.9120360000	0.5224070000
B	-1.1142110000	-2.7440600000	-0.6253600000
B	-1.5415410000	-1.1036750000	-0.1665360000
B	0.4138370000	-3.0354590000	-0.6773110000
B	-3.1723510000	-0.5657760000	0.0283760000
B	-2.4482460000	2.1969180000	0.7841430000
B	-0.2390410000	0.0803890000	0.1093820000
B	-1.3068310000	3.2741110000	0.8335790000
B	2.8261700000	1.7575030000	0.5209470000
B	-0.7573010000	1.6060410000	0.6697180000
B	1.7597600000	2.8191300000	0.7839220000

B	2.9841740000	-1.3511590000	-0.0213190000
B	2.9807540000	0.2301700000	0.1425820000
B	1.3238310000	-0.5913600000	-0.0735710000
B	0.2344420000	3.2191480000	0.8952750000

12

energy

Al	1.8199660000	0.0003720000	1.3227770000
Al	2.5862170000	-1.2854110000	-1.0003640000
Al	2.5877370000	1.2857200000	-0.9984590000
Al	0.7853260000	2.4850240000	0.5049360000
Al	-0.0095460000	0.0011530000	-0.8635640000
Al	-1.6735710000	2.1138710000	-0.1894580000
Al	-2.9320770000	-0.0006300000	-1.5040140000
Al	-1.6714250000	-2.1144570000	-0.1903160000
Al	0.7867670000	-2.4848140000	0.5063550000
Al	-2.1512490000	-0.0008820000	1.3518160000
B	-0.1668800000	0.8127190000	1.3784240000
B	-0.1662930000	-0.8125780000	1.3783320000

13

energy

Al	-0.0130280000	2.0739330000	-1.8508030000
Al	0.0119610000	-1.9401880000	1.2929870000
Al	-2.0426160000	1.2745740000	-0.4167890000
Al	-0.0117100000	1.9617670000	1.2612600000
Al	-1.7223430000	0.0060100000	2.0700290000
Al	-2.0261540000	-1.3080640000	-0.3984340000
Al	1.7227770000	0.0268020000	2.0695290000
Al	2.0418290000	-1.2831810000	-0.3990010000
Al	2.0268230000	1.2994850000	-0.4173920000
Al	0.0126110000	-2.1007640000	-1.8224320000
B	-0.8214100000	-0.0175730000	-1.7390900000
B	0.8210440000	-0.0074340000	-1.7393050000
B	-0.0000270000	-0.0019630000	-0.1328880000

14

energy

Al	-3.3107570000	-0.0003910000	-0.8695140000
Al	-1.2525880000	1.9676960000	-0.5566820000
Al	2.4088120000	0.0004420000	-1.7025080000
Al	-1.2520360000	-1.9676470000	-0.5558060000
Al	1.4095640000	-2.1256570000	-0.4228520000
Al	2.0956670000	-0.0002900000	1.2663240000
Al	1.4089910000	2.1260040000	-0.4222270000
Al	0.1526230000	-1.8686380000	1.9066830000
Al	-1.7174870000	0.0003470000	1.4106410000
Al	0.1530160000	1.8682890000	1.9073960000
B	0.3192250000	0.8306910000	-1.7557770000
B	-1.1373290000	-0.0001940000	-1.4806250000
B	0.3193040000	-0.8307150000	-1.7559570000
B	0.2497070000	-0.0001880000	-0.1074240000

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energy

Al	-3.5685780000	-0.0058690000	-0.9974490000
Al	-1.3303830000	-2.0288340000	-0.4725640000
Al	1.3265700000	-2.0297960000	-0.4713790000
Al	2.2251240000	0.0013000000	1.2558120000
Al	-0.0008400000	-1.4157130000	1.9604660000
Al	-0.0001100000	1.4308000000	1.9497030000
Al	1.3307630000	2.0259800000	-0.4811110000
Al	-2.2240800000	0.0034440000	1.2558770000
Al	-1.3280590000	2.0293590000	-0.4825060000
Al	3.5707280000	-0.0066990000	-0.9977340000
B	-0.0000730000	-0.8541960000	-1.7544780000
B	-1.4273090000	-0.0016810000	-1.4751170000
B	1.4279980000	-0.0035950000	-1.4738020000
B	-0.0044620000	0.0007650000	-0.0880780000
B	0.0008910000	0.8483780000	-1.7582280000

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energy

Al	0.4323940000	2.4964120000	0.2734770000
Al	-1.3971080000	-0.2006300000	1.3495190000
Al	3.0223010000	1.7774010000	-0.6930360000
Al	1.3972550000	0.1999950000	1.3482570000
Al	-2.1619230000	2.1611720000	0.0873670000
Al	-4.1026510000	0.5091330000	0.2289880000
Al	-0.4302800000	-2.4970670000	0.2756170000
Al	-3.0239080000	-1.7767860000	-0.6921830000
Al	4.1013330000	-0.5071600000	0.2327930000
Al	2.1631640000	-2.1615990000	0.0823470000
B	1.0664740000	0.9254260000	-1.1933300000
B	-0.5420770000	0.6728490000	-1.1001190000
B	-2.1547000000	0.2537320000	-0.9500310000
B	-1.0673220000	-0.9265740000	-1.1899460000
B	0.5415940000	-0.6739060000	-1.0975350000
B	2.1545310000	-0.2537910000	-0.9512180000

17
energy

Al	1.2661970000	-0.4691280000	1.3748180000
Al	-1.2793040000	-1.8248730000	2.4336020000
Al	2.9567080000	-1.5361150000	-0.5121160000
Al	-2.5181510000	-1.1354340000	0.0073730000
Al	-0.0274000000	-2.4542480000	0.1176530000
Al	-2.2583910000	1.7737150000	-0.8761990000
Al	-1.0220370000	0.7657140000	1.3622600000
Al	1.3983330000	2.1806890000	1.3337260000
Al	-0.3187880000	3.1812720000	-0.1663140000
Al	2.6464300000	1.1321210000	-0.7482430000
B	-1.5622160000	-1.1521030000	-2.3514440000
B	-0.1107810000	-1.7079500000	-2.1362750000
B	0.9151920000	-0.4456220000	-1.1753100000
B	0.3612790000	0.9885330000	-0.5748930000
B	-0.7169130000	0.1108540000	-1.5027850000
B	-2.3909190000	0.0561420000	-1.9163150000
B	1.3110050000	-2.0455080000	-1.5920350000

18
energy

Al	0.9297530000	2.6071960000	-0.2127860000
Al	1.2693230000	0.0123560000	-1.1654280000
Al	2.4849480000	-2.3173480000	0.2622540000
Al	3.2635600000	1.6955500000	0.2506150000
Al	3.9780080000	-0.6161590000	-0.9929150000
Al	-1.7070160000	2.5799890000	0.0545510000
Al	-1.4725990000	-0.1458600000	-1.1585540000
Al	-3.7892980000	-1.7856530000	-0.7876710000
Al	-0.0136390000	-2.6182260000	0.5913000000
Al	-3.7843610000	1.0664520000	-0.1163100000
B	-0.2081810000	0.8918120000	1.3137840000
B	0.7791150000	-0.5668350000	1.3171180000
B	2.3360040000	-0.2769490000	0.8528830000
B	1.3915290000	0.9947160000	1.1958150000
B	-1.9149650000	-1.9026340000	0.4421460000
B	-2.6205140000	-0.5292070000	0.9051220000
B	-0.9743680000	-0.6818300000	1.2368200000
B	-1.8011860000	0.8273580000	1.2511670000

19
energy

Al	3.9265510000	-0.0202950000	-0.0328920000
Al	2.5641900000	-2.3050860000	-0.6260420000
Al	-0.0966090000	-2.3093720000	-0.8558190000
Al	-1.3682860000	0.0348200000	-1.4182700000
Al	1.3813370000	0.3037660000	-1.1981770000
Al	-0.1921140000	2.5060160000	-0.4708680000
Al	-2.6727990000	-1.9107220000	0.5535640000
Al	-3.9501370000	0.0259810000	-0.5829190000
Al	-2.7261500000	2.2183240000	0.2671850000

Al	2.5129040000	2.6031860000	0.1152390000
B	-0.8971790000	-0.8175740000	1.3217660000
B	2.1123580000	0.6094370000	1.0644420000
B	1.9941520000	-1.0568380000	1.1069450000
B	0.6915330000	-0.0901970000	1.4882960000
B	0.8048250000	1.5752850000	1.2164250000
B	-0.7129530000	0.8985760000	1.2663770000
B	-2.1171110000	0.2461790000	0.8753780000
B	0.5732040000	-1.8460880000	1.4597160000
B	-0.8339350000	-2.4999840000	1.2480570000

11

energy

Al	0.0008310000	-1.3307900000	1.3558380000
Al	-0.0000860000	1.3307060000	1.3578890000
Al	-0.0009450000	2.8558400000	-1.0601310000
Al	-2.4156590000	-0.0001920000	1.4865600000
Al	-2.2275850000	1.5570020000	-0.6250940000
Al	2.2272340000	-1.5588690000	-0.6236970000
Al	0.0001480000	0.0004490000	-1.0666480000
Al	2.4161060000	0.0011020000	1.4854160000
Al	-2.2269720000	-1.5580860000	-0.6242810000
Al	2.2269860000	1.5586670000	-0.6256900000
Al	-0.0000580000	-2.8558300000	-1.0601630000

12

energy

Al	-2.7884710000	-0.4103840000	-1.4279660000
Al	-1.3500610000	-2.3309980000	-0.3788890000
Al	-0.0003610000	0.0910570000	-0.6849480000
Al	-2.0009160000	0.1397110000	1.2723220000
Al	-2.0883090000	1.9677170000	-0.7697960000
Al	2.7886830000	-0.4093940000	-1.4286500000
Al	2.0875960000	1.9681870000	-0.7687430000
Al	-0.0003410000	2.5035970000	0.8689860000
Al	1.3509600000	-2.3296360000	-0.3783830000
Al	-0.0000940000	-1.5482070000	1.7739650000
Al	2.0012060000	0.1390310000	1.2717160000
B	0.0002820000	0.5702270000	1.6910020000

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energy

Al	2.0450400000	-2.6919180000	0.6746550000
Al	1.1597070000	-0.6410630000	-1.3829690000
Al	3.7401900000	-1.6424630000	-1.0156530000
Al	3.3554590000	0.8362460000	-0.5856320000
Al	-0.4880550000	-2.2404230000	0.3450300000
Al	-2.5853620000	2.0257840000	0.1254040000
Al	2.2070500000	3.0197180000	0.0707190000
Al	-0.0561550000	2.1288180000	-0.9078210000
Al	-1.4697070000	-0.1718590000	-1.5137710000
Al	-3.1962190000	-2.1763360000	-0.0177040000
Al	-4.0954050000	0.1446350000	-1.2059240000
B	1.6759660000	0.9121270000	1.1148330000
B	2.4452650000	-0.5382610000	0.8426680000
B	-0.4936230000	-0.7323030000	2.1032540000
B	1.0422650000	-0.6163000000	1.6351680000
B	0.1270930000	0.8483580000	1.8846320000
B	-1.9505640000	-1.0839100000	1.5793420000
B	-0.8697860000	2.1093290000	1.3993050000
B	-2.7864050000	-0.1128520000	0.5894180000
B	-1.5363140000	0.5676850000	1.5489740000
B	0.7430950000	2.3091620000	1.3779420000

22

energy

Al	0.3276920000	-1.9586460000	0.7234240000
Al	-1.1570130000	-0.3343090000	-1.2244450000
Al	1.4251500000	-0.6619020000	-1.4181970000
Al	-3.6014380000	0.7698610000	-0.8780090000
Al	0.5172370000	1.9361120000	-0.8236740000

Al	3.3230950000	1.3696310000	-0.4894070000
Al	-3.5998590000	-1.7338800000	-1.3085510000
Al	4.1096240000	-0.8636850000	-1.9296450000
Al	-2.1658450000	-2.5881610000	0.6868970000
Al	-1.9606790000	2.7340520000	-0.6927200000
Al	3.1264570000	-1.5966770000	0.6955250000
B	-2.0142810000	0.9854910000	1.0127020000
B	-2.6923210000	-0.4749080000	0.7173740000
B	0.0117560000	-0.4859290000	2.4837610000
B	-1.4300040000	-0.5167050000	1.7657480000
B	-0.6526120000	1.0287400000	2.0906800000
B	-1.2058880000	2.3914000000	1.2991890000
B	0.3504070000	2.3639740000	1.6137090000
B	2.3521700000	0.3715670000	1.1749640000
B	1.0119310000	0.8023760000	2.0495440000
B	1.5735460000	-0.8008870000	2.0778650000
B	1.7998010000	1.9466510000	1.0273500000

23

energy

Al	-3.9126000000	0.6306390000	-0.5796270000
Al	-1.4315860000	-0.3732060000	-1.3125470000
Al	2.6123110000	2.5704060000	0.0854720000
Al	0.2723770000	3.6109390000	0.3857230000
Al	0.6347370000	1.2480290000	-1.1148540000
Al	-1.9258930000	2.4885040000	-0.6365080000
Al	-1.5105350000	-2.4918310000	0.7857130000
Al	3.6183810000	-2.5707200000	-0.8195030000
Al	3.2467360000	0.2489510000	-0.9670550000
Al	1.0092620000	-1.5718700000	-1.3120540000
Al	-3.7260860000	-2.0647680000	-0.6709970000
B	-2.1274220000	0.9146430000	0.9350660000
B	-2.5704190000	-0.6253080000	0.7279610000
B	0.9538130000	1.7232560000	1.4650610000
B	-0.6467980000	1.4428850000	1.3089160000
B	-0.1335950000	-1.2720040000	2.3328130000
B	-1.2443670000	-0.2395970000	1.7132240000
B	0.4225870000	0.2704270000	2.0765950000
B	0.4826780000	-2.5904130000	1.4882590000
B	1.2955970000	-1.1212930000	1.5562510000
B	2.6390810000	-0.9697270000	0.6446520000
B	1.9095750000	0.4428450000	1.0495960000
B	1.9128020000	-2.4609050000	0.7078230000

24

energy

Al	2.8303540000	0.2662480000	-1.6997610000
Al	0.1795530000	0.6533380000	-2.2271310000
Al	-0.8042380000	-1.9881660000	-1.9103600000
Al	-1.7388320000	-0.1717740000	2.1728780000
Al	-0.2777010000	2.3311500000	1.7263010000
Al	-2.9561640000	-1.5964740000	0.0369530000
Al	-0.2503000000	3.2570490000	-0.8509080000
Al	-2.4095550000	0.1929040000	-1.9380980000
Al	-0.5701380000	-2.2848040000	0.9244080000
Al	2.9478520000	-0.6813770000	0.7026880000
Al	-2.3331750000	1.4633320000	0.2608490000
B	1.5541790000	1.9283480000	-1.1415340000
B	1.0090400000	0.7062310000	0.0068020000
B	1.6005310000	2.2569050000	0.4568100000
B	1.6684910000	-0.3532320000	2.4491610000
B	0.8167130000	-0.8856700000	-0.4188720000
B	1.3856730000	-1.8767290000	1.8872310000
B	1.6723750000	1.1397940000	1.6462930000
B	0.2072130000	-1.0617940000	2.7383160000
B	0.3770150000	0.5742120000	2.7175410000
B	-0.7514390000	-0.1646670000	-0.1197500000
B	1.6236770000	-2.2972720000	-1.1354740000
B	1.5718100000	-2.4759710000	0.4185200000

B	1.2588150000	-1.2378640000	-2.2193740000
25			
energy			
Al	1.5232200000	-1.2899870000	1.9673710000
Al	1.7984740000	1.5154180000	1.6901080000
Al	-2.1876240000	2.0629980000	-0.7364900000
Al	0.2867350000	0.1191570000	-0.1675060000
Al	2.3124380000	2.1098160000	-1.2846980000
Al	3.2084920000	-0.2096240000	0.3454940000
Al	-2.4799910000	-1.8809600000	0.4947160000
Al	-1.9667240000	-0.5380100000	-1.9475380000
Al	1.5380570000	-2.5517950000	-0.6666950000
Al	-4.1218580000	0.1989030000	-0.5984290000
Al	2.5303650000	-0.6722070000	-2.4773470000
B	0.0455340000	2.6561960000	-0.5535310000
B	-1.1616080000	1.3572480000	1.4740200000
B	-1.2492460000	-0.3538580000	1.8394630000
B	-0.2159220000	-2.5872630000	0.6566310000
B	-0.6191840000	-1.9980080000	2.1109680000
B	-0.6363890000	-2.0777360000	-0.8323980000
B	-0.2963970000	0.7350370000	3.0245040000
B	-0.2978280000	-0.8512130000	3.1449640000
B	-0.1895030000	2.7883050000	1.0260950000
B	-0.1148800000	2.2278740000	2.4779250000
B	-0.0056240000	1.7222630000	-1.7950510000
B	0.1714540000	-1.2402680000	-1.9465520000
B	0.1900350000	0.2828910000	-2.3900120000
B	-1.9685620000	0.2928880000	0.5536130000
26			
energy			
Al	2.0584880000	-1.8235230000	-0.0893700000
Al	2.9634880000	-0.0024410000	1.4728030000
Al	-1.1655190000	0.0003260000	2.8783160000
Al	-1.2190230000	-2.0549350000	0.9741380000
Al	-1.2177170000	2.0570680000	0.9759340000
Al	-1.3498260000	-1.3806450000	-1.9319290000
Al	2.6417280000	-0.0027760000	-2.3360180000
Al	2.0607860000	1.8208420000	-0.0878980000
Al	-1.3456670000	1.3856050000	-1.9317950000
Al	-3.2764580000	1.3152670000	-0.2404890000
Al	-3.2799840000	-1.3138650000	-0.2395980000
B	1.1503000000	-0.0005150000	2.6960890000
B	0.7544390000	-2.8666480000	1.4880560000
B	0.7319370000	-1.4389410000	2.2101360000
B	0.3972490000	-0.0001050000	0.9701360000
B	0.5354200000	-3.4812670000	0.0988660000
B	0.4628090000	-2.8065720000	-1.2952110000
B	0.8977070000	-1.4205360000	-1.9994740000
B	0.5403180000	3.4809500000	0.0984450000
B	0.7337910000	1.4382940000	2.2097880000
B	0.3291210000	0.0000540000	-2.5467850000
B	0.9016750000	1.4191300000	-1.9989360000
B	-1.1097950000	0.0014310000	0.0749540000
B	0.5865940000	-0.0001620000	-0.7527370000
B	0.7573110000	2.8660820000	1.4878160000
B	0.4683520000	2.8064110000	-1.2957930000
27			
energy			
Al	0.8467680000	2.1470850000	2.1458080000
Al	2.2847810000	0.0006420000	-1.9694490000
Al	0.8531270000	2.1587920000	-2.1411740000
Al	-1.6211970000	1.2945690000	-2.0207750000
Al	0.8438120000	-2.1502860000	-2.1458320000
Al	-1.6309000000	-1.2863350000	-2.0272750000
Al	-1.6294970000	-1.2906710000	2.0190600000
Al	-1.6296360000	1.2904960000	2.0250350000
Al	0.8430280000	-2.1572010000	2.1411060000

Al	2.2842810000	-0.0063520000	1.9736540000
Al	-3.8308440000	0.0045570000	-0.0006890000
B	2.7342840000	1.4925830000	0.0040470000
B	1.8135000000	-2.8071880000	-0.0029150000
B	0.9412990000	1.2810290000	0.0006560000
B	1.8206020000	2.8021480000	0.0059730000
B	-1.2769450000	2.6578270000	0.0038050000
B	0.2792090000	3.0220370000	0.0038150000
B	0.1219830000	0.0001500000	-0.8531390000
B	-2.3983150000	1.5536060000	0.0004090000
B	-1.2830520000	-2.6549020000	-0.0051410000
B	0.2717090000	-3.0247130000	-0.0046510000
B	0.9369170000	-1.2848750000	-0.0010880000
B	-2.4021920000	-1.5481270000	-0.0039480000
B	0.1213170000	-0.0013660000	0.8533310000
B	-1.4555250000	0.0017700000	-0.0008010000
B	2.7296060000	-1.4995440000	-0.0011060000
B	3.2499230000	-0.0042040000	0.0021340000

13

energy

Al	-2.0721270000	-1.3709720000	-0.1874180000
Al	2.3446890000	-1.2413810000	-0.1157710000
Al	0.3306210000	-2.1039960000	-1.4941120000
Al	0.0117230000	-2.0952450000	1.2277800000
Al	-0.1066450000	2.1244080000	1.1781470000
Al	0.2106330000	2.0773690000	-1.5451630000
Al	-0.9846670000	-0.0587870000	-2.3179440000
Al	-2.1444090000	1.2522550000	-0.2216500000
Al	2.2705050000	1.3671190000	-0.1491200000
Al	1.2514200000	0.0597320000	2.0029360000
Al	-1.5617690000	-0.0147930000	2.2288390000
B	0.0785650000	0.0002970000	-0.0798200000
B	1.0915030000	0.0108590000	-1.4971440000

14

energy

Al	0.0512590000	1.3311390000	-2.1659020000
Al	-1.4082070000	2.1415960000	0.0007950000
Al	0.0512180000	1.3301860000	2.1667250000
Al	1.3957590000	2.1436970000	0.0004330000
Al	3.4418590000	-0.0015280000	-0.0008140000
Al	0.0489390000	-1.3318290000	2.1652900000
Al	1.3928890000	-2.1460520000	-0.0004410000
Al	0.0484100000	-1.3310000000	-2.1654220000
Al	-2.2755160000	0.0027420000	-1.4783150000
Al	-2.2748730000	0.0015560000	1.4777760000
Al	-1.4123630000	-2.1399680000	-0.0003950000
B	1.3113560000	-0.0010030000	-0.8768500000
B	1.3119400000	-0.0012380000	0.8767720000
B	-0.1776670000	0.0008400000	0.0007850000

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energy

Al	0.0343960000	0.3346300000	-2.1087230000
Al	-2.0931030000	1.5706330000	-0.9980340000
Al	0.5022750000	2.3176180000	-0.0781090000
Al	2.5344880000	1.0042260000	-1.3344850000
Al	-0.1755380000	-2.1943820000	-0.7476560000
Al	2.4250040000	-1.5556600000	-0.7286400000
Al	-2.4141870000	-0.9389950000	-1.5206160000
Al	-1.5470580000	1.9598850000	1.6333740000
Al	2.6050610000	0.4160820000	1.5226660000
Al	0.5243940000	-1.5860090000	1.8545510000
Al	-2.1930640000	-1.5468780000	1.0680370000
B	0.9391200000	-0.0668540000	0.0024360000
B	0.3393550000	0.6638320000	1.4751430000
B	-1.0586080000	-0.0331710000	2.0385790000
B	-0.7468040000	0.0052050000	0.2216940000

16

energy
Al -1.9741020000 1.9309130000 -0.0068530000
Al -2.0599970000 0.0625030000 1.9151990000
Al 0.1236700000 -1.2926310000 2.0559260000
Al -2.8469930000 -1.4667890000 -0.1141130000
Al 1.9428370000 1.2353250000 1.4953900000
Al -0.2925280000 -2.4387160000 -0.4767310000
Al 2.5789310000 -1.2874620000 1.0103220000
Al 0.4732180000 3.1112630000 0.1124510000
Al 1.9359090000 1.1252600000 -1.6917470000
Al 1.9999640000 -1.5513870000 -1.5440270000
Al -1.8295820000 0.1952840000 -2.2275940000
B -0.9238890000 -0.2909320000 -0.0709410000
B -0.1257800000 0.8467550000 1.0191190000
B -0.0489970000 1.1123760000 -0.7748680000
B 0.8711270000 -0.2538180000 0.0069880000
B 0.0940910000 -0.4356470000 -1.5536730000

17

energy
Al -2.2019340000 -0.5439310000 1.1482240000
Al -3.5159170000 -0.6243980000 -1.2463990000
Al -0.3123710000 -2.2748300000 0.2100700000
Al -0.3907160000 -1.5444640000 2.8153860000
Al 0.0102470000 3.3702550000 -0.2891440000
Al -2.2121110000 2.0029330000 -0.2829420000
Al 2.1587000000 1.9748870000 0.3023380000
Al 3.5676830000 -0.1273840000 -0.5199580000
Al -0.1359850000 1.0514210000 1.5173830000
Al 1.7309760000 -0.8168650000 1.3258690000
Al 1.9492320000 -1.6897600000 -1.7772360000
B -1.5042040000 0.2801550000 -1.2528250000
B -0.0945210000 1.1253100000 -0.8697330000
B 0.0252020000 -0.3900450000 -1.5732310000
B 1.3713830000 0.3381620000 -0.9266950000
B -1.4195640000 -1.2994710000 -1.7724890000
B -0.0625840000 -2.0765580000 -1.9343620000

18

energy
Al 2.4985420000 -2.3927870000 0.1696990000
Al 0.0068290000 -2.5758220000 0.5786990000
Al -2.4845420000 -2.3960360000 0.1611190000
Al -1.3224170000 2.6741810000 -0.1150770000
Al -4.0921890000 -0.7545010000 -1.0163780000
Al -3.5471270000 1.5312200000 0.3156010000
Al -1.3891530000 0.0584240000 -1.1642820000
Al 1.3117450000 2.6770470000 -0.1097600000
Al 3.5420940000 1.5400400000 0.3052250000
Al 1.3822810000 0.0539840000 -1.1592040000
Al 4.0900970000 -0.7443470000 -1.0217290000
B 0.8745780000 -0.5878210000 1.2480800000
B -2.4577550000 -0.3923580000 0.8490740000
B -0.8695790000 -0.5894820000 1.2439830000
B 1.5987470000 0.9419030000 1.2183490000
B -1.5978330000 0.9382650000 1.2160520000
B 0.0005140000 0.9298110000 1.3210030000
B 2.4613120000 -0.3859670000 0.8492870000

19

energy
Al 1.2950660000 -0.7330920000 -1.4322870000
Al 1.0663630000 3.2242980000 1.2027170000
Al -2.1216200000 2.5964400000 -0.7012550000
Al 0.3033560000 1.7665400000 -1.2964490000
Al -1.4808860000 -0.5475110000 -1.2366110000
Al 2.7302080000 1.5681830000 -0.0278000000
Al 3.8851090000 -0.6386210000 -0.5353740000
Al -0.0680380000 -2.8743450000 -0.0937670000
Al 2.4201080000 -2.4366790000 0.5820190000

Al	-2.9093540000	-2.5484030000	0.2914870000
Al	-3.9822410000	0.3453400000	-0.1552040000
B	-0.4966370000	1.8117270000	1.1006770000
B	-0.9556190000	-1.4783290000	1.2618580000
B	0.8611100000	0.8230120000	1.0871800000
B	2.0459600000	-0.3024990000	0.8651980000
B	0.5874020000	-0.9289060000	1.1762190000
B	-2.0051800000	1.1349910000	0.9068110000
B	-0.7527420000	0.1697510000	1.3901330000
B	-2.2432780000	-0.5073380000	1.0584880000

20

energy

Al	1.4747820000	0.0705040000	-1.3392910000
Al	1.7929470000	-2.1711270000	0.4743590000
Al	3.4691010000	1.7208500000	0.1386230000
Al	3.9565460000	-0.9463310000	-0.6116110000
Al	0.9686770000	2.5728090000	-0.3626130000
Al	-1.2102210000	0.9332190000	-1.2860910000
Al	-1.4417640000	3.2990930000	0.3358550000
Al	-3.5503410000	1.6625580000	-0.0710870000
Al	-3.3929510000	-1.6163050000	-0.6909370000
Al	-0.9394080000	-3.7469360000	0.6611410000
Al	-0.5021440000	-1.8214520000	-1.3271800000
B	0.8684720000	-0.2948370000	1.3926620000
B	2.4334090000	-0.0584170000	0.8604000000
B	1.5989820000	1.2268820000	1.3778240000
B	0.0116700000	1.3419700000	1.4893390000
B	-0.0833970000	-1.6587380000	1.3297620000
B	-1.5790610000	1.3244510000	1.2229620000
B	-2.3692750000	-0.0420530000	0.6986200000
B	-0.8540900000	-0.1668890000	1.3597380000
B	-1.6522960000	-1.5602640000	0.8736570000

12

energy

Al	-1.3128940000	-2.3306800000	-0.4191290000
Al	2.3635980000	1.6114520000	-0.8708980000
Al	-0.0918470000	-1.3384810000	1.8581010000
Al	-0.1556730000	1.3079430000	1.8451800000
Al	2.0609470000	-0.0267590000	1.2758430000
Al	1.3220570000	-2.4396510000	0.0012050000
Al	-2.2446370000	-0.1534740000	1.1714160000
Al	0.2273590000	2.8878560000	-0.0691440000
Al	-2.6368550000	-0.5257320000	-1.7367580000
Al	-2.1088340000	1.7899970000	-0.7262920000
Al	0.0230960000	0.0481880000	-0.7183450000
Al	2.5536820000	-0.8306600000	-1.6111810000

13

energy

Al	-0.3198790000	-2.3056190000	1.1293110000
Al	1.0959340000	-2.0542630000	-1.1281620000
Al	-1.6146640000	-1.6777170000	-1.1261290000
Al	-0.0017090000	-0.0017030000	-2.3555340000
Al	-2.2933740000	-0.4074370000	1.1303510000
Al	-2.0940550000	1.0165350000	-1.1275420000
Al	1.6152490000	1.6792500000	1.1272800000
Al	2.2913120000	0.4071240000	-1.1280490000
Al	2.0953880000	-1.0176670000	1.1286420000
Al	0.3202500000	2.3050940000	-1.1303260000
Al	-1.0959040000	2.0548490000	1.1272800000
Al	0.0011800000	0.0015240000	2.3532170000
B	0.0007050000	0.0000820000	-0.0008800000

22

energy

Al	1.7710720000	0.4334940000	-1.2101910000
Al	-1.3915930000	-1.0236770000	-1.1492760000
Al	-2.0861410000	-3.3347820000	0.1686640000
Al	2.8045650000	-2.0847890000	-0.6743540000

Al	0.4538980000	-3.2112270000	-0.6751440000
Al	4.4546790000	-0.1680800000	-0.5580670000
Al	-0.6048540000	1.6653710000	-1.4652670000
Al	-3.3560130000	1.0036380000	-0.5587920000
Al	1.4506940000	2.7057700000	0.5541260000
Al	-2.3755020000	3.5757650000	-0.7099450000
Al	-3.8789650000	-1.2504340000	0.9216220000
Al	3.5199120000	1.3882340000	1.3660890000
B	-0.3108370000	-2.1370300000	1.0628880000
B	1.1372800000	-1.3455490000	0.9628170000
B	2.5074140000	-0.4872150000	0.8235730000
B	1.1751180000	0.4041440000	1.2548690000
B	-1.7987230000	1.8346890000	0.7594560000
B	-0.6006680000	2.8528580000	0.5288050000
B	-0.2639950000	1.2701270000	1.2123740000
B	-1.7155110000	-1.3691440000	1.3079400000
B	-0.3057580000	-0.4878620000	1.3559380000
B	-1.8048780000	0.2468470000	1.1067290000

23

energy

Al	0.2887970000	1.2372520000	-0.8475060000
Al	-0.5767030000	-2.1929630000	0.4501090000
Al	-1.4688380000	-0.5234150000	-1.7274860000
Al	-4.0613970000	0.2132640000	-1.4688890000
Al	1.0461140000	-1.4046390000	-1.5081480000
Al	3.2233020000	0.8182770000	-1.3177340000
Al	3.6872880000	-2.0147540000	-1.0709610000
Al	2.2008910000	3.0979810000	-0.0967270000
Al	2.0869600000	-2.4986290000	1.1906760000
Al	-0.3735760000	3.5639580000	0.5529710000
Al	-2.3246900000	1.9306670000	-0.1139740000
Al	-3.4361410000	-2.1824220000	-0.2496270000
B	-0.6834060000	1.6397740000	1.6258830000
B	-0.0232270000	0.2121590000	2.2202420000
B	0.5617080000	-1.3899060000	2.3374860000
B	-1.0078340000	-1.1671960000	2.4144800000
B	-2.7875060000	-0.1295480000	0.4025490000
B	-1.6702220000	0.3094840000	1.6089380000
B	-2.3303860000	-1.2535450000	1.4973910000
B	1.5165120000	-0.2699180000	1.5522320000
B	2.1922950000	1.0151700000	0.6646290000
B	0.9012990000	1.4572210000	1.5387870000
B	2.5715470000	-0.5395980000	0.2763530000

24

energy

Al	-2.4526120000	-1.2677670000	-1.7164690000
Al	-0.1451490000	0.0084060000	-2.4363720000
Al	-0.6359660000	2.6279260000	-1.4142950000
Al	1.6257220000	0.8573770000	2.1440070000
Al	1.4878390000	-1.7448070000	1.2790640000
Al	1.6742180000	2.3105590000	0.0298560000
Al	1.7782580000	-1.8577890000	-1.4791810000
Al	2.2751090000	0.8215300000	-1.9227290000
Al	-0.6760470000	2.4226230000	1.3409870000
Al	-2.9452480000	1.6725350000	0.0504420000
Al	3.4606130000	-0.2612960000	0.2802940000
Al	-2.3766300000	-1.6958380000	0.8497980000
B	-0.3724440000	-2.0615300000	-1.9819760000
B	-0.2752750000	-1.2037360000	-0.2790340000
B	-0.4070810000	-2.8553280000	0.8364800000
B	-0.3354870000	-2.9561870000	-0.7148340000
B	-1.3842050000	-0.7000770000	2.5815660000
B	-1.2222280000	0.2183620000	-0.1143690000
B	-1.9672390000	0.4640620000	1.4929170000
B	-0.5225600000	-2.0316620000	2.1847320000
B	-0.6029790000	0.7160290000	2.5971710000
B	0.2375500000	-0.6849920000	2.8573530000

B	0.8192040000	0.1391200000	-0.0857420000
B	-1.9495320000	0.8329440000	-1.5883080000

25

energy			
Al	1.3239190000	1.8547030000	-2.0498990000
Al	-1.2322130000	1.6545140000	-2.1076680000
Al	0.3967120000	-2.2052230000	-2.1574650000
Al	2.3865530000	-0.5309760000	-2.1136220000
Al	1.3224410000	1.8668260000	2.0408870000
Al	2.3849540000	-0.5184450000	2.1164220000
Al	0.3966020000	-2.1941350000	2.1701550000
Al	-1.8430230000	-0.9380690000	-2.1401430000
Al	-3.0004090000	0.9430240000	-0.0031810000
Al	-1.2334460000	1.6654540000	2.0981970000
Al	-1.8432430000	-0.9271360000	2.1443060000
Al	-3.1769680000	-1.6568040000	0.0039130000
B	-0.1548620000	1.3670200000	-0.0036040000
B	1.3174830000	2.7486130000	-0.0072730000
B	0.0073490000	-0.1235990000	-0.8799820000
B	3.0599610000	-1.3398840000	0.0042110000
B	3.0351340000	0.2062070000	-0.0005810000
B	2.4605190000	1.6965410000	-0.0034710000
B	1.3281260000	-0.8547440000	0.0022530000
B	-0.2141240000	3.1543950000	-0.0083190000
B	-1.6222340000	2.4850650000	-0.0070350000
B	1.9531380000	-2.4963090000	0.0068690000
B	0.4106320000	-2.6616530000	0.0074400000
B	0.0073820000	-0.1188720000	0.8807160000
B	-0.8813890000	-1.4984860000	0.0038320000

26

energy			
Al	1.8242540000	2.3956180000	0.0031720000
Al	-2.1413810000	0.6990870000	2.0471860000
Al	1.9955410000	0.5162870000	2.0657010000
Al	0.9732930000	-1.8123170000	2.0717930000
Al	-1.6330040000	-1.8661680000	2.1318130000
Al	-0.0726180000	2.2103450000	-2.1098740000
Al	0.9760110000	-1.8083240000	-2.0749750000
Al	1.9988710000	0.5201630000	-2.0632220000
Al	-1.6294660000	-1.8572460000	-2.1369700000
Al	-2.1437130000	0.7061270000	-2.0478570000
Al	-0.0740220000	2.2083470000	2.1149120000
Al	3.3370040000	-1.5052780000	-0.0008640000
B	-2.5843190000	1.5943460000	0.0013710000
B	-0.6794900000	1.4431550000	0.0013280000
B	2.7853080000	0.5477510000	0.0018940000
B	-0.0899520000	3.1061650000	0.0030310000
B	-0.1359600000	0.0280580000	0.8607840000
B	-0.1360650000	0.0294930000	-0.8617980000
B	-0.2102820000	-2.7599960000	-0.0018120000
B	1.3843910000	-2.2768490000	-0.0017660000
B	-1.7830090000	-2.7026190000	-0.0041210000
B	-2.8592410000	-1.5043200000	-0.0022200000
B	-3.0629480000	0.0521550000	-0.0006630000
B	-1.1700650000	-1.0684750000	-0.0008990000
B	1.3432200000	-0.4349160000	-0.0001540000
B	-1.6695910000	2.8887810000	0.0029020000

27

energy			
Al	2.7444420000	2.1797770000	0.0002230000
Al	-2.0274260000	1.1685140000	1.9932340000
Al	2.0079310000	0.0977720000	2.0452500000
Al	0.5711180000	-2.0364590000	2.0316860000
Al	-1.9950300000	-1.4490400000	2.1421820000
Al	0.3624670000	2.1613000000	-2.0901840000
Al	0.5698090000	-2.0358690000	-2.0327430000
Al	2.0073710000	0.0980950000	-2.0451710000

Al	-1.9953530000	-1.4453250000	-2.1437150000
Al	-2.0270410000	1.1719590000	-1.9918740000
Al	0.3615020000	2.1593260000	2.0916410000
Al	3.2490360000	-1.9132980000	-0.0008490000
B	-2.0361730000	2.4761900000	0.0015810000
B	-0.4057820000	1.5250370000	0.0002240000
B	2.7896620000	0.0961270000	-0.0000060000
B	0.8099410000	2.9315680000	0.0010150000
B	-0.1840580000	-0.0063420000	0.8516790000
B	-0.1841090000	-0.0058620000	-0.8517490000
B	-0.1790890000	-3.0853710000	-0.0005460000
B	1.3072980000	-2.5966500000	-0.0008630000
B	-1.6985370000	-2.6844420000	-0.0016560000
B	-2.9755250000	-1.8005650000	-0.0009630000
B	-3.2049140000	-0.2532620000	-0.0004060000
B	-1.4600240000	-0.8621270000	-0.0002040000
B	1.2174910000	-0.7682760000	-0.0000340000
B	-0.6871090000	3.3079920000	0.0020390000
B	-3.0640230000	1.3184280000	0.0007240000

28

energy

Al	-0.2156810000	2.2884100000	2.1460940000
Al	0.7079380000	-1.8982740000	2.0055800000
Al	1.6853200000	0.4886040000	2.0279150000
Al	-1.9069780000	-1.6995560000	2.1440250000
Al	-2.3761450000	0.8487610000	1.9812200000
Al	-1.9103230000	-1.6968600000	-2.1419550000
Al	0.7053870000	-1.8966960000	-2.0127370000
Al	3.3615230000	-1.5789090000	-0.0000770000
Al	1.6787250000	0.4917350000	-2.0322210000
Al	-2.3806540000	0.8506510000	-1.9750190000
Al	-0.2221670000	2.2926830000	-2.1452540000
Al	4.8192000000	0.8001610000	0.0013060000
B	-2.2651780000	2.3659560000	0.0033360000
B	-0.3848410000	0.0218820000	0.8490710000
B	-0.0551020000	-2.9866690000	-0.0025700000
B	-1.6385350000	-2.7385130000	-0.0002690000
B	-3.3743610000	-0.4156360000	0.0032120000
B	-3.2927780000	1.1608910000	0.0043520000
B	-1.6293400000	-0.8512150000	0.0013850000
B	1.3802620000	-2.3803150000	-0.0039230000
B	1.0749060000	-0.6067540000	-0.0027590000
B	2.4915660000	0.5325200000	-0.0035780000
B	-0.3872650000	0.0225230000	-0.8492570000
B	-0.9480310000	3.2577560000	0.0026780000
B	0.5746200000	2.9368800000	0.0000680000
B	-0.6536060000	1.5235190000	0.0007170000
B	1.8354700000	1.9675980000	-0.0014210000
B	-2.9877650000	-1.9662610000	0.0018790000

14

energy

Al	1.2959240000	-1.6568360000	-1.5954140000
Al	-3.5911810000	0.0002610000	-0.0004410000
Al	-1.0313320000	2.0140930000	-1.0767060000
Al	-1.0313590000	-0.3985860000	-2.2484370000
Al	-1.0334340000	-2.2599100000	-0.3168580000
Al	1.2983320000	1.0048940000	-2.0667170000
Al	2.7552530000	-0.0015590000	0.0053210000
Al	1.2923020000	-2.0302750000	1.0832550000
Al	-1.0358090000	-0.9977170000	2.0517880000
Al	1.2908510000	0.4027270000	2.2666840000
Al	-1.0352240000	1.6445100000	1.5800010000
Al	1.2952150000	2.2784240000	0.3182240000
B	0.2170750000	0.0001610000	-0.0005770000
B	-1.4378730000	-0.0002260000	-0.0012430000

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energy

Al	-1.2047140000	0.7277620000	2.1058350000
Al	-0.5618020000	-2.1024740000	1.0182890000
Al	1.1467060000	-0.5879450000	2.3381710000
Al	0.9822270000	2.0705670000	1.3082560000
Al	2.7838290000	0.2783430000	0.3992190000
Al	1.8660260000	-2.2305720000	-0.1875690000
Al	-3.0022160000	-0.8492620000	0.8217810000
Al	1.6363380000	-0.2908030000	-2.1719770000
Al	1.2060220000	2.0871070000	-1.3438780000
Al	-0.5791700000	-1.7662790000	-1.6851000000
Al	-1.4359270000	2.2938900000	-0.2986860000
Al	-2.5193920000	0.2258410000	-1.7627580000
B	-1.0887200000	-0.1176080000	-0.0069180000
B	0.6036070000	-0.0337900000	-0.0258880000
B	-0.3414990000	0.5253410000	-1.3753110000

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energy

Al	2.0223140000	0.8836060000	-1.8405130000
Al	2.5772470000	-1.5151270000	-0.8101480000
Al	-2.0944760000	1.1827180000	-1.5359950000
Al	1.6655000000	2.1368230000	0.5437630000
Al	-0.8578630000	3.1031220000	0.1230270000
Al	-2.0576330000	-1.8262600000	1.1912240000
Al	-2.3690620000	-1.4537760000	-1.3343290000
Al	2.7214570000	-0.2921650000	1.5151510000
Al	0.3564470000	-2.3139890000	0.2769270000
Al	0.0775450000	-0.8996210000	-2.1338020000
Al	-2.2031040000	0.7744500000	1.5564700000
Al	0.1949620000	-0.4546870000	2.4615600000
B	-0.0183210000	1.0784080000	-0.8891640000
B	-0.1580500000	1.0556870000	0.8645640000
B	0.9275900000	-0.1023910000	0.0270650000
B	-0.8378900000	-0.2769520000	-0.0371300000

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energy

Al	3.6044570000	-1.1136210000	-0.8691560000
Al	1.2773230000	-2.0889630000	-0.5328470000
Al	-1.2793210000	-2.0872050000	-0.5368080000
Al	2.1647900000	-0.1481770000	1.2790210000
Al	-3.6067170000	-1.1118780000	-0.8700000000
Al	-0.0004850000	-1.6854680000	1.9640860000
Al	0.0005340000	1.0927230000	2.3197940000
Al	1.2833290000	2.1394340000	0.0529880000
Al	-2.1639220000	-0.1491630000	1.2783740000
Al	-1.2814760000	2.1394030000	0.0566440000
Al	3.4537950000	1.3951000000	-1.0768880000
Al	-3.4522100000	1.3971090000	-1.0744310000
B	-0.0003560000	-0.6535000000	-1.6051640000
B	1.4246680000	0.1237140000	-1.1874480000
B	0.0000640000	1.0153800000	-1.3607850000
B	-1.4252570000	0.1253900000	-1.1880760000
B	0.0006270000	-0.0371460000	0.1654520000

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energy

Al	1.3149860000	-1.5069810000	1.1428100000
Al	0.7555650000	-2.4546450000	-1.5637810000
Al	3.1995800000	0.5819080000	0.0242050000
Al	3.1451900000	-1.9333840000	-0.8003730000
Al	2.1621820000	2.9354420000	-0.6129140000
Al	0.8247020000	1.1131860000	1.4488130000
Al	-0.4894870000	-0.7499600000	3.1005540000
Al	-0.5080700000	3.1782510000	-0.2156570000
Al	-1.2816040000	-1.9702610000	0.7330100000
Al	-1.7867490000	0.7101080000	1.2241640000
Al	-3.1234950000	1.5515490000	-0.9006430000
Al	-3.5483170000	-1.4377900000	-0.8078780000
B	-0.1100040000	-0.2833300000	-1.3431600000

B	1.5532820000	-0.3104160000	-1.0824310000
B	0.7148360000	1.1079940000	-0.9276230000
B	-1.1479380000	-1.6386020000	-1.4168200000
B	-0.9241440000	1.2400640000	-1.1026650000
B	-1.8136930000	-0.1610120000	-1.3353080000

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energy

Al	1.4833120000	-0.5080950000	1.2324250000
Al	-1.4199280000	-0.5842250000	1.2086260000
Al	-0.1049570000	-2.9235780000	-0.1219560000
Al	-2.6155920000	-2.8453640000	0.0489070000
Al	2.3011870000	-2.3629600000	-0.8833950000
Al	-3.2480850000	-0.6376350000	-1.0110160000
Al	0.0137580000	0.3180050000	3.2924020000
Al	2.6650740000	1.6501000000	-0.7266740000
Al	3.9711070000	-0.5062090000	-0.0950540000
Al	-2.5017660000	1.7026140000	-0.2570010000
Al	0.0833220000	1.9043820000	1.1724170000
Al	-0.9258320000	3.7604510000	-0.5292930000
B	-1.2228260000	-1.3956880000	-1.1529250000
B	1.8711070000	-0.3187200000	-1.1942460000
B	0.3466820000	-0.9139940000	-1.1394660000
B	-1.0390600000	0.2077820000	-1.3873550000
B	0.7136490000	0.8307830000	-1.3424170000
B	-0.6464210000	1.7756960000	-1.4506780000
B	0.7527080000	2.4986770000	-0.9919240000

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energy

Al	-0.3160680000	3.4317200000	-0.9168860000
Al	-1.4779560000	-0.5661950000	1.1953490000
Al	-2.8544270000	-1.9317110000	-0.8301800000
Al	-0.5435640000	-2.9564910000	-0.2584180000
Al	-2.3014990000	1.9524350000	-0.0420410000
Al	-4.0418350000	0.1030160000	0.1593820000
Al	2.3918630000	2.8967080000	-0.3118970000
Al	0.1729360000	-0.0060320000	3.2357880000
Al	3.9182830000	-0.1639160000	0.1084670000
Al	2.3616820000	-3.0805440000	-0.7019300000
Al	1.2575590000	-1.2449380000	1.1702420000
Al	0.4423340000	1.5373190000	1.1329070000
B	-0.7529750000	0.9327670000	-1.3803670000
B	-0.7946470000	-0.8552600000	-1.3847610000
B	-2.1275130000	0.0814620000	-1.1433790000
B	0.7346620000	1.6561810000	-1.3563290000
B	0.6469310000	-1.6520700000	-1.4073120000
B	0.7034050000	0.0060560000	-1.5045580000
B	2.0909040000	0.7913370000	-0.9942740000
B	2.0750340000	-0.8860370000	-1.0750590000

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energy

Al	-0.0009910000	-2.5362240000	0.4054310000
Al	1.3474400000	-0.8163270000	-1.4669560000
Al	4.0735980000	-0.7770220000	-1.0181500000
Al	1.2952700000	3.2665280000	0.5122160000
Al	2.8179220000	1.4180390000	-0.5528060000
Al	-1.3494720000	-0.8133350000	-1.4701620000
Al	-2.8180970000	1.4190020000	-0.5491320000
Al	0.0008850000	1.5309470000	-1.1742810000
Al	-1.2918520000	3.2670590000	0.5094270000
Al	-2.6822030000	-2.4991210000	0.3795530000
Al	2.6817330000	-2.5002340000	0.3820050000
Al	-4.0756730000	-0.7747890000	-1.0156150000
B	-1.3784590000	-0.9121980000	1.7852160000
B	0.0006250000	-1.4714690000	2.3154500000
B	1.3792020000	-0.9113350000	1.7844310000
B	0.0003840000	0.1373980000	1.9276230000
B	0.0003200000	1.6637570000	1.3504620000

B	2.514910000	-0.323408000	0.781289000
B	1.402454000	0.830469000	1.212648000
B	-1.401603000	0.830524000	1.212766000
B	-2.514088000	-0.323497000	0.782140000

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energy

Al	-0.955090000	-1.429766000	-2.053488000
Al	-1.486566000	-2.212401000	0.564132000
Al	1.158856000	-2.404391000	-0.540784000
Al	2.657284000	-0.197701000	0.564509000
Al	0.744197000	-1.522517000	2.067363000
Al	1.711545000	-0.153102000	-2.052402000
Al	-0.004260000	0.004564000	-0.000574000
Al	-1.162335000	2.393055000	0.602374000
Al	-0.759162000	1.590143000	-2.027859000
Al	0.987229000	1.443366000	2.033633000
Al	-1.748522000	0.107693000	2.034077000
Al	-2.653972000	0.190369000	-0.597204000
Al	1.510795000	2.190688000	-0.593776000

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energy

Al	0.148970000	0.735577000	-2.468780000
Al	-0.815201000	2.473003000	-0.591370000
Al	0.147503000	1.770930000	1.871140000
Al	-0.814165000	-0.724708000	2.437202000
Al	0.150912000	-2.505247000	0.597819000
Al	-0.813127000	-1.748615000	-1.846248000
Al	1.638969000	1.533601000	-0.363579000
Al	-2.288122000	1.060767000	1.119685000
Al	1.639838000	-0.449794000	1.510149000
Al	-2.286225000	-1.503024000	0.359577000
Al	1.640463000	-1.080811000	-1.145584000
Al	-2.287286000	0.438008000	-1.479984000
Al	4.053577000	0.000308000	0.000046000
B	-0.301873000	0.000013000	-0.000188000

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energy

Al	-1.383241000	-3.325743000	-0.853771000
Al	-0.443303000	-1.281717000	1.070340000
Al	2.040246000	-0.491836000	1.693749000
Al	4.517712000	0.130443000	0.706603000
Al	1.132040000	-3.067368000	-0.301451000
Al	3.408941000	-1.856789000	-0.388056000
Al	1.014559000	3.418548000	-1.085179000
Al	2.785406000	2.012681000	0.247636000
Al	-2.319366000	0.640218000	1.647258000
Al	-4.781931000	0.488007000	0.427149000
Al	0.214273000	1.437756000	1.206895000
Al	-1.510674000	3.048159000	-0.348672000
Al	-3.153599000	-1.814166000	0.392256000
B	-1.489787000	-0.913646000	-1.171135000
B	-0.073560000	-1.600107000	-1.562214000
B	1.315704000	-0.857063000	-1.122834000
B	-0.119488000	0.018327000	-1.756119000
B	-0.117667000	1.640437000	-1.630434000
B	2.595114000	0.081503000	-0.719260000
B	1.272021000	0.945643000	-1.154143000
B	-1.527091000	0.922062000	-1.157854000
B	-2.842258000	-0.035198000	-0.786449000
B	-2.967753000	1.518739000	-0.417934000

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energy

Al	-2.729381000	-1.883787000	-0.501804000
Al	-0.730780000	-1.064977000	-2.533387000
Al	-2.718212000	0.507605000	-1.534806000
Al	-1.993776000	-1.068991000	1.812098000
Al	-0.440445000	1.890169000	-1.889735000

Al	2.2403160000	1.1944120000	1.5147110000
Al	1.5712700000	-1.3872450000	1.4040120000
Al	1.4767560000	-2.4720010000	-1.1067680000
Al	1.7060460000	0.0393800000	-2.3387360000
Al	3.4563240000	-0.5140510000	-0.2903070000
Al	-0.0740760000	2.7608350000	0.5948950000
Al	-2.6734510000	2.2706220000	0.2969580000
Al	2.1419850000	2.1235160000	-0.9160240000
B	-0.7008880000	-2.5505770000	-0.9791070000
B	-0.3853740000	-1.0025800000	-0.1526450000
B	-0.2252130000	-2.4723310000	2.0751760000
B	-0.4173760000	-2.7887480000	0.5631800000
B	-0.7248430000	0.2832840000	2.9346270000
B	-1.5195930000	1.1682680000	1.7331760000
B	-1.1221420000	0.4614080000	0.1829460000
B	0.0051690000	-1.2104090000	2.9938280000
B	0.1487940000	1.4815890000	2.2515450000
B	0.9380110000	0.1595790000	2.8969690000
B	0.7987490000	0.2422470000	-0.2285740000

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energy

Al	-1.0265920000	-1.4386820000	-1.7780460000
Al	-1.1991260000	-0.2497230000	2.0631480000
Al	-3.4246220000	0.9972540000	0.9031940000
Al	-1.1549410000	1.4098090000	-1.9234740000
Al	2.8759400000	0.6267820000	-1.7524370000
Al	2.4162260000	1.8133270000	0.5734570000
Al	3.0822520000	-1.9431050000	-0.7823430000
Al	-3.2536880000	-0.0640840000	-1.6702170000
Al	-0.6450730000	-2.6747510000	0.7231700000
Al	-2.9787870000	-1.5975130000	0.4990790000
Al	2.6305310000	-0.4660420000	1.8222070000
Al	-1.0989830000	2.1255640000	0.6533380000
Al	0.7281130000	-0.0854880000	-0.1697590000
B	0.6097950000	1.2149740000	2.7501670000
B	0.5434270000	2.7579960000	-1.0416540000
B	0.7455240000	3.2044390000	0.4747930000
B	0.7994820000	0.1873810000	-2.5712750000
B	0.9477210000	1.7179700000	-2.1937110000
B	1.4643670000	-2.1357940000	0.7282690000
B	0.8599790000	-2.2546440000	-0.8191840000
B	0.7343300000	-0.3239580000	3.0002460000
B	0.7400690000	-1.6612820000	2.1252670000
B	0.6713620000	2.5477270000	1.8957180000
B	-1.3891300000	0.0360430000	-0.0996620000
B	1.1998230000	-1.2695570000	-2.0683960000

26

energy

Al	0.7710060000	2.2108860000	1.7112210000
Al	3.0134470000	1.7033240000	-0.0511630000
Al	0.7763060000	1.3116000000	-2.3819000000
Al	2.2468740000	-0.1485810000	1.5994270000
Al	-1.2319130000	2.1065610000	-0.1961460000
Al	1.0718510000	3.4135530000	-0.6621230000
Al	2.5805260000	-0.5352400000	-1.1469660000
Al	0.2262380000	-2.8072130000	-0.4404780000
Al	-1.8854520000	-1.9719590000	-1.8349300000
Al	-2.2130910000	-1.9684890000	1.3365800000
Al	-3.8202150000	1.3023750000	-0.6951480000
Al	-2.6355370000	0.6477010000	1.6821700000
Al	-0.3728130000	0.0979020000	2.9072400000
B	0.7156640000	0.6921160000	-0.1079580000
B	-0.9878580000	-0.1030380000	-2.8112350000
B	1.7872810000	-2.3330360000	1.8652330000
B	2.3955970000	-2.5553070000	0.4045000000
B	0.0236560000	-1.7800900000	1.5137080000
B	-2.0213360000	0.5159780000	-1.7227910000

B	-2.0451600000	-0.3452560000	-0.2396620000
B	0.1870960000	-1.1387420000	-2.5856450000
B	-0.4500600000	-0.1296730000	-1.1063040000
B	-0.4860440000	-0.4945550000	0.5525840000
B	2.2884920000	-2.6923540000	-1.1384570000
B	1.4374180000	-2.0597890000	-2.2591420000
B	0.9844660000	-1.5185460000	2.8829300000

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energy

Al	-1.3803190000	-2.3023730000	-1.1732950000
Al	2.5896530000	1.1198060000	-0.5580150000
Al	2.6533530000	-2.1784890000	1.4589600000
Al	0.0748830000	-1.6819460000	1.5059360000
Al	-1.6362580000	1.9729940000	1.6323710000
Al	-0.1370560000	2.7252520000	-0.5538980000
Al	-2.4973020000	1.6524630000	-1.4245970000
Al	2.0630650000	0.1789680000	2.5180350000
Al	1.1666100000	-2.7868250000	-0.6470520000
Al	1.0599630000	-0.4699370000	-2.3966370000
Al	3.3070750000	-1.2435240000	-1.1723740000
Al	-3.6997460000	0.2903170000	0.9518500000
Al	-3.8991350000	-2.0246040000	-0.4143380000
B	1.4642020000	2.3836880000	1.3669620000
B	-0.2929510000	0.3599560000	2.4932940000
B	-2.1338370000	-1.4033530000	0.7822910000
B	-1.6150260000	-0.3740470000	1.8917110000
B	-1.1620180000	-0.1692340000	-1.9220340000
B	1.9660580000	3.1219230000	0.0308220000
B	1.0719340000	1.9477940000	-2.3971050000
B	0.4620040000	1.7648040000	2.4225940000
B	1.2562000000	-0.5171920000	-0.0210500000
B	0.4954150000	0.8074360000	0.8667720000
B	-0.2463390000	0.4534810000	-0.5927070000
B	-1.8898830000	-0.2369260000	-0.4379730000
B	-0.3660000000	1.2311110000	-2.2629180000
B	1.8617990000	2.9750950000	-1.5107180000

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energy

Al	-1.9888910000	1.8505140000	0.9975830000
Al	0.4692840000	1.5003120000	-2.5027280000
Al	-2.4985400000	1.3441860000	-1.8250290000
Al	-0.9360640000	-0.7635240000	-2.3303290000
Al	-0.6047210000	-2.2587460000	1.2271230000
Al	2.1488520000	-2.2047980000	0.4873230000
Al	1.2051670000	-0.9539820000	2.9737160000
Al	-2.8787640000	-0.5212790000	-0.1924020000
Al	1.0936870000	2.3929020000	0.0598520000
Al	-0.9827080000	3.3742220000	-1.1150550000
Al	3.5987840000	1.5464800000	1.1811710000
Al	2.1005780000	-1.8319140000	-2.2351800000
Al	2.7831890000	0.4136610000	-1.1209250000
B	-2.1197760000	-2.7089160000	-0.4854390000
B	-2.7001830000	-1.1960530000	1.9895760000
B	-2.7300670000	-2.3351520000	0.8901410000
B	1.5216690000	1.2167240000	1.9154050000
B	0.1195940000	1.2052790000	2.7450840000
B	1.8695820000	-0.0669590000	0.8527480000
B	-1.0635130000	-2.9736720000	-1.6430830000
B	-0.5860920000	0.7050200000	-0.4772420000
B	0.7115450000	-0.4890580000	-0.4515540000
B	0.1711530000	0.3662310000	1.0636310000
B	-0.9384670000	-0.2726190000	2.2326270000
B	-2.5020500000	0.0748570000	2.8808780000
B	-1.4232760000	1.1585360000	3.1391550000
B	0.3205190000	-2.1013650000	-0.8020170000
B	0.2237430000	-2.6917400000	-2.4232220000

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energy

Al	-2.2925300000	1.8616040000	0.4896190000
Al	-0.2059590000	-2.1813540000	1.7791320000
Al	-1.3594960000	1.0561460000	2.7181180000
Al	1.1952060000	0.1065590000	2.3784740000
Al	-0.5845420000	0.8789780000	-1.8010660000
Al	2.2822120000	-0.2007300000	-2.1084460000
Al	0.3469780000	2.3504730000	1.0885960000
Al	-2.5430160000	-1.1254620000	1.6746000000
Al	2.0305920000	-3.5817380000	0.5251400000
Al	3.0479840000	1.2693350000	0.5644000000
Al	3.1588990000	-1.2554630000	0.5398020000
Al	2.4387510000	3.5496830000	-0.4179170000
Al	0.1277040000	-2.0978020000	-2.7424250000
B	-1.0118250000	2.9837130000	-1.3614140000
B	-3.0431200000	-0.4481320000	-1.2723580000
B	-2.3638150000	2.3370160000	-1.6466260000
B	0.2769010000	-2.8511080000	-0.4336620000
B	-1.2614140000	-2.5898410000	-0.9316840000
B	1.3950060000	-1.6015000000	-0.6635920000
B	-0.4556890000	0.0231150000	0.8638970000
B	1.0100090000	0.0525240000	-0.0944700000
B	-0.3400220000	-1.1279040000	-0.3697750000
B	-1.5562130000	-1.0902550000	-1.7260850000
B	-3.9526790000	-1.2143540000	-0.0442750000
B	-2.7721030000	-2.0764360000	-0.6409220000
B	1.4288090000	1.4559220000	-1.0549780000
B	0.5635990000	2.9175210000	-1.0817810000
B	-4.2687440000	0.2940470000	-0.4153910000
B	-3.5199400000	1.2970760000	-1.3157540000

15
energy

Al	-0.1727960000	0.0011730000	2.6078730000
Al	2.3700760000	-0.0009020000	1.7608720000
Al	2.8321400000	1.4608820000	-0.5333920000
Al	2.8303020000	-1.4617030000	-0.5346050000
Al	0.4870040000	-1.3438590000	-1.9563060000
Al	0.3745860000	-1.9692720000	0.7809630000
Al	-1.6719900000	-2.4053070000	-0.8668220000
Al	-1.6685750000	2.4066770000	-0.8698170000
Al	0.4894350000	1.3400120000	-1.9571410000
Al	-2.1967160000	1.3283360000	1.3915950000
Al	-1.9866100000	0.0003380000	-1.9471740000
Al	-2.1974760000	-1.3244750000	1.3936590000
Al	0.3763470000	1.9684430000	0.7794090000
B	-0.6761930000	-0.0000040000	-0.0406450000
B	1.0253080000	-0.0008830000	-0.0870500000

16
energy

Al	2.2398470000	-2.1273400000	-0.0097550000
Al	2.3987960000	-0.3666880000	1.9394640000
Al	0.0011990000	-1.7238310000	1.5247660000
Al	-0.0016120000	1.0645040000	2.2140150000
Al	-2.3983220000	-0.3718480000	1.9409840000
Al	-2.2374540000	-2.1281760000	-0.0119860000
Al	-0.0043050000	3.4490190000	0.0087490000
Al	-2.1407770000	1.6078000000	0.0108490000
Al	2.1369670000	1.6138670000	0.0107730000
Al	-2.3965070000	-0.3489220000	-1.9442630000
Al	2.3998320000	-0.3455240000	-1.9403680000
Al	-0.0001100000	1.0865570000	-2.2030310000
Al	0.0023630000	-1.7088500000	-1.5419010000
B	0.8741930000	-0.2311990000	-0.0006410000
B	-0.0009610000	1.2425350000	0.0064820000
B	-0.8730150000	-0.2328090000	-0.0014140000

17
energy

Al	-2.2122180000	0.4126220000	1.3525500000
Al	-0.0009410000	-0.6696250000	2.5859080000
Al	0.0003900000	1.8344270000	1.6267910000
Al	1.3112670000	2.1362660000	-0.8251640000
Al	-3.3615320000	-1.4235400000	-0.8746910000
Al	-3.6858900000	1.1401050000	-0.7844150000
Al	-1.3119920000	2.1352610000	-0.8246320000
Al	2.2129330000	0.4134290000	1.3540870000
Al	3.6847280000	1.1406930000	-0.7821890000
Al	1.3106290000	-2.0344770000	0.5989520000
Al	3.3594720000	-1.4238100000	-0.8788170000
Al	0.0033020000	-1.6692800000	-1.8509280000
Al	-1.3091110000	-2.0352340000	0.5970950000
B	0.0000090000	0.5011980000	-1.5322150000
B	-0.0020080000	-0.1501730000	0.1380010000
B	-1.4317730000	-0.1206630000	-0.9886150000
B	1.4310760000	-0.1181380000	-0.9829940000

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energy

Al	-0.4067160000	3.1547630000	-0.6203240000
Al	-0.1239510000	-0.0669580000	3.2457040000
Al	-1.6059400000	1.0529650000	1.3074600000
Al	-1.1452530000	-1.5901080000	1.1237160000
Al	-1.7517220000	-2.4004020000	-1.3447590000
Al	-3.7904070000	-0.9468000000	-0.2616590000
Al	3.2386830000	-2.0447700000	-0.5848990000
Al	0.7887500000	-2.7203540000	-0.9829220000
Al	1.4750550000	-1.2139520000	1.3770630000
Al	2.1490850000	2.7607590000	-1.0182260000
Al	3.2350280000	0.5394760000	-0.3576440000
Al	1.0217860000	1.4595910000	1.2814070000
Al	-2.9195620000	1.7267740000	-0.9173370000
B	-1.8161730000	-0.2196680000	-1.0627510000
B	-0.1238880000	-0.4463080000	-1.2666990000
B	1.5109340000	-0.6057380000	-1.1101270000
B	0.8195940000	0.9458970000	-1.1577670000
B	-0.8190360000	1.0772610000	-1.2463620000

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energy

Al	-1.0392120000	-1.2869630000	1.2525730000
Al	-1.3068010000	-3.0623210000	-1.1300660000
Al	1.6356690000	-0.2562790000	1.2527210000
Al	-3.3636850000	-2.0351800000	-0.0445700000
Al	3.4440820000	-1.8960090000	-0.0473320000
Al	1.0980930000	-2.8485110000	-0.2715370000
Al	0.0013510000	-0.0006580000	3.3613240000
Al	3.3055150000	0.3997590000	-1.1301940000
Al	-0.5947300000	1.5424600000	1.2516840000
Al	-1.9994170000	2.6635970000	-1.1293810000
Al	1.9179110000	2.3763530000	-0.2727480000
Al	-0.0807490000	3.9303760000	-0.0440110000
Al	-3.0170870000	0.4728820000	-0.2727940000
B	0.0008140000	-1.0665130000	-1.2299700000
B	-1.6284040000	-0.9274260000	-1.1769980000
B	1.6167610000	-0.9460140000	-1.1765080000
B	0.9225750000	0.5347140000	-1.2285360000
B	-0.9246580000	0.5324110000	-1.2281520000
B	0.0104690000	1.8741130000	-1.1765790000

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energy

Al	-0.0560720000	1.6066700000	1.1417650000
Al	1.3800530000	-0.8562110000	1.1591930000
Al	-2.7800290000	1.4092230000	-0.0361630000
Al	-0.0007160000	0.0249990000	3.2706880000
Al	-1.4589610000	-0.9235010000	1.2439860000
Al	-2.4667580000	-2.4441660000	-0.9783650000
Al	1.2473540000	3.7899080000	-0.1727730000

Al	2.6018690000	-2.7355250000	-0.6564100000
Al	4.1575680000	-0.6038870000	0.1960810000
Al	2.4396180000	1.4827080000	-0.5851590000
Al	-4.0668820000	-0.7966160000	0.1466280000
Al	-0.0478580000	-2.9670010000	-0.2482010000
Al	-1.1957780000	3.1851990000	-1.0066940000
B	0.3881700000	1.8190290000	-1.2423280000
B	2.2219780000	-0.5983380000	-1.0730220000
B	-2.0970390000	-0.3222040000	-1.1296680000
B	-0.6232470000	-0.9405840000	-1.4259240000
B	-0.9140580000	0.8152140000	-1.2920850000
B	0.7626840000	0.2223750000	-1.4120120000
B	0.9026570000	-1.4421700000	-1.4588600000

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energy

Al	-3.9209430000	-1.7011730000	0.1841520000
Al	-1.6702800000	2.6729050000	0.1083400000
Al	2.9587740000	2.8275020000	0.0851380000
Al	-3.8334620000	1.0306000000	-0.3455440000
Al	0.6280940000	3.5967700000	-1.0356090000
Al	1.1222900000	-3.5645070000	-0.9517960000
Al	0.1129300000	-0.0470650000	3.2098440000
Al	0.7869260000	-1.4713780000	1.0329590000
Al	-1.6666720000	-0.1019580000	1.2195540000
Al	-1.4093380000	-2.4344470000	-0.5970060000
Al	3.3957750000	-2.5263690000	0.3405310000
Al	0.6995950000	1.4861460000	1.1372250000
Al	3.0000050000	0.2555830000	-0.3922800000
B	-2.4144120000	-0.5111310000	-1.0230460000
B	-1.7510350000	0.9429480000	-1.3152040000
B	-0.7735650000	-0.3797610000	-1.5350020000
B	0.9914200000	-0.0173160000	-1.3842830000
B	-0.1908700000	1.3202470000	-1.3671320000
B	1.3953400000	1.5819160000	-1.1471410000
B	0.3445340000	-1.5531270000	-1.5645850000
B	1.8689880000	-1.4425590000	-1.0519220000

22

energy

Al	3.1108030000	2.4991320000	0.2317820000
Al	0.7768080000	1.7260020000	-1.1670720000
Al	-1.5249680000	0.1094850000	-1.5129230000
Al	-1.4622310000	3.0404090000	-0.4317190000
Al	-4.1331520000	-0.9073960000	-0.9325670000
Al	0.2209760000	-1.7440010000	-0.9928640000
Al	1.6908980000	-3.5020900000	0.3164500000
Al	-2.4980940000	-2.3700920000	0.4946970000
Al	-0.3833790000	-3.0705170000	1.8516350000
Al	3.3199780000	0.1084940000	-0.7679190000
Al	3.1327670000	-2.3501480000	-1.3887670000
Al	0.8945230000	4.1063820000	0.9523910000
Al	-3.5265020000	1.4585770000	-0.1865710000
B	1.8272470000	0.2053900000	1.0067460000
B	1.3021460000	1.7743900000	1.1856190000
B	-0.2763690000	2.1291920000	1.2256670000
B	0.2039770000	0.5569360000	1.4080790000
B	-0.9172250000	-0.7186920000	0.9532800000
B	-1.4427010000	0.9986170000	0.9714660000
B	-2.4685940000	-0.2207540000	0.7035530000
B	2.0827360000	-1.3034520000	0.4100470000
B	0.6808760000	-1.0926440000	1.3225060000

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energy

Al	-0.7840060000	-1.3880250000	-2.3096940000
Al	-2.6363610000	-1.2769660000	-0.1872000000
Al	1.6658750000	-1.5011390000	-1.1561360000
Al	1.5248180000	-1.1151530000	1.6485840000
Al	-1.2167900000	-1.1787840000	2.3138040000

Al	-0.3616520000	-2.7132440000	0.2269260000
Al	3.9174860000	0.0011510000	0.0003970000
Al	-0.2941640000	0.0001240000	0.0002460000
Al	-0.3631260000	2.7127500000	-0.2267990000
Al	-1.2179480000	1.1803270000	-2.3139110000
Al	-0.7857600000	1.3907450000	2.3096840000
Al	1.6648640000	1.5010560000	1.1562050000
Al	-2.6374360000	1.2725340000	0.1870100000
Al	1.5241980000	1.1146240000	-1.6491150000

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energy

Al	-0.7773700000	2.1837740000	-0.0002400000
Al	1.8835670000	2.2784560000	-0.0003980000
Al	-1.4921480000	0.0016080000	-1.3984960000
Al	0.6108860000	1.3875380000	-2.1916340000
Al	0.6108030000	1.3882010000	2.1912180000
Al	2.6668430000	-0.0032860000	-1.2828930000
Al	-1.4922360000	0.0018850000	1.3986040000
Al	0.6078190000	-1.3883720000	2.1943020000
Al	2.6669140000	-0.0024730000	1.2824870000
Al	0.6074730000	-1.3893730000	-2.1937220000
Al	1.8761470000	-2.2791190000	0.0004770000
Al	-3.5980420000	1.4491370000	-0.0001390000
Al	-3.5985020000	-1.4460800000	-0.0000400000
Al	-0.7818490000	-2.1813480000	0.0004760000
B	0.5452070000	-0.0014240000	-0.0000040000

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energy

Al	2.5358520000	0.1937580000	1.5769260000
Al	0.0605920000	1.2658180000	1.2594190000
Al	-2.5721510000	2.4303110000	0.4920560000
Al	-2.3697750000	-0.1308440000	1.4672700000
Al	-4.4653770000	-1.8607760000	0.3970000000
Al	-4.6533010000	0.8300580000	-0.3672480000
Al	-1.9113970000	-2.4267850000	-0.2253080000
Al	0.2414780000	-1.4590630000	1.3504040000
Al	-0.3098580000	3.4784860000	-0.2105960000
Al	4.7397650000	-0.9660580000	0.4687830000
Al	2.1269950000	2.7586650000	0.0743920000
Al	4.1030380000	1.2333940000	-0.8712910000
Al	0.4599020000	-3.2734010000	-0.8202160000
Al	2.6774590000	-2.4380360000	0.2046840000
B	-3.0167310000	-0.6260370000	-0.7655800000
B	-1.0227930000	1.4007070000	-1.3739640000
B	0.5407150000	1.7676740000	-1.4113910000
B	1.7424640000	0.7015260000	-1.0721720000
B	0.1504340000	0.1854610000	-1.6735100000
B	-0.2084420000	-1.4151490000	-1.6735940000
B	2.7990040000	-0.5146550000	-0.7756010000
B	1.2976310000	-1.0545430000	-1.1859390000
B	-1.4494370000	-0.3773090000	-1.3861770000
B	-2.5572240000	0.8799570000	-1.1523890000

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energy

Al	1.4738590000	2.0001350000	-1.2667520000
Al	1.8970640000	-2.0870680000	-1.2755350000
Al	3.6378930000	-0.2396350000	0.4398510000
Al	1.7705960000	-1.2225640000	1.9051890000
Al	-1.8506720000	-1.5062400000	1.6859090000
Al	-2.3065940000	1.4954660000	1.2170570000
Al	2.0085200000	1.5814790000	1.4420580000
Al	0.0847530000	-0.0387290000	-2.5991140000
Al	3.0107770000	0.0784670000	-2.1042230000
Al	-3.3475190000	-1.4695510000	-0.4090980000
Al	-1.2559000000	2.0331140000	-1.5409370000
Al	-0.0547680000	3.3805290000	0.5511230000
Al	-3.5319780000	0.9681500000	-1.0120630000

Al	-1.2840490000	-2.1883340000	-1.9080530000
B	0.0569040000	-2.9298090000	1.0640710000
B	0.6138720000	0.5284740000	2.8703220000
B	-0.1830700000	1.6019040000	1.8709660000
B	-1.4571080000	-0.1537510000	-0.5101870000
B	-0.0031280000	-2.3599180000	2.5048360000
B	1.4060750000	-0.0711630000	-0.2166830000
B	-0.0266020000	-1.0727070000	-0.2797910000
B	-0.1005450000	0.6432250000	0.1225950000
B	-0.0852000000	-0.9096050000	3.1405190000
B	-1.0021110000	0.3767860000	2.6081170000
B	0.1257540000	-2.8950040000	-0.5008330000

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energy

Al	-0.5854340000	-2.6407840000	0.3184220000
Al	-2.3483540000	0.1126500000	-2.2302170000
Al	-3.2720000000	-1.4375610000	0.7665700000
Al	-2.6542510000	0.9783800000	1.2083860000
Al	0.2395500000	2.4165250000	1.0004980000
Al	0.7326580000	2.9817400000	-1.7157570000
Al	2.4927060000	1.0843240000	1.3279300000
Al	-1.1374880000	-0.9683070000	2.3752350000
Al	0.1586820000	-1.2242460000	-2.0092860000
Al	-2.3276590000	-2.4069020000	-1.6487710000
Al	3.3777260000	1.0827510000	-1.3664330000
Al	2.0855530000	-2.7647810000	-0.5778120000
Al	1.5732420000	-1.4076150000	1.9130890000
Al	3.8436530000	-1.1069940000	0.4523240000
B	-1.3389750000	2.0045220000	-2.0981570000
B	-0.7735710000	1.2493600000	2.7039840000
B	-1.5475040000	2.5481200000	2.2878700000
B	0.5537060000	0.4750480000	2.1155570000
B	-0.1420000000	0.9638780000	-2.4242090000
B	1.0798160000	0.7049540000	-1.3428120000
B	-1.5957950000	2.6563640000	-0.6570700000
B	-1.3597840000	-0.4937510000	-0.0861140000
B	-0.6872070000	1.0460650000	-0.7303370000
B	0.2583930000	0.0590080000	0.3619520000
B	-1.9056490000	3.0473100000	0.8665830000
B	1.7942550000	-0.4787470000	-0.5141130000

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energy

Al	1.4147900000	1.9236600000	1.7508560000
Al	3.3721430000	1.2080280000	-0.2865880000
Al	1.0162810000	1.3903880000	-2.4848590000
Al	2.4420890000	-0.5901040000	1.4128420000
Al	-0.6435260000	2.2861450000	-0.0155990000
Al	1.7477050000	3.2971900000	-0.5772450000
Al	2.4925400000	-0.9107290000	-1.3935650000
Al	-0.1262860000	-2.6038700000	-0.5646070000
Al	-2.2251070000	-1.5146700000	-1.8534090000
Al	-2.0285790000	-1.7253560000	1.3428580000
Al	-3.2470150000	2.1934340000	-0.3518020000
Al	-3.9753810000	-0.4473420000	-0.0863010000
Al	-2.0581090000	0.9662170000	1.9537250000
Al	0.1088020000	-0.0260730000	3.1218600000
B	1.1035860000	0.6281390000	-0.2278640000
B	-0.9160500000	0.1756000000	-2.7494100000
B	1.7371480000	-2.6875090000	1.7515410000
B	2.0844150000	-2.9584120000	0.2295640000
B	0.2056300000	-1.7240180000	1.4657830000
B	-1.7741450000	0.8594090000	-1.5436930000
B	-1.7046530000	0.0799820000	-0.0501780000
B	-0.0001360000	-1.1230950000	-2.6199840000
B	-0.2681020000	-0.0318410000	-1.1041550000
B	-0.1566020000	-0.3054210000	0.6030000000
B	1.8741020000	-3.0137990000	-1.3184610000

B	1.1243210000	-2.2486310000	-2.4289790000
B	1.1355790000	-1.8123910000	2.8756040000

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energy

Al	-1.6474280000	-2.4536870000	-0.1376110000
Al	-0.9196230000	2.1671590000	1.3376890000
Al	-1.6705240000	-1.8944570000	2.3083220000
Al	0.6827650000	0.2865330000	2.6734260000
Al	0.4329730000	-1.1971970000	-2.2568990000
Al	2.2330680000	0.7845720000	-1.8381050000
Al	0.7845640000	-2.0437190000	1.3751830000
Al	-2.9497470000	-0.0153040000	0.5755550000
Al	-2.0082060000	0.6050970000	3.0778460000
Al	0.2807440000	4.1492440000	-0.2763530000
Al	3.3490290000	0.3442320000	0.6331580000
Al	-0.3243890000	1.4420480000	-3.0387160000
Al	1.8478420000	2.3632160000	0.8766360000
Al	3.6567270000	-2.2248070000	0.4343970000
B	0.5252640000	-3.1871600000	-1.1474930000
B	-3.1099430000	-1.0421210000	-2.0810150000
B	-0.7360080000	-3.0032460000	-2.0166640000
B	-0.9889420000	2.4851080000	-0.9123480000
B	-2.2152630000	1.5772210000	-1.4581420000
B	0.5726600000	1.8095820000	-0.8276420000
B	-0.6738770000	-0.2167070000	0.8389010000
B	0.8646490000	0.2807830000	0.1036160000
B	-0.7737030000	0.6781910000	-0.6582470000
B	-1.6419130000	-0.1090280000	-1.9905940000
B	-3.3020420000	0.4281530000	-1.6052530000
B	1.8874110000	-0.9618440000	-0.4596340000
B	1.8382570000	-2.6665240000	-0.4177000000
B	-1.9908170000	-2.0860270000	-2.3035580000

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energy

Al	0.7929410000	1.6672630000	2.7612470000
Al	2.2474790000	-1.9625910000	0.5927670000
Al	3.1169800000	0.9780200000	1.3523000000
Al	2.7574920000	0.2314390000	-1.0290240000
Al	0.1952700000	-0.3931200000	-2.5066210000
Al	-1.8213510000	-2.1103390000	-1.6521830000
Al	-2.3023120000	0.8257190000	-1.6871770000
Al	1.1159540000	2.4153310000	0.1790440000
Al	-0.5485560000	-0.7574880000	2.4343430000
Al	1.9940840000	-0.8167360000	3.0029020000
Al	-3.1856460000	-0.7219880000	2.1466590000
Al	-1.8676280000	1.6528680000	1.3380660000
Al	-1.5774070000	3.4052220000	-0.8331900000
Al	-3.8921620000	-1.0523350000	-0.3878850000
B	-0.5271150000	-2.8909280000	0.1960800000
B	1.2694390000	2.2533230000	-2.4770070000
B	2.0136680000	0.9327500000	-2.9816150000
B	-0.2302670000	1.6114720000	-1.6101430000
B	-1.6071160000	-1.8313750000	0.8197190000
B	-1.7258870000	-0.2764730000	0.1621310000
B	0.4556420000	-2.1371280000	-1.1363440000
B	1.0502420000	0.0941450000	0.6923030000
B	-0.1052020000	-1.0406480000	0.0752980000
B	-0.3759430000	0.6885440000	-0.1933190000
B	2.3393640000	-0.5678000000	-2.9679280000
B	2.2192910000	-1.9062730000	-2.1051590000
B	1.8766720000	-3.1959120000	-1.2894700000
B	0.3415290000	3.2041890000	-1.6912410000
B	0.7403250000	-3.6771730000	-0.3425480000

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energy

Al	3.0344390000	0.4692730000	0.0309490000
Al	-0.6499890000	-1.5921710000	2.1558870000

Al	2.3330640000	0.5234110000	2.4694460000
Al	-0.2695820000	1.2115650000	2.5916310000
Al	1.8799020000	-2.0797840000	1.7429220000
Al	0.8212980000	0.2737870000	-1.9893820000
Al	-2.1448740000	0.8543020000	-1.7989100000
Al	-1.2889750000	-2.0463840000	-2.2873850000
Al	1.1818630000	2.4129270000	0.7263630000
Al	-3.4119180000	-1.7110710000	1.2859680000
Al	-1.7236920000	2.9241140000	0.4585840000
Al	-3.6894060000	-1.4578100000	-1.4470470000
Al	-2.6875100000	0.7857820000	1.4577390000
Al	-0.0398110000	4.3049920000	-0.9169430000
B	2.3116060000	-2.1319090000	-1.2516080000
B	3.1465950000	0.4842060000	-2.1390820000
B	-0.1966700000	-2.8466780000	-0.3807320000
B	0.7497620000	-0.0159060000	0.9254460000
B	-0.0701230000	-1.0473630000	-0.1423540000
B	0.6783890000	-1.8734460000	-1.5554220000
B	2.8710640000	-3.1601070000	0.0016110000
B	1.3506110000	-3.3218320000	-0.2664740000
B	3.8604080000	-2.0958150000	-0.6248870000
B	3.6098920000	-0.9513580000	-1.6271100000
B	-1.5991500000	-2.1832120000	0.1549700000
B	-1.8366130000	-0.5427820000	-0.1476570000
B	-0.6135000000	0.6576520000	0.0381570000
B	-0.4207930000	1.9379500000	-1.1699100000
B	1.0736400000	2.6302930000	-1.5426200000
B	2.3883740000	1.7906820000	-1.9198650000

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energy

Al	2.2802250000	1.7369450000	1.4072200000
Al	0.1301350000	0.5333740000	2.3711920000
Al	-2.3514760000	0.5921290000	1.4678390000
Al	2.4265470000	-0.8314920000	1.8492950000
Al	-2.3669710000	-1.5985910000	-0.2231570000
Al	0.0127740000	-1.6760850000	-1.5510780000
Al	-2.3613740000	0.9721490000	-1.2612640000
Al	-0.0277930000	-1.8695460000	1.2226800000
Al	2.2360990000	2.0053010000	-1.1449000000
Al	0.1091770000	0.8900320000	-2.2322620000
Al	-0.0990870000	2.1426480000	0.1935230000
Al	2.4689710000	-0.4828790000	-1.9119970000
Al	2.1693980000	-2.4175600000	-0.1900060000
Al	-4.7493190000	0.0164660000	0.0114790000
B	-0.6889860000	-0.0312200000	-0.0201010000
B	1.0079910000	-0.0022960000	-0.0021670000

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energy

Al	-2.3772960000	-1.4220200000	-1.7791830000
Al	-2.2357160000	0.3547960000	1.7678520000
Al	-0.0026400000	-2.4693360000	-0.7823230000
Al	-2.6242650000	-2.1092650000	0.7722530000
Al	-0.1808060000	-1.6252110000	1.8780310000
Al	-1.1825760000	2.8788430000	0.9769100000
Al	-0.0091190000	0.0418490000	-2.2391960000
Al	-2.4358150000	1.0891070000	-0.9347230000
Al	1.8094940000	1.4355330000	-0.3089670000
Al	0.4076230000	1.0190920000	2.1689240000
Al	2.3882200000	-0.7918400000	1.4631220000
Al	2.3769790000	-1.1034970000	-1.3456560000
Al	-0.2988850000	2.7354300000	-1.5362240000
Al	4.6417700000	-0.0075910000	-0.0404710000
B	-1.0306220000	-0.5931940000	-0.1061330000
B	0.6693080000	-0.4399010000	0.0096950000
B	-0.3588030000	0.9657790000	-0.0604730000

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energy

Al	0.1206720000	-1.2705000000	-2.1392830000
Al	-2.0216430000	-0.6590510000	1.5549920000
Al	0.6670050000	-1.1467690000	2.1561010000
Al	-0.0900130000	-3.1086500000	0.4289660000
Al	-2.1518050000	-2.2812920000	-0.8010370000
Al	2.1955330000	-2.0881560000	-0.4012060000
Al	2.4495370000	0.7427250000	1.9022000000
Al	-0.3063210000	1.4100930000	1.5102460000
Al	3.6302120000	0.0711010000	-0.3477910000
Al	-0.8806420000	2.9510110000	-0.8531310000
Al	1.8408930000	0.6995420000	-2.1571190000
Al	-3.7956310000	-0.2714120000	-0.5112140000
Al	1.6793850000	2.5495690000	-0.0734880000
Al	-3.1171560000	2.0648060000	0.1934350000
B	-0.3570640000	-0.5885410000	0.0766260000
B	1.2637700000	0.0402690000	0.0190050000
B	-1.5225930000	0.5854690000	-0.4215600000
B	0.0438210000	0.8389590000	-0.8744180000

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energy

Al	-1.3487110000	-2.3237490000	-1.0785710000
Al	0.0475640000	-0.2532260000	3.1586550000
Al	-1.9170630000	-0.9594440000	1.5674560000
Al	-0.4158770000	1.3381260000	1.0577820000
Al	-0.0273750000	3.3612580000	-0.7952000000
Al	-2.5272720000	3.1434500000	-0.3043020000
Al	4.1288560000	0.5308010000	-0.2722400000
Al	2.2014420000	2.1959250000	-0.5533090000
Al	2.0958980000	0.2665270000	1.5868520000
Al	1.0288670000	-3.0514190000	-1.5420610000
Al	2.8619500000	-1.6728500000	-0.4720880000
Al	0.5007200000	-1.8302750000	0.9357680000
Al	-3.0139100000	0.5758830000	-0.7617630000
Al	-3.8384720000	-1.8720310000	-0.1150670000
B	-1.1239200000	1.5143610000	-1.1737810000
B	0.3955910000	0.8132980000	-1.3074720000
B	1.8440120000	0.1205860000	-1.0954400000
B	0.4793650000	-0.8881630000	-1.3677190000
B	-1.0142540000	-0.1274200000	-1.3265520000

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energy

Al	0.0214670000	-0.1303350000	3.2877500000
Al	-2.2025760000	-0.4292940000	1.4551050000
Al	-1.8772900000	-2.4508140000	-0.7294350000
Al	-4.1643040000	-1.0878810000	-0.3895190000
Al	2.2130720000	-0.1839250000	1.2018930000
Al	2.8425410000	-2.6124950000	0.1056210000
Al	0.1172080000	-1.7251000000	1.1232830000
Al	0.5745320000	-3.1090820000	-1.1820500000
Al	2.5186450000	1.9689910000	-0.4046000000
Al	-0.0488000000	1.3920980000	1.1629070000
Al	-1.3227730000	3.0927330000	-0.7358720000
Al	-3.0885040000	1.2313630000	-0.8333650000
Al	0.9824650000	4.0738590000	-0.0120910000
Al	3.4500180000	-0.3644740000	-1.4462260000
B	-1.8079080000	-0.3958700000	-1.2170200000
B	1.3618850000	-1.1334480000	-0.9155890000
B	-0.2446310000	-0.8500690000	-1.2304660000
B	0.9716050000	0.4249570000	-1.1078850000
B	-0.7680660000	0.8553900000	-1.2552210000
B	0.4462890000	1.9683670000	-1.0426610000

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energy

Al	2.8739920000	1.0009160000	-0.8138860000
Al	2.3595230000	-0.3412200000	1.6013740000
Al	1.3719960000	3.1717010000	-1.0753430000
Al	2.6510070000	-1.8517950000	-0.7514570000

Al	-0.0124780000	-1.6352090000	0.8367060000
Al	0.2551480000	1.3793830000	0.8058360000
Al	0.1085260000	-0.1162100000	2.9759980000
Al	-0.7872930000	-3.7561750000	-1.2645830000
Al	-2.6867080000	-2.2905410000	-0.0206150000
Al	-2.1717620000	0.0596800000	1.6295600000
Al	-2.5531170000	1.6856530000	-0.6882930000
Al	-4.3205960000	-0.1423820000	-0.0007330000
Al	4.7639830000	-0.6121740000	0.3437250000
Al	-1.0826250000	3.8680160000	0.0072000000
B	0.7909470000	1.0530440000	-1.5566700000
B	-0.7548650000	0.3690980000	-1.4319300000
B	0.6330820000	-2.1644760000	-1.2595250000
B	0.7476800000	-0.5633290000	-1.5395680000
B	-0.8116430000	-1.3620690000	-1.3457330000
B	-2.1092130000	-0.4663480000	-0.9298680000
B	-0.4969400000	2.0430030000	-1.2589750000

22

energy

Al	-2.3100760000	-0.0048630000	1.2522110000
Al	-4.4948570000	-1.5090180000	-0.0422560000
Al	-4.1911980000	1.1482710000	-0.7260970000
Al	-1.9475070000	-2.3866090000	-0.2832130000
Al	-2.1574340000	2.6020180000	0.2171830000
Al	0.1494940000	1.3828610000	1.5719580000
Al	0.2262340000	3.4685140000	-0.1977150000
Al	3.8283810000	-1.2455080000	-1.0211660000
Al	0.2044690000	-1.4430320000	1.5122800000
Al	2.3643030000	0.1256500000	0.8320190000
Al	2.5495620000	2.9499190000	0.6680650000
Al	0.4355990000	-3.5886870000	-0.2062130000
Al	2.8068200000	-2.8173900000	0.7583820000
Al	3.5414380000	1.4849030000	-1.2363710000
B	-1.9656210000	0.9434720000	-1.2672640000
B	-2.7233830000	-0.4708240000	-1.0102480000
B	-1.0463120000	-0.4196560000	-1.2280300000
B	-0.3799810000	1.2965750000	-1.0913320000
B	0.7275690000	-0.0893830000	-0.8477740000
B	0.0384310000	-1.6096340000	-1.1612880000
B	1.5476560000	-1.5987390000	-0.6972680000
B	1.1880500000	1.5139140000	-0.7543650000

23

energy

Al	2.1918810000	-0.4149450000	1.6850540000
Al	4.6625670000	0.2551140000	0.7247070000
Al	3.5984700000	-1.7406970000	-0.4389800000
Al	1.0720460000	3.4495770000	-1.0105990000
Al	2.8658880000	2.0862530000	0.2739250000
Al	0.2549000000	1.3897230000	1.1924820000
Al	-1.3839700000	3.0420190000	-0.3463940000
Al	-2.1954520000	0.4127840000	1.6916240000
Al	-4.6626860000	-0.2564410000	0.7189930000
Al	-3.5959130000	1.7412770000	-0.4362250000
Al	-1.0692860000	-3.4487280000	-1.0142060000
Al	-2.8660390000	-2.0883970000	0.2692060000
Al	-0.2598370000	-1.3905550000	1.1991760000
Al	1.3843880000	-3.0375180000	-0.3420240000
B	2.6942320000	0.1574950000	-0.6948260000
B	1.3420450000	0.9790390000	-1.1251020000
B	-0.0940680000	1.6130110000	-1.5819290000
B	-1.4515190000	0.8173050000	-1.1280400000
B	0.0003270000	0.0002710000	-1.7742820000
B	0.0954390000	-1.6124780000	-1.5834760000
B	-2.6920930000	-0.1572100000	-0.6921990000
B	-1.3399400000	-0.9790420000	-1.1237500000
B	1.4534910000	-0.8170040000	-1.1299150000

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energy
Al 2.1653660000 1.7071000000 -0.0016080000
Al 2.1652730000 -1.7070350000 0.0006900000
Al 1.4802010000 0.0013560000 2.2183530000
Al -0.0228110000 -2.2692440000 1.4716160000
Al 4.1588920000 -0.0000610000 0.0018590000
Al 0.0136270000 0.0000240000 -0.0005870000
Al 1.4802720000 -0.0014390000 -2.2202340000
Al -0.0232450000 -2.2704190000 -1.4694230000
Al -0.0234720000 2.2688130000 -1.4719000000
Al -1.3317860000 -0.0012020000 -2.3255560000
Al -1.3308480000 0.0011630000 2.3250170000
Al -0.0225360000 2.2709070000 1.4691320000
Al -2.1989300000 1.5795630000 0.0004480000
Al -4.3110180000 0.0000410000 0.0009070000
Al -2.1989850000 -1.5795660000 0.0012850000

16
energy
Al 0.1997810000 2.1700250000 -1.3396760000
Al 1.6812850000 0.0020340000 1.7830440000
Al 2.4696040000 -1.7984700000 -0.0130080000
Al 2.4699450000 1.7984520000 -0.0172630000
Al 1.6556810000 -0.0021380000 -1.8183090000
Al 4.4346180000 -0.0001130000 -0.0612060000
Al 0.2304820000 2.1776330000 1.3949650000
Al 0.2302140000 -2.1744640000 1.4001600000
Al -3.8304280000 -0.0014310000 -1.4234330000
Al -4.0873450000 0.0012930000 1.2169880000
Al -1.8718420000 -1.3437670000 0.0628580000
Al -0.9924370000 -0.0025450000 -2.2950960000
Al 0.1996760000 -2.1734510000 -1.3349480000
Al -0.9572710000 0.0029040000 2.3786720000
Al -1.8717850000 1.3442000000 0.0601110000
B 0.1035380000 -0.0004180000 0.0159640000

25
energy
Al 0.9604300000 1.7627410000 -1.9121990000
Al 2.1892170000 2.2840140000 0.4022370000
Al -3.6312410000 -0.3456600000 0.8109970000
Al 1.1510350000 -2.1504180000 -1.8794720000
Al 2.2900950000 -2.2691350000 0.5777330000
Al -1.7778330000 -2.3437560000 -0.8012810000
Al -1.9553550000 1.6183560000 1.3924460000
Al -0.6304180000 -0.3697470000 -2.5729510000
Al -0.2772050000 3.4985950000 0.0357660000
Al -1.8047620000 1.7763360000 -1.4294740000
Al -1.6600860000 -1.1860690000 2.1193980000
Al -3.2561950000 -0.4114000000 -1.7996200000
Al 2.8839880000 -0.1114450000 -2.0503100000
Al 1.6365640000 0.0969990000 2.1242300000
Al 3.6367570000 -0.0040530000 0.4691870000
B 0.1939250000 -2.8145100000 -0.0429570000
B 0.0177270000 -1.0083050000 -0.0843320000
B 1.3818680000 -0.0406380000 -0.3693500000
B -0.0255820000 0.7835280000 0.1412220000
B -1.4652420000 -0.1353970000 -0.1348290000
B 0.2228720000 1.9608410000 1.5651720000
B 0.2072500000 -2.5693410000 1.5165570000
B -0.0319040000 -0.3417170000 3.4400310000
B -0.1597660000 1.1027350000 2.8543460000
B 0.2958710000 -1.7351240000 2.8487500000

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energy
Al 0.7665290000 -2.8203360000 -0.8649860000
Al -2.3083820000 -0.1780450000 -1.6003350000
Al -2.5835820000 -2.4767600000 0.2809120000
Al -2.2621810000 -0.3103960000 1.6357210000

Al	0.2201570000	2.5420930000	1.3187590000
Al	2.6069030000	0.7035530000	1.5424720000
Al	-0.4049020000	-2.4213740000	1.7645300000
Al	0.4949290000	-0.4453370000	-2.4934810000
Al	-1.5418760000	-2.6127610000	-2.1320970000
Al	1.6268400000	2.9808060000	-0.8529580000
Al	2.8047170000	-1.0300480000	-1.1001200000
Al	2.3827250000	-2.3374800000	1.3317380000
Al	3.6214710000	1.4352890000	-0.7396440000
Al	-0.4411470000	2.1248530000	-2.2183630000
Al	-3.3563930000	2.7067780000	0.3337250000
B	-0.4176030000	-0.4028740000	2.9027900000
B	1.0453640000	-0.7561400000	2.1551420000
B	1.4059350000	0.7295510000	-0.5389010000
B	-1.9465310000	1.9232080000	1.6826530000
B	-0.7273540000	-1.1549590000	-0.2746180000
B	-0.2628580000	0.5058430000	-0.4088620000
B	0.8469730000	-0.6776290000	0.2502650000
B	-0.9561340000	1.1160000000	2.7237990000
B	0.6524650000	0.7892400000	2.6190470000
B	-1.5038160000	1.5703690000	0.0819490000
B	-2.3635370000	1.9192200000	-1.3285400000

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energy

Al	1.2497380000	0.9368410000	-2.4546140000
Al	0.2408380000	2.8874770000	1.2298990000
Al	3.0342960000	1.9218320000	-0.3769990000
Al	2.2989300000	0.7926060000	1.7951340000
Al	0.2402180000	-1.7302740000	1.9965780000
Al	-2.1742130000	-0.5307970000	2.3628010000
Al	-1.5369190000	-2.4349970000	-0.1005040000
Al	2.6091600000	-0.6668700000	-0.6426060000
Al	-1.0542590000	1.8237300000	-1.2678690000
Al	1.0608580000	3.4268260000	-1.3544520000
Al	-3.6407440000	1.3977740000	-0.8762560000
Al	-2.0867860000	-0.5439930000	-2.1274530000
Al	0.2779820000	-1.5964590000	-2.4765970000
Al	1.9832460000	-3.3843220000	-1.5972060000
Al	-3.8480090000	-1.1018620000	0.2994350000
B	-1.3361680000	1.6212620000	2.2010340000
B	2.1538320000	-2.6014190000	0.3012520000
B	2.5255530000	-1.9331210000	1.6922460000
B	0.6113630000	-2.0757710000	-0.2369590000
B	-2.1125470000	1.3378970000	0.8024880000
B	-1.7428720000	-0.1207210000	0.0151650000
B	-0.2180330000	0.6848390000	2.8429640000
B	0.9075520000	0.9935790000	-0.0986740000
B	-0.4321350000	0.6502930000	0.9728920000
B	-0.0745630000	-0.4946570000	-0.2817530000
B	2.1280880000	-1.1176560000	2.9535890000
B	1.0886560000	-0.0580580000	3.3716040000

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energy

Al	2.6601320000	0.8568540000	0.1794210000
Al	-0.8427120000	-1.8693030000	1.6977310000
Al	1.9230700000	1.2299650000	2.5647110000
Al	-1.0111110000	0.9173130000	2.3846480000
Al	0.2205670000	1.0804050000	-2.3258690000
Al	-2.3137060000	0.0509520000	-2.0826780000
Al	-0.2835650000	-1.9281170000	-2.7694290000
Al	0.5297890000	2.6034880000	0.8508150000
Al	2.0411300000	-1.5347750000	1.4968630000
Al	0.6607520000	-0.8886530000	3.6964270000
Al	-2.1615770000	-3.6447820000	-0.0480490000
Al	-3.0129640000	1.4226240000	0.4206780000
Al	-3.1515760000	-1.1535640000	0.3403210000
Al	-2.1066830000	3.7920810000	-0.3491750000

Al	2.0157510000	-0.9191010000	-2.3113800000
B	1.2821830000	2.7911200000	-1.4735180000
B	3.5200480000	0.6523380000	-1.7746900000
B	-0.1325880000	-2.7026270000	-0.3851810000
B	2.9480580000	-1.9120470000	-0.5171890000
B	-1.2460230000	-1.4531170000	-0.6584610000
B	0.5371600000	0.1083820000	0.9485100000
B	-0.9478390000	0.1502240000	-0.0099390000
B	0.4080870000	-1.0047840000	-0.3481350000
B	-1.2481280000	1.6585880000	-0.8010680000
B	-0.2673400000	2.9781090000	-1.1128200000
B	2.4664810000	1.8505910000	-1.8344490000
B	3.8063230000	-0.7110690000	-1.0881740000
B	1.4386030000	-2.4457170000	-0.6819750000

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energy

Al	2.5828800000	-1.0125040000	1.0199330000
Al	-1.1970650000	-1.3001910000	-1.9106590000
Al	2.9782680000	-1.1737690000	-1.5068780000
Al	0.8237720000	0.4123210000	-2.7112430000
Al	0.3823090000	0.6226960000	2.4051290000
Al	-1.5826430000	2.1248780000	1.1693970000
Al	-2.0866750000	-0.6433290000	2.3998420000
Al	2.3655250000	1.2812280000	-0.7101640000
Al	0.9141130000	-2.9688490000	-0.2975070000
Al	1.0147910000	-2.2970700000	-2.9572680000
Al	-3.7549890000	-0.9302430000	-1.2160810000
Al	-0.2001440000	2.8460660000	-1.4479500000
Al	-3.8840510000	0.7781590000	0.9406560000
Al	-2.1804790000	1.2636440000	-1.6725750000
Al	1.6404920000	4.2109810000	-0.0440010000
B	2.4155360000	0.0560320000	2.9036880000
B	1.1640200000	-2.7364660000	2.6190470000
B	1.8382240000	-1.4107450000	3.0462250000
B	-2.0995720000	-1.6225190000	0.1442430000
B	-1.2473840000	-2.5808620000	1.1412450000
B	-1.7840020000	0.0493680000	0.1038970000
B	0.8752970000	-0.7141880000	-0.6362380000
B	-0.1741380000	0.6829650000	-0.2966540000
B	-0.4065660000	-0.9801030000	0.4736030000
B	-0.0503360000	-1.5834710000	2.0767290000
B	0.5195350000	2.0278900000	0.5677720000
B	2.5573270000	1.3232990000	2.0333690000
B	2.0860660000	2.4786020000	1.0364420000
B	-0.0158810000	-3.3462530000	1.7889880000

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energy

Al	2.9855700000	0.5037540000	-0.2519200000
Al	-0.9052400000	-1.7661040000	1.4260390000
Al	2.9432600000	-0.3133820000	2.1102630000
Al	0.3446890000	0.0675790000	2.8872050000
Al	0.4297790000	1.2636670000	-2.1115310000
Al	-2.1488620000	2.0225860000	-0.4228780000
Al	-1.7828470000	-0.4118450000	-2.5918020000
Al	1.4775900000	2.0465060000	1.6740520000
Al	1.9084640000	-2.3085930000	0.0164460000
Al	1.3866110000	-2.4492680000	2.6363840000
Al	-3.6486670000	-1.5909870000	1.1685370000
Al	-2.3414440000	0.7199960000	1.9734640000
Al	-2.1731610000	-2.4494540000	-0.8161440000
Al	-3.8379400000	0.0281630000	-1.0760030000
Al	-0.9847070000	4.4098390000	0.3140600000
B	0.9508420000	3.5529940000	0.3059800000
B	1.9388790000	-0.8185730000	-2.5486910000
B	2.5417220000	1.9372440000	-1.8763880000
B	-0.4065670000	-2.2568110000	-1.9169070000
B	1.1490360000	-2.4891210000	-2.3017710000

B	-1.7248970000	-0.2373470000	-0.1261810000
B	1.0276800000	-0.4409130000	0.6803140000
B	-0.3145850000	0.6265350000	0.3383170000
B	-0.0985930000	-0.8129230000	-0.6745970000
B	0.2949990000	-0.8086650000	-2.4092510000
B	3.5209820000	-0.9445770000	-2.1224980000
B	2.6955400000	-2.2928630000	-2.0436660000
B	0.0330690000	2.2368830000	-0.1608240000
B	3.0780650000	0.5458880000	-2.3981620000
B	1.8157780000	2.7938600000	-0.7797240000

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energy

Al	-2.8456430000	0.6406450000	-0.3627440000
Al	0.8402020000	-1.6491760000	1.9445330000
Al	-2.5271790000	0.8148240000	2.1428750000
Al	0.1551160000	0.9093140000	2.5400210000
Al	-0.4981160000	0.6541400000	-2.1645150000
Al	2.3699340000	0.9898080000	-1.5595830000
Al	1.2844790000	-1.7791310000	-2.5129740000
Al	-0.9586180000	2.6566540000	0.8959060000
Al	-1.9419450000	-2.0560200000	0.9618630000
Al	-1.3338500000	-1.2747410000	3.4711570000
Al	3.2311030000	-2.3872650000	0.9474800000
Al	1.9354900000	2.6891920000	0.9459240000
Al	2.7659660000	0.2705890000	1.3978180000
Al	0.6986130000	4.4789020000	-0.6690200000
Al	3.6877060000	-1.3441680000	-1.5402990000
B	-1.9837680000	2.2769440000	-1.9524540000
B	-2.3845520000	-1.6830650000	-1.8764560000
B	-2.8129860000	1.1093050000	-2.4685310000
B	1.2311880000	-2.3901720000	-0.1316700000
B	-0.1316070000	-2.8343360000	-0.9136420000
B	1.7081140000	-0.7748190000	-0.2540390000
B	-0.8951000000	-0.0912970000	0.7569790000
B	0.6376490000	0.5400340000	0.1034520000
B	-0.0703820000	-1.0428690000	-0.4481760000
B	-0.7334910000	-1.5581110000	-1.9873300000
B	-3.1946540000	-2.8160900000	-0.8463420000
B	-1.7142050000	-3.2303890000	-0.9915810000
B	0.6478210000	2.0062440000	-0.8635600000
B	-0.6874180000	2.9577540000	-1.2574180000
B	-3.9708470000	-1.5301790000	-1.3796780000
B	-3.4902310000	-0.3342280000	-2.2295050000

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energy

Al	-1.0789310000	2.3901400000	0.0021200000
Al	-3.6752660000	1.5538740000	0.0008610000
Al	-1.8254930000	-2.5330540000	-0.0010610000
Al	0.2510310000	-1.6315860000	1.4680360000
Al	-1.8998930000	-0.0417610000	1.4392740000
Al	-4.1133920000	-0.9846830000	-0.0001520000
Al	-1.9003920000	-0.0416080000	-1.4391860000
Al	0.2510680000	-1.6290450000	-1.4695420000
Al	2.4967550000	-0.3280900000	-2.0925340000
Al	2.5543510000	-2.1601150000	-0.0028110000
Al	3.6316230000	0.7077940000	0.0009330000
Al	0.3972330000	1.2501630000	2.1317200000
Al	2.4975800000	-0.3333950000	2.0918390000
Al	1.5933730000	2.4358320000	0.0007100000
Al	0.3950190000	1.2534150000	-2.1304670000
B	1.3544920000	0.0397040000	0.0004660000
B	-0.2486260000	0.1998060000	0.0002110000

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energy

Al	-3.7870490000	0.4300830000	0.2678400000
Al	2.1422280000	2.3579490000	0.1744970000
Al	-0.0034380000	3.8035860000	0.0017780000

Al	-2.9732790000	-1.4820060000	-1.1858090000
Al	0.1371860000	1.3120970000	-1.4345430000
Al	1.9882780000	-0.5870010000	-1.8746970000
Al	3.7863820000	0.4367670000	-0.2665850000
Al	1.2185760000	-2.6627340000	-0.3729140000
Al	-0.5779430000	-1.2034010000	-2.2427410000
Al	2.9778660000	-1.4788980000	1.1857480000
Al	-2.1470640000	2.3547290000	-0.1737210000
Al	-1.2143590000	-2.6642970000	0.3731830000
Al	-0.1406040000	1.3097360000	1.4308630000
Al	-1.9881420000	-0.5902760000	1.8770980000
Al	0.5802180000	-1.2032000000	2.2390130000
B	-1.4824150000	0.0900460000	-0.3396500000
B	1.4839870000	0.0900320000	0.3437120000
B	0.0014030000	-0.5262350000	-0.0014890000

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energy

Al	-1.2747700000	1.4951050000	-1.9220990000
Al	-3.5556150000	0.9575660000	-0.6108370000
Al	0.0016890000	3.2517820000	-0.1334070000
Al	1.4017210000	1.3240070000	-1.6156910000
Al	1.8469930000	1.8713190000	1.1170160000
Al	-1.8318780000	1.9434530000	1.1451800000
Al	0.0624600000	-0.9869780000	-1.9411810000
Al	-2.1147580000	-0.7887350000	1.9102860000
Al	0.2932120000	0.1783610000	2.3577830000
Al	-1.3968010000	-2.8014820000	-0.4613760000
Al	1.1203400000	-2.7796950000	0.2396000000
Al	2.8098730000	-1.5494620000	-1.3733000000
Al	-3.6084060000	-1.5119470000	-0.0766780000
Al	2.8729310000	-0.9387870000	1.6814300000
Al	3.6678650000	0.7102870000	-0.3414980000
B	-0.1663330000	0.6743720000	-0.0847990000
B	-1.5881300000	-0.3087880000	-0.3954850000
B	1.2635700000	-0.3413560000	0.0830930000
B	-0.2757300000	-0.9986940000	0.4615980000

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energy

Al	2.1954190000	-1.7498210000	-1.5217680000
Al	-0.3235060000	-2.7540460000	-1.4232880000
Al	2.1252020000	-1.5035680000	1.4827420000
Al	-2.6880920000	-1.4983630000	-1.4185680000
Al	-0.1421100000	-2.9130140000	1.4105650000
Al	-0.1557270000	0.0011140000	2.2167410000
Al	-2.4167140000	-1.4790500000	1.4849550000
Al	-2.6879450000	1.4954000000	-1.4197080000
Al	-0.0948010000	-0.0003380000	-2.1058140000
Al	3.8162990000	0.0005910000	-0.0776630000
Al	2.1916020000	1.7494630000	-1.5216870000
Al	-0.3262600000	2.7544300000	-1.4239100000
Al	-2.4159320000	1.4791420000	1.4843540000
Al	-0.1416070000	2.9141590000	1.4093180000
Al	2.1254510000	1.5045470000	1.4811230000
B	-1.3391000000	-0.0003980000	-0.0967190000
B	0.0821310000	-0.9070410000	0.0560250000
B	-3.0664880000	-0.0003800000	0.0692130000
B	1.4817800000	-0.0009740000	-0.2326240000
B	0.0823500000	0.9071140000	0.0548870000

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energy

Al	-2.6408700000	1.3446740000	-0.8340780000
Al	-2.6411510000	-1.3422880000	-0.8397180000
Al	-1.5841340000	3.7311960000	-0.5032440000
Al	-1.5828990000	-3.7269960000	-0.5007930000
Al	0.8689190000	-3.2567720000	-1.2012210000
Al	2.8230560000	-1.9159860000	-0.3238040000
Al	2.8242850000	1.9173120000	-0.3193900000

Al	4.5312280000	-0.0001640000	0.0475660000
Al	-4.6503550000	-0.0015320000	0.4749880000
Al	0.8694690000	3.2585630000	-1.1947000000
Al	0.0513420000	-0.0026990000	3.0597930000
Al	-2.1502470000	-0.0028070000	1.6249230000
Al	0.0793170000	-1.5374560000	0.8975130000
Al	0.0784090000	1.5328860000	0.8989880000
Al	2.3098850000	-0.0017530000	1.6875520000
B	-0.5868560000	1.6586250000	-1.3149920000
B	0.8729720000	0.8788970000	-1.3624490000
B	-0.5864820000	-1.6554390000	-1.3174110000
B	-0.6640750000	0.0015040000	-1.3731120000
B	0.8730730000	-0.8753390000	-1.3632640000
B	2.2071030000	0.0016880000	-1.0021440000

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energy

Al	2.2056520000	0.5499430000	1.1182460000
Al	-1.5080310000	-2.9268330000	-0.2601020000
Al	3.6658770000	1.9103000000	-0.8096420000
Al	0.1954500000	-1.3181070000	1.3350780000
Al	0.9628580000	-3.3819650000	-0.2430470000
Al	2.8947500000	-2.1909160000	1.1107120000
Al	2.1115140000	-0.9899440000	-1.2749900000
Al	-2.3783250000	-0.6113770000	1.2639860000
Al	-3.6926490000	-1.7575740000	-1.0265290000
Al	-3.0675520000	2.0027710000	0.2697020000
Al	-4.8112800000	0.1942600000	0.1858540000
Al	-0.3629800000	1.4123660000	1.4467210000
Al	-1.0526590000	3.5225030000	-0.1633020000
Al	1.5672320000	3.2712860000	0.0151820000
Al	4.5783450000	-0.6068210000	-0.1038900000
B	0.0569080000	-1.5155760000	-1.1546890000
B	1.5750580000	1.2166690000	-1.0456220000
B	-1.3428480000	-0.6865710000	-1.1253670000
B	-2.6923380000	0.2242310000	-0.9524010000
B	0.2492080000	0.1694590000	-1.0255730000
B	-1.3424920000	1.1373520000	-1.0299080000
B	0.0951700000	1.8467170000	-1.1127880000

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energy

Al	-2.1591130000	0.3898380000	-1.7061680000
Al	-3.6019520000	1.7402080000	0.2930500000
Al	-2.9139170000	-2.1382590000	-0.2916580000
Al	-4.6595740000	-0.2802490000	-0.8833050000
Al	1.0179790000	3.5460140000	0.8059860000
Al	-1.4387040000	3.1434060000	0.1490370000
Al	0.2507260000	1.3722880000	-1.1943310000
Al	-0.0002670000	0.0002860000	2.6979880000
Al	1.4389780000	-3.1422780000	0.1493230000
Al	-0.2513510000	-1.3728000000	-1.1953670000
Al	-1.0182720000	-3.5452720000	0.8065150000
Al	2.1588000000	-0.3902510000	-1.7056090000
Al	2.9134320000	2.1378820000	-0.2916740000
Al	3.6028600000	-1.7402480000	0.2928630000
Al	4.6596250000	0.2803490000	-0.8839960000
B	-2.7078660000	-0.1649280000	0.5766260000
B	-0.0909810000	1.6469900000	1.2917110000
B	-1.4727430000	0.8369950000	0.9774320000
B	-1.3553440000	-0.9666580000	0.9976540000
B	1.4736690000	-0.8379200000	0.9782960000
B	0.0913910000	-1.6468600000	1.2923430000
B	1.3554680000	0.9653540000	0.9979230000
B	2.7083540000	0.1646530000	0.5771120000

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energy

Al	1.8464040000	-2.8827040000	-0.1524600000
Al	0.2382080000	-1.3422170000	1.4745170000

Al	-4.4620870000	-0.2457510000	1.0639070000
Al	-0.6622180000	-3.3418210000	-0.2348240000
Al	-2.6436130000	-2.0426780000	0.7060940000
Al	-1.9886720000	0.5023310000	1.6570070000
Al	-3.5638540000	1.7824990000	-0.7034780000
Al	3.9070000000	-1.6367740000	-1.0939530000
Al	1.0948130000	3.3602080000	-0.4522570000
Al	0.6883990000	1.3665300000	1.4201390000
Al	2.8638650000	-0.4633240000	1.3936530000
Al	5.1318500000	0.3731640000	0.0199700000
Al	3.2321360000	2.0813150000	0.1143010000
Al	-1.3448290000	2.9370010000	0.1226930000
Al	-4.8040000000	-0.4444530000	-1.6215160000
B	0.2701320000	-1.6288450000	-1.2872110000
B	-1.2160810000	-1.0491480000	-0.9691950000
B	-2.6336720000	-0.2577050000	-0.6054920000
B	0.1049510000	-0.0012080000	-1.3605300000
B	-0.0221980000	1.6276950000	-1.2566070000
B	-1.3790420000	0.7698090000	-0.9233620000
B	1.6631040000	-0.7688990000	-1.1358400000
B	2.9341750000	0.2611860000	-1.0030220000
B	1.4917860000	1.0384680000	-1.1146010000

16

energy

Al	0.4735810000	-1.3253090000	2.2651290000
Al	-3.6703320000	1.2234030000	-0.0006140000
Al	-1.8796470000	-0.1502770000	-1.5274980000
Al	-1.8797520000	-0.1493930000	1.5272080000
Al	1.6145570000	-2.5309330000	0.0017060000
Al	-3.9560010000	-1.4693210000	0.0003190000
Al	-1.0157930000	-2.2810440000	0.0004430000
Al	0.4739970000	-1.3272510000	-2.2641070000
Al	0.1064920000	1.4728680000	2.2727980000
Al	-1.2000170000	2.2590120000	0.0003540000
Al	0.1055740000	1.4725000000	-2.2730700000
Al	2.5570300000	0.6054500000	-1.7876640000
Al	0.5443670000	0.0213050000	-0.0002100000
Al	3.6427940000	-0.9300970000	-0.0008980000
Al	2.5583250000	0.6062230000	1.7863100000
Al	1.5248240000	2.5028640000	-0.0002060000

17

energy

Al	1.3317830000	-2.2105620000	-0.0000600000
Al	-1.3314530000	-2.2098640000	0.0000500000
Al	2.0980560000	0.0010800000	1.4450090000
Al	4.0300230000	-1.3235940000	0.0019470000
Al	-4.0314030000	-1.3239090000	-0.0003110000
Al	2.0991450000	-0.0005150000	-1.4476370000
Al	-0.0000170000	-1.3598380000	2.1722170000
Al	0.0000230000	-1.3599900000	-2.1726870000
Al	-2.0990130000	0.0000170000	1.4451800000
Al	-0.0009390000	1.3582690000	2.1728960000
Al	1.3316100000	2.2094660000	0.0007430000
Al	-4.0307340000	1.3233060000	-0.0006700000
Al	-1.3318300000	2.2116610000	0.0011350000
Al	4.0318860000	1.3235770000	-0.0001940000
Al	-2.0977660000	0.0005050000	-1.4459160000
Al	0.0004020000	1.3605940000	-2.1717050000
B	0.0005890000	-0.0005240000	0.0000060000

26

energy

Al	2.7090590000	-1.3978360000	-0.9857630000
Al	-1.6199640000	-1.8307620000	-1.4242850000
Al	-0.0514640000	-3.6957860000	0.1175680000
Al	-1.2934860000	-1.8944530000	1.5581880000
Al	-1.2976040000	1.8917550000	1.5579020000
Al	1.6691420000	2.1630100000	1.5165270000

Al	1.6739900000	-2.1594990000	1.5167900000
Al	0.7348050000	0.0006840000	-2.3504860000
Al	0.7704340000	-2.7778530000	-2.2248780000
Al	-0.0603890000	3.6954960000	0.1173660000
Al	2.7059640000	1.4033150000	-0.9855060000
Al	3.5837580000	0.0036380000	1.2572060000
Al	-1.6230190000	1.8262520000	-1.4266590000
Al	0.7652490000	2.7795300000	-2.2243710000
Al	-4.3043840000	-0.0026750000	0.9070980000
Al	-3.5089420000	-0.0037730000	-1.5660150000
B	0.2875620000	-0.8121350000	2.7839160000
B	1.6030800000	0.0017080000	2.1679510000
B	0.3964170000	1.4092760000	-0.3214890000
B	-2.1752600000	-0.0027730000	0.2534390000
B	0.4001750000	-1.4085200000	-0.3220850000
B	-0.5546180000	-0.0009250000	-0.3169570000
B	1.1714110000	0.0012000000	0.2705030000
B	-1.1276280000	-0.0010000000	2.8332180000
B	0.2859650000	0.8128210000	2.7841690000
B	-2.5052900000	-0.0023660000	1.9295640000

27

energy

Al	1.3101400000	1.0513050000	-2.5436510000
Al	0.0935030000	2.8931090000	1.1016110000
Al	2.8120370000	2.2893060000	-0.4699900000
Al	2.3254590000	1.0461840000	1.6877160000
Al	0.6733180000	-1.7683310000	2.0176560000
Al	-1.7351670000	-0.7425910000	2.4515130000
Al	-1.1353260000	-2.6713840000	0.0798370000
Al	2.7535800000	-0.3784760000	-0.6963730000
Al	-1.1582690000	1.4145810000	-1.3777100000
Al	0.6268490000	3.4708510000	-1.5257730000
Al	-3.8796140000	0.7541470000	-1.3839700000
Al	-2.1101830000	-1.1463530000	-1.9848820000
Al	0.4380110000	-1.5768020000	-2.4185230000
Al	-3.5524140000	-1.5002180000	0.5395360000
Al	-2.8066700000	1.3488980000	0.9363980000
Al	2.4098500000	-3.1330270000	-1.6587370000
B	-1.2426390000	1.5454100000	2.2830130000
B	2.9068690000	-1.6236140000	1.5999390000
B	2.4540950000	-0.8303510000	2.8640650000
B	2.5606680000	-2.3578430000	0.2425990000
B	-1.6437980000	-0.3514600000	0.0642370000
B	-0.0354500000	0.8357640000	2.9849320000
B	0.8516500000	1.0422360000	-0.1570820000
B	-0.5157660000	0.7080570000	0.8617520000
B	0.0558560000	-0.5331390000	-0.2077230000
B	1.3136400000	0.0868290000	3.3378990000
B	0.9256080000	-2.0350030000	-0.2357380000

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energy

Al	-0.5085230000	1.5957550000	2.4696980000
Al	-1.5960770000	-2.2939680000	1.1937390000
Al	-2.7462770000	-0.5531280000	-0.6287120000
Al	-0.2095310000	0.2784520000	-2.5627920000
Al	1.6432180000	-1.8300560000	-1.9820220000
Al	2.1871100000	1.1110730000	-1.5655190000
Al	-1.9644190000	-3.5331890000	-1.5375240000
Al	-1.8585190000	2.1300000000	0.1248070000
Al	0.8543400000	-0.8184930000	2.2575870000
Al	-1.4928210000	-0.7359890000	3.4150590000
Al	3.1535150000	-1.9334740000	1.5551380000
Al	3.8781290000	-0.8484150000	-0.8826380000
Al	2.7667940000	0.8733690000	1.2751960000
Al	1.1861610000	2.8983010000	0.7870440000
Al	-0.0103460000	4.2932210000	-1.1280670000
Al	-3.1186260000	0.4954090000	1.7157840000

B	-0.0081300000	-2.7933420000	-0.5392010000
B	-2.0787710000	1.5363260000	-2.4511860000
B	-2.4175580000	0.0487440000	-2.7810340000
B	-1.1013430000	2.6248510000	-1.8384300000
B	1.2234200000	-2.1853890000	0.3629690000
B	1.6683550000	-0.5557020000	0.0229770000
B	-0.5423060000	-1.7785580000	-1.7442610000
B	-1.0185770000	-0.0188070000	0.8521080000
B	-0.0330130000	-1.0180900000	-0.2132580000
B	0.4372200000	0.6657770000	0.0915180000
B	-1.9879740000	-1.4267030000	-2.4670120000
B	0.2319460000	1.9658330000	-1.0128080000

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energy

Al	2.5909520000	-1.3141060000	-0.3178230000
Al	-0.3817620000	1.2134540000	2.1730660000
Al	1.7665210000	-2.4243860000	1.9190920000
Al	-0.9885240000	-1.5613820000	2.2972140000
Al	0.3833050000	-0.4478300000	-2.4986540000
Al	-2.0608980000	0.5716660000	-1.9417020000
Al	0.3140450000	2.3885120000	-2.0414670000
Al	0.0935050000	-2.7719300000	-0.0259000000
Al	2.4756040000	0.6153650000	1.6223590000
Al	1.0744360000	-0.4542520000	3.6274810000
Al	-1.2082840000	3.6339120000	1.3455750000
Al	-3.1227040000	-1.0545430000	0.6535160000
Al	-2.1339570000	3.1834550000	-1.2953330000
Al	-2.7862910000	1.4421310000	0.9447370000
Al	-3.2390120000	-3.1315150000	-0.8439090000
Al	3.9637970000	1.5825320000	-0.7133040000
B	0.0960120000	-2.9297430000	-2.2922100000
B	3.2143730000	0.0526380000	-1.9886070000
B	1.5083630000	-2.3390890000	-2.5202400000
B	0.4491610000	2.4728010000	0.3919480000
B	1.8837620000	2.1672530000	-0.2903960000
B	-0.8765280000	1.5109390000	-0.1483190000
B	0.6489960000	-0.6528740000	0.8958780000
B	-0.8122180000	-0.2152700000	0.0096870000
B	0.7338090000	0.7244510000	-0.1583800000
B	1.9178730000	0.9775330000	-1.4833340000
B	-1.6185170000	-1.3883790000	-0.9746770000
B	-1.3446710000	-2.8900010000	-1.6633950000
B	2.6736830000	-1.3150730000	-2.5308250000

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energy

Al	-3.2235910000	-0.1535520000	0.2739590000
Al	0.9473970000	-1.3508420000	2.1336820000
Al	-2.5578590000	1.4016090000	2.2112300000
Al	0.1613060000	1.2772670000	2.5469260000
Al	-0.1517950000	0.8353120000	-2.3668670000
Al	2.4832990000	0.7746230000	-1.5563270000
Al	1.1500020000	-1.7740220000	-2.2865320000
Al	-1.3552330000	2.2917920000	0.1491070000
Al	-1.4941450000	-2.1368670000	1.1566600000
Al	-1.3235750000	-0.7629350000	3.4367750000
Al	2.6578890000	-2.9467640000	0.8575000000
Al	2.1697170000	2.2760960000	1.1984890000
Al	3.6022020000	-1.5597390000	-1.3943500000
Al	3.1136620000	-0.1634830000	1.0470090000
Al	1.4638600000	4.2707920000	-0.4844290000
Al	-2.7500370000	-2.6246110000	-1.1925220000
B	-2.4777870000	1.4613350000	-2.2507960000
B	-2.2846530000	-0.2953870000	-2.2593390000
B	-3.7164440000	0.5216600000	-2.0496060000
B	0.6116300000	-2.4499290000	-0.0063600000
B	-0.6311050000	-2.5764770000	-1.0599200000
B	1.5212700000	-1.0015830000	-0.1609960000

B	-0.9391690000	0.0861890000	0.8881730000
B	0.6815560000	0.5207790000	0.2413460000
B	-0.2641190000	-0.8813060000	-0.4088060000
B	-0.8975100000	-1.1871270000	-2.0353740000
B	0.9579450000	1.9768000000	-0.6487210000
B	-1.3876100000	2.5988640000	-2.0886080000
B	-3.8199520000	-0.9680760000	-1.6392860000
B	-0.0761180000	3.0920970000	-1.4205180000

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energy

Al	3.0471450000	0.0430770000	-0.2541750000
Al	-1.1465950000	-1.2912940000	1.8222410000
Al	2.6504010000	0.1831280000	2.2234940000
Al	0.0855030000	0.9662480000	2.6183260000
Al	0.8063070000	0.5544460000	-2.1197000000
Al	-1.9517310000	1.5588540000	-1.5971850000
Al	-1.4494350000	-1.2879890000	-2.5931580000
Al	1.5526750000	2.3806890000	0.9378810000
Al	1.4129830000	-2.4180500000	0.9957160000
Al	0.9526930000	-1.5390220000	3.5182490000
Al	-3.9248030000	-1.0726420000	1.0595920000
Al	-1.2070810000	3.2665220000	0.8402480000
Al	-3.7360470000	-0.3797940000	-1.6378510000
Al	-2.4971290000	1.0934480000	1.3460620000
Al	-2.2960430000	-2.5405950000	-0.2263150000
Al	0.4870500000	4.5856670000	-0.7581340000
B	2.6019690000	1.8008600000	-1.8695420000
B	2.0989660000	-2.1185360000	-1.7854760000
B	3.1640100000	0.4804980000	-2.3658920000
B	-0.3907550000	-2.8237420000	-1.0169010000
B	1.0855710000	-3.5071260000	-1.0033350000
B	-1.7827970000	-0.3135580000	-0.2807850000
B	0.8890240000	-0.2510350000	0.7740260000
B	-0.4252640000	0.6839320000	0.0768700000
B	-0.1420990000	-1.0300820000	-0.4269820000
B	0.5037520000	-1.6563790000	-1.9472440000
B	3.6658970000	-2.3403380000	-1.2439520000
B	2.6063740000	-3.4205210000	-0.7598320000
B	-0.0753600000	2.1508890000	-0.8856780000
B	1.4682980000	2.7499910000	-1.2138200000
B	3.4890900000	-1.0718490000	-2.1072150000

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energy

Al	-1.6554190000	-2.2606220000	1.9788630000
Al	-0.8736840000	0.4048870000	2.5238520000
Al	-2.6698390000	1.2951950000	-1.3213770000
Al	0.7366270000	2.3480170000	1.2424860000
Al	0.5963440000	-1.8744580000	3.2134610000
Al	-2.8784710000	-2.8971340000	-0.1178910000
Al	-2.1551440000	2.6013470000	1.3265010000
Al	-3.4639180000	-1.1350760000	-2.0387910000
Al	-3.0865390000	-0.1185060000	0.9192010000
Al	1.7909040000	0.4615280000	2.9397420000
Al	-0.5966010000	4.4369420000	-0.0118130000
Al	2.8309360000	0.5860290000	0.6443080000
Al	-0.1082900000	1.0682190000	-2.3396660000
Al	1.4608630000	-2.2011760000	0.7629370000
Al	4.3217420000	-2.0038200000	-0.5293370000
Al	-0.9342160000	-1.4005030000	-2.8149960000
B	-1.6198770000	-0.8741040000	-0.5850060000
B	0.6875280000	-0.0492290000	0.8920360000
B	-0.8263010000	0.5212730000	0.1446530000
B	0.6201910000	2.8155240000	-1.1335400000
B	-0.8376370000	2.1782560000	-0.5247650000
B	2.2393020000	0.4951910000	-2.1805370000
B	2.1435170000	2.5629660000	-0.4898260000
B	-0.7933040000	-2.3686930000	-0.5567580000

B	0.5917960000	-2.4590490000	-1.4131110000
B	0.1191380000	-0.7886730000	-0.5486550000
B	1.1607370000	-0.8400100000	-2.0447910000
B	2.8993050000	-1.0136370000	-1.9890450000
B	2.1981320000	-2.3250720000	-1.3913520000
B	3.2275010000	1.6531470000	-1.2765880000
B	3.8059060000	0.1763600000	-1.4367620000
B	1.7643030000	2.1074930000	-2.0473980000

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energy

Al	1.8910320000	-0.2126010000	1.4365600000
Al	3.7234980000	-1.7290270000	0.0001490000
Al	4.0480380000	0.7862720000	-0.0000310000
Al	1.8901450000	2.3803610000	0.0003810000
Al	1.1953680000	-2.6299360000	-0.0010110000
Al	-0.2370180000	1.2896490000	-1.4859810000
Al	-2.6535870000	0.1887380000	1.8462810000
Al	-0.4635150000	-1.3762900000	2.2123090000
Al	-3.5410960000	-1.4073710000	-0.0000650000
Al	-0.2374660000	1.2898470000	1.4851120000
Al	-0.2537690000	3.8576750000	0.0003180000
Al	-2.3240640000	2.2076150000	-0.0006150000
Al	-1.3934710000	-2.8701670000	0.0013060000
Al	-2.6535580000	0.1887020000	-1.8463640000
Al	1.8909960000	-0.2127490000	-1.4368460000
Al	-0.4641530000	-1.3772430000	-2.2115110000
B	0.2578380000	-0.5436800000	0.0000870000
B	-1.3430250000	-0.4273590000	-0.0000630000

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energy

Al	-3.7799950000	0.7714230000	0.4003480000
Al	2.3315380000	2.1487480000	-0.2792230000
Al	0.2818590000	3.7500180000	-0.5619720000
Al	-3.4574330000	-1.3493060000	-0.9345620000
Al	0.0985300000	1.0506640000	-1.6416560000
Al	1.4697870000	-1.2005420000	-2.2897040000
Al	3.4807490000	-0.0817270000	-0.9969790000
Al	-1.1691020000	-1.4019820000	-2.1655420000
Al	-1.9919480000	2.4769210000	-0.3875670000
Al	0.6374630000	-2.7848910000	-0.1920840000
Al	0.4718790000	-1.0925300000	2.1275940000
Al	-1.7186430000	-2.2825530000	0.8199170000
Al	2.8703660000	-1.8693300000	0.8230780000
Al	2.6356750000	0.5657560000	1.9798090000
Al	0.0693150000	1.4490540000	1.1720740000
Al	-1.9988390000	0.1461870000	2.2479300000
B	-1.6990050000	0.0870570000	-0.2308260000
B	-0.2520400000	-0.5843430000	-0.0607000000
B	1.3499230000	-0.2720780000	-0.0242710000

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energy

Al	2.2360130000	-1.5480940000	1.4919510000
Al	-2.2381420000	-1.5484180000	1.4901590000
Al	3.8450240000	0.0029820000	0.0103420000
Al	2.3477800000	-1.6258520000	-1.4965810000
Al	0.0051890000	-2.8581220000	-1.4386270000
Al	-2.3392610000	-1.6309960000	-1.4977520000
Al	-0.0009990000	-2.9567200000	1.4092660000
Al	0.0008950000	-0.0004350000	-2.1116080000
Al	2.3420690000	1.6295680000	-1.4958560000
Al	-3.8437180000	-0.0025780000	0.0034740000
Al	-0.0020120000	0.0002170000	2.2269430000
Al	-0.0045020000	2.9572110000	1.4087500000
Al	-2.3434650000	1.6263640000	-1.4988990000
Al	-2.2400720000	1.5456270000	1.4901370000
Al	2.2334390000	1.5508850000	1.4911480000
Al	-0.0017570000	2.8584510000	-1.4384270000

B	1.4329780000	-0.0005450000	-0.1052960000
B	0.0020630000	-0.9061130000	0.0480170000
B	-1.4286270000	0.0000410000	-0.1058690000
B	0.0027370000	0.9063830000	0.0476570000

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energy

Al	-3.5513910000	-1.9779150000	-0.9611340000
Al	-2.0852760000	-1.3421830000	1.4302320000
Al	1.6441020000	-2.2924290000	-1.3180470000
Al	0.1516170000	0.1507830000	2.2064680000
Al	0.2782590000	-2.6479640000	1.3433420000
Al	-1.0049700000	-2.6123660000	-1.2111930000
Al	2.6161580000	-1.4760540000	1.6786970000
Al	3.7932080000	-0.9886430000	-0.5797850000
Al	2.8786160000	1.3885860000	-1.1734930000
Al	-0.2234040000	2.8188870000	1.1423080000
Al	0.3112540000	0.0465630000	-2.1633650000
Al	0.8147050000	2.9324740000	-1.5467710000
Al	2.3561060000	1.5479280000	1.4756070000
Al	-1.7306840000	2.0981740000	-1.6464200000
Al	-2.4959920000	1.6613550000	1.8716220000
Al	-3.4840370000	0.5933880000	-0.3320190000
B	-1.6199310000	-0.5394600000	-0.7938150000
B	-0.1221330000	-0.6681790000	-0.0135820000
B	1.5567730000	-0.3412540000	-0.0473330000
B	0.5959770000	1.0383510000	0.0479890000
B	-1.1081940000	0.7690210000	0.2450160000

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energy

Al	-0.8627790000	-0.6834230000	2.2241900000
Al	-3.0514950000	0.0006530000	1.0319850000
Al	-2.8723620000	-2.6803870000	0.8208500000
Al	2.8252250000	1.5045190000	-1.2640550000
Al	1.8157310000	1.6374530000	1.5131210000
Al	0.8536110000	3.2328240000	-0.5238300000
Al	-0.9830190000	2.1679060000	1.4806630000
Al	-1.7278030000	4.0254700000	-0.4963870000
Al	-2.8512560000	1.6731090000	-1.0717360000
Al	1.6493680000	-1.3035920000	1.7995970000
Al	-0.2139380000	-2.9960850000	0.8061040000
Al	3.7615290000	-0.0629520000	1.0833650000
Al	-2.9141400000	-0.9604930000	-1.6820270000
Al	1.7186480000	-2.4340070000	-1.1691270000
Al	3.8240980000	-0.8745020000	-1.4041600000
Al	-0.8194480000	-2.5259960000	-2.1218340000
B	-1.3068080000	-1.2667750000	-0.0885480000
B	0.6093310000	0.9166950000	-0.6606470000
B	0.2807290000	-0.8466740000	-0.1861710000
B	-1.0602260000	0.3048990000	-0.5130510000
B	1.7868080000	-0.2147800000	-0.3164220000
B	-0.7049570000	1.8333460000	-0.9046350000

23

energy

Al	0.9008640000	-3.2739890000	-0.5709670000
Al	-1.5793020000	-2.9925160000	-0.3505140000
Al	-3.8543470000	-1.9306900000	-0.8091890000
Al	1.7690280000	-0.8419770000	-1.6811990000
Al	-5.1247480000	-0.1560910000	0.6116880000
Al	4.2344330000	-0.2368220000	-0.7666970000
Al	2.7514520000	-2.1312780000	0.8700800000
Al	0.1089980000	-1.2533710000	1.0649390000
Al	-2.4471640000	-0.5162570000	1.4220320000
Al	-3.5978390000	1.8331350000	0.3291520000
Al	2.2676740000	0.6766030000	1.1163140000
Al	1.0069260000	3.5430110000	-0.5189440000
Al	-0.1986160000	1.4916190000	1.5013400000
Al	-1.5605340000	3.3622850000	0.0808460000

Al	4.6650070000	-0.4576740000	1.8320420000
Al	3.0681280000	2.0627020000	-1.3578830000
B	-0.2364920000	-1.4737260000	-1.3743520000
B	-1.6937810000	-0.7569130000	-1.1237030000
B	-0.1732940000	0.1763870000	-1.1479700000
B	-1.7896630000	1.0380420000	-0.9308080000
B	-3.0797020000	0.0767050000	-0.8425240000
B	1.0931910000	1.2325300000	-0.7938120000
B	-0.3861580000	1.8423860000	-0.9967300000

24

energy

Al	-0.7558890000	-3.3700170000	0.3090380000
Al	0.0875740000	-0.9372650000	1.0532190000
Al	2.7643650000	-0.3635350000	1.4919120000
Al	5.2213210000	0.1476320000	0.2187050000
Al	1.7464630000	-2.9385940000	0.1176230000
Al	3.9200420000	-1.8910100000	-0.7497170000
Al	1.3793690000	3.3434350000	-0.6757430000
Al	3.4311960000	1.9736340000	-0.0756060000
Al	-1.9003600000	0.9871160000	1.4694290000
Al	-3.5995200000	2.1635440000	-0.6763140000
Al	0.8084050000	1.6717460000	1.3958380000
Al	-1.1100910000	3.1676230000	-0.1575890000
Al	-2.5790800000	-1.6012030000	1.2228290000
Al	-4.5694430000	0.2646520000	1.0104260000
Al	-1.7120480000	-1.4663950000	-1.5665370000
Al	-4.2904950000	-1.4032240000	-1.1215560000
B	0.3091220000	-1.7250860000	-1.2163150000
B	1.7402940000	-0.9341270000	-1.2251320000
B	0.1670570000	-0.0924970000	-1.2967490000
B	0.1332570000	1.5574310000	-1.2010800000
B	3.0281250000	0.0372030000	-0.9612250000
B	1.6274640000	0.8775980000	-1.0946830000
B	-1.2750050000	0.8067720000	-0.9340450000
B	-2.7190170000	0.1275430000	-0.5622600000

25

energy

Al	-1.0789290000	-3.3046120000	-0.3868290000
Al	0.4596620000	-1.2058660000	1.3791070000
Al	3.0210850000	-0.4593090000	1.4982930000
Al	5.2333230000	-0.0362940000	-0.0166810000
Al	1.5760100000	-3.1454330000	-0.1717390000
Al	3.8099640000	-2.0011410000	-0.8923240000
Al	1.5708250000	3.4165950000	-0.8474620000
Al	3.5838540000	1.9517860000	-0.1806790000
Al	-1.5386210000	0.9099110000	1.6331790000
Al	-3.1989570000	2.2080190000	-0.3989380000
Al	1.1483280000	1.5602500000	1.3056150000
Al	-0.8120340000	3.1787810000	0.1826520000
Al	-2.1439570000	-1.6822930000	1.5140950000
Al	-4.0906160000	0.0421720000	1.2449990000
Al	-4.9153230000	0.4090600000	-1.3219360000
Al	-3.4812300000	-1.9142420000	-0.9974580000
B	-1.1892950000	-0.8786260000	-0.8938170000
B	0.2142240000	-1.6119530000	-1.2278200000
B	1.6773670000	-0.9006840000	-1.0752370000
B	0.2040690000	0.0209580000	-1.4066950000
B	0.2426390000	1.6590090000	-1.2733600000
B	3.0396500000	-0.0073730000	-0.9192990000
B	1.6915360000	0.9059460000	-1.0930700000
B	-1.1706980000	0.9564590000	-0.8930600000
B	-2.4822920000	0.0450660000	-0.4317700000

2

energy

Al	0.0000000000	0.0000000000	1.5271450000
Al	0.0000000000	0.0000000000	-1.5271450000

3

energy
Al -0.4966620000 -1.2057820000 0.0000000000
Al 0.0000000000 1.3040610000 0.0000000000
B 1.2913210000 -0.2555270000 0.0000000000

12
energy
Al -1.5112670000 1.4630830000 0.0004500000
Al -2.6125390000 -0.8151000000 0.0006810000
B 1.7001820000 2.1734950000 0.0003360000
B 0.6010140000 0.8925700000 -0.0010590000
B -0.3641060000 -0.5001870000 -0.0006070000
B 0.5553070000 -2.1869960000 -0.0001470000
B 1.3779390000 -0.6007140000 -0.0001430000
B 2.1636260000 -2.0282060000 0.0006170000
B 3.0040970000 -0.7365970000 -0.0001260000
B -1.0029940000 -1.9930350000 -0.0011240000
B 2.4813010000 0.7757430000 -0.0000210000
B 0.2055300000 2.5191700000 -0.0006650000

13
energy
Al 1.0433570000 2.3154540000 0.2286790000
Al 3.4507500000 -0.8267800000 -0.2106660000
B -2.6640480000 -1.2805510000 -0.0741310000
B -1.6994690000 0.3074610000 -0.4196670000
B -3.3283940000 0.1858080000 -0.0707730000
B -2.6388250000 1.5805270000 -0.0502940000
B -1.0543350000 1.8380430000 -0.0088450000
B -0.1305000000 -2.4388630000 0.4088860000
B -0.8783310000 -1.1057430000 -0.1402010000
B 0.8024030000 -1.1273810000 0.2930200000
B -0.0160060000 0.4179250000 -0.1465200000
B -1.6691130000 -2.5068420000 0.1788420000
B 1.5919420000 0.2590650000 -0.0171520000

14
energy
Al 1.4124850000 1.8375680000 -0.0343140000
Al -1.6602830000 -0.2876500000 1.6008330000
B 0.1186430000 -0.1013140000 -0.2474620000
B -3.0367740000 0.2080570000 -0.7263350000
B -1.3494730000 0.1315580000 -0.9699230000
B -2.4107130000 -1.2073510000 -0.7807120000
B -0.8616830000 -1.5428300000 -0.6811600000
B -0.6207620000 1.4612580000 -0.1092710000
B -2.1963830000 1.4589830000 -0.3403330000
B 0.6645650000 -1.7999980000 -0.2540280000
B 2.2137000000 -1.9902140000 0.1119830000
B 3.3095450000 -0.8804900000 0.1431560000
B 1.7684410000 -0.3999690000 -0.2979680000
B 3.0451680000 0.6325230000 0.0791030000

15
energy
Al -1.5980660000 1.5999230000 -0.0055350000
Al 1.6025060000 1.6001960000 -0.0033050000
B 0.8193410000 -0.7068230000 -1.5651930000
B 2.3745650000 -0.4335910000 -1.3737250000
B 3.1279980000 -0.3950890000 0.0000660000
B 2.3754660000 -0.4253440000 1.3746210000
B 1.6041610000 -1.0719430000 0.0026150000
B 0.8203270000 -0.6972540000 1.5686670000
B -0.0010910000 -0.8718700000 0.0024230000
B -0.8211850000 -0.6963340000 1.5689940000
B -3.1294260000 -0.3912190000 0.0019580000
B -0.8222070000 -0.7063290000 -1.5646600000
B -2.3761190000 -0.4226120000 1.3759890000
B -1.6064320000 -1.0707580000 0.0035410000
B -2.3769420000 -0.4311430000 -1.3723100000

16

energy
Al -1.8392190000 -0.3671890000 1.3229830000
Al 1.9497900000 -0.4858930000 -1.3159660000
B -0.5941550000 0.7962980000 -0.8691030000
B -0.9310960000 2.3879520000 -0.3271030000
B -0.5145770000 -2.2186360000 -0.1815830000
B -2.1325830000 1.4754030000 -0.7337340000
B -2.1527700000 -0.0920610000 -1.0203580000
B -0.4856760000 -0.7967320000 -1.1496900000
B -1.8691370000 -1.6146070000 -0.6655430000
B 2.0668360000 -1.1671660000 0.9391350000
B 2.0991220000 0.4137150000 0.9879390000
B 0.5395610000 -0.5159370000 1.1397600000
B 0.3912790000 1.0443790000 0.6104540000
B 0.5699390000 2.6628220000 0.1046600000
B 1.8402270000 1.9283430000 0.6029510000
B 0.8855450000 -2.0857610000 0.5439720000

17

energy
Al 3.7367740000 0.3360730000 0.7138980000
Al 1.9563190000 -1.9881450000 -0.1189380000
B -1.0272720000 0.7281180000 -0.4809220000
B -1.3818370000 -0.9571540000 -0.5123080000
B 0.5690120000 1.1015080000 -0.2066130000
B -0.2780320000 -2.1026550000 -0.0620520000
B 1.8141930000 0.0685270000 -0.6079730000
B -1.8022350000 -2.4135100000 0.1795000000
B -3.0840400000 -1.4896380000 0.2807480000
B -0.6181560000 2.3791670000 -0.1558590000
B 0.9507990000 2.7095740000 -0.2429740000
B -2.1517170000 1.8928150000 0.1687470000
B -2.5356550000 0.2113870000 -0.0339060000
B -4.0121510000 -0.2086390000 0.5116180000
B 2.1095070000 1.6471030000 -0.3246600000
B 0.2693710000 -0.5584640000 -0.5674650000
B -3.6238270000 1.2872470000 0.5072260000

18

energy
Al 3.2444650000 -1.6735200000 -0.9576950000
Al -3.2386680000 -1.6733200000 -0.9606520000
B 1.6260540000 -1.6311060000 0.7988560000
B 1.6475280000 1.2158880000 0.4384470000
B 0.8424270000 -0.1879260000 1.0657340000
B 2.4775500000 -0.3014940000 0.6823060000
B 3.1384680000 0.8710980000 -0.2068760000
B 2.3902210000 2.1612310000 -0.6607540000
B 0.8338140000 2.4476740000 -0.4065770000
B -0.8416690000 -0.1897160000 1.0671670000
B -2.4770310000 -0.3079480000 0.6863990000
B 0.0023760000 -1.7194370000 0.9318660000
B -1.6215090000 -1.6352060000 0.7995370000
B -0.0019070000 1.3071390000 0.6227720000
B -1.6513670000 1.2112030000 0.4396740000
B -2.3971120000 2.1539020000 -0.6595780000
B -3.1413440000 0.8613360000 -0.2052390000
B -0.8415700000 2.4451440000 -0.4060300000

4

energy
Al 1.7680460000 -0.2948780000 0.0000040000
Al -1.7682030000 -0.2947840000 0.0000250000
B 0.0002690000 0.7666170000 0.7373880000
B 0.0001390000 0.7665060000 -0.7374650000

5

energy
Al 1.7298050000 -0.0761710000 0.0000000000
Al -0.6110410000 -1.2866540000 -0.0000000000
B -1.6375010000 0.4706820000 -0.0000000000

B	-1.2712840000	1.9559660000	0.0000000000
B	0.0000000000	1.1166970000	0.0000000000

6

energy			
Al	2.1062880000	-0.8454200000	-0.0001460000
Al	-2.1058980000	-0.8459020000	-0.0000990000
B	-0.8559600000	1.1210780000	0.0000830000
B	-0.0005950000	2.4195560000	-0.0003770000
B	0.8553560000	1.1215250000	0.0003810000
B	0.0001850000	-0.2647190000	0.0005490000

7

energy			
Al	1.7318960000	-0.4301080000	0.0001240000
Al	-1.1779070000	-1.2008130000	0.0003670000
B	-1.1191800000	1.0665790000	0.7788310000
B	-1.1198460000	1.0649280000	-0.7788110000
B	0.2272460000	0.3414090000	-1.2718650000
B	0.3437920000	1.4249390000	-0.0009370000
B	0.2276170000	0.3425370000	1.2715050000

8

energy			
Al	2.2689740000	0.1187630000	-0.0000090000
Al	-1.1691440000	1.3937030000	0.0000330000
B	-0.0482950000	-1.2981790000	-0.0000990000
B	0.5007890000	-0.0537670000	1.0299520000
B	-1.7835180000	-1.2528000000	0.0000420000
B	-1.0145510000	-0.6370320000	1.2142330000
B	-1.0146830000	-0.6369710000	-1.2142160000
B	0.5007010000	-0.0536620000	-1.0299750000

9

energy			
Al	0.0001700000	0.0000030000	1.2934620000
Al	-0.0001700000	0.0000070000	-1.2931360000
B	1.6599600000	0.7507210000	-0.0002640000
B	1.6218920000	-0.8297290000	-0.0002640000
B	0.3624770000	-1.7851180000	-0.0001880000
B	-1.1697550000	-1.3964950000	-0.0000080000
B	0.4479630000	1.7655990000	-0.0001920000
B	-1.1011920000	1.4511500000	-0.0000130000
B	-1.8213440000	0.0438450000	0.0000810000

10

energy			
Al	-2.3254280000	-0.5510180000	0.0017230000
Al	2.3295910000	-0.5433400000	-0.0017400000
B	-0.0000140000	0.4030190000	0.0000350000
B	-0.0021530000	1.4377280000	1.4134720000
B	0.0045500000	-1.2686100000	0.7476220000
B	0.0034270000	-0.0770230000	1.7277820000
B	0.0023650000	-1.2443540000	-0.7973420000
B	-0.0082310000	1.4812520000	-1.3790370000
B	-0.0031180000	-0.0231870000	-1.7403370000
B	-0.0076480000	2.1365060000	0.0278500000

11

energy			
Al	-0.6954730000	0.3337510000	1.6464350000
Al	2.4179070000	-0.6507830000	0.0881280000
B	-0.9101250000	-0.3811760000	-0.8701800000
B	-1.0549690000	-1.9173410000	-0.2043070000
B	0.6108610000	0.2540050000	-0.7435890000
B	0.4108590000	-1.3768780000	-0.4057950000
B	-1.0663080000	1.4463260000	-0.7235640000
B	0.4169300000	1.9735540000	-0.5217000000
B	1.7757480000	1.3058910000	-0.2289850000
B	-2.3417130000	-1.0131170000	-0.2813220000
B	-2.3196110000	0.5330200000	-0.5304210000

3

energy

Al	-0.0000000000	-1.4648710000	0.0000000000
Al	-1.2686210000	0.7324380000	0.0000000000
Al	1.2686210000	0.7324320000	0.0000000000

4

energy

Al	1.2787390000	-1.2906740000	-0.0000030000
Al	-2.4519050000	-0.0003140000	-0.0000050000
Al	1.2776600000	1.2911320000	-0.0000030000
B	-0.2716850000	-0.0003760000	0.0000300000

13

energy

Al	0.9354260000	-2.4086700000	-0.2622090000
Al	3.6303100000	0.4187410000	0.1895140000
Al	-1.6538660000	-2.0247080000	0.1987150000
B	-2.0661110000	2.1587730000	-0.0626610000
B	-0.7762160000	3.0882990000	-0.0812310000
B	-3.0626980000	-0.5569980000	0.1214770000
B	-1.6108710000	0.2241730000	-0.0330770000
B	-3.1370850000	0.9669960000	0.0211380000
B	-0.4611240000	1.4857120000	-0.1079140000
B	0.0228680000	-0.1999610000	-0.0419280000
B	0.6997770000	2.6309970000	-0.0637660000
B	1.2115340000	1.0962320000	-0.0503770000
B	1.6090640000	-0.4561650000	-0.0293120000

14

energy

Al	3.4271710000	-0.5914170000	0.1954620000
Al	-2.0500360000	0.0815210000	1.6212420000
Al	1.1394990000	-1.5986640000	-0.2169100000
B	-2.4611070000	-1.5526730000	-0.4240990000
B	-1.6850960000	-0.1303600000	-0.9425490000
B	-0.2369990000	0.1849390000	-0.1577830000
B	-0.8862370000	-1.4833230000	-0.2008930000
B	1.7256500000	2.2851550000	-0.0128370000
B	1.4400750000	0.6157310000	-0.2184690000
B	0.2010220000	1.9450050000	-0.2732070000
B	2.9142580000	1.3370760000	0.0027990000
B	-1.3252670000	1.5237670000	-0.5337510000
B	-3.3818440000	-0.3488790000	-0.7263800000
B	-2.8477020000	1.1058160000	-0.6722970000

15

energy

Al	-1.8807520000	-0.0007920000	1.2363040000
Al	0.6924070000	0.0000870000	1.3361960000
Al	1.5668410000	-0.0001940000	-1.3557740000
B	-0.4770400000	-0.8302260000	-0.6949840000
B	-2.0742240000	-1.5129190000	-0.6800260000
B	-2.4467080000	0.0001910000	-0.9332900000
B	2.0917470000	-1.4114000000	0.3481270000
B	-0.8612620000	-2.3978500000	-0.3120720000
B	0.6912460000	-2.0263850000	-0.0456360000
B	-0.8616970000	2.3980590000	-0.3116260000
B	-0.4777630000	0.8304730000	-0.6948180000
B	0.6907670000	2.0268980000	-0.0454520000
B	2.0913410000	1.4118600000	0.3478180000
B	2.7243120000	0.0003700000	0.5380140000
B	-2.0748090000	1.5132680000	-0.6795420000

16

energy

Al	2.0842820000	0.0210560000	-1.4188220000
Al	0.8163800000	-0.0178820000	1.2597960000
Al	-1.8585970000	-0.0283420000	1.4433710000
B	0.4769660000	1.6164930000	-0.5009660000
B	1.8801870000	1.7399980000	0.1836340000
B	2.8576180000	0.7594200000	0.8753780000
B	2.8560530000	-0.7889780000	0.8504400000
B	1.8767800000	-1.7459730000	0.1289230000

B	-0.1915980000	0.0132850000	-0.7980610000
B	-2.6819480000	1.4032290000	-0.4056690000
B	-2.6850960000	-1.3832240000	-0.4496640000
B	-3.4180900000	0.0098030000	-0.3446980000
B	-1.1582440000	-1.5849630000	-0.7139940000
B	-1.1544790000	1.6091130000	-0.6640730000
B	0.4725150000	-1.6002650000	-0.5492780000
B	-1.8400340000	0.0174990000	-0.9512690000

17

energy

Al	-0.2915470000	2.6227150000	-0.9550700000
Al	-1.1777830000	0.1458930000	-1.3113550000
Al	-1.1245200000	-1.0140460000	1.4718580000
B	-2.8466610000	-0.5131870000	0.0900340000
B	-2.1015820000	-1.7412200000	-0.4734620000
B	-0.6168910000	-2.3485570000	-0.5838420000
B	0.9018450000	-2.6937520000	-0.6685990000
B	0.5466580000	-1.0947190000	-0.1693410000
B	2.2365780000	-1.8812160000	-0.4555210000
B	-2.2630710000	0.7754590000	0.7315880000
B	0.4351710000	0.4268310000	0.4476010000
B	-0.8655450000	1.4201740000	1.1304720000
B	2.0065880000	1.4517150000	0.7193290000
B	0.5827800000	2.0613040000	1.0565710000
B	1.9686350000	-0.2337530000	0.1634550000
B	3.4303100000	-0.8281680000	-0.2052070000
B	3.3291930000	0.6372280000	0.2827990000

18

energy

Al	1.8389610000	-2.1665310000	-0.4313110000
Al	-1.3181800000	-1.2657700000	1.6698750000
Al	3.3450160000	0.0857850000	0.8320700000
B	-1.5138180000	-1.0122940000	-0.9099040000
B	-2.7827180000	0.1122340000	-0.1822070000
B	-1.8845650000	-2.5441840000	-0.4106620000
B	-0.3220640000	-2.2578160000	-0.5528870000
B	-2.9731960000	-1.4658420000	-0.2011210000
B	-2.3285090000	1.6692440000	0.0345560000
B	-1.7209730000	3.1422510000	0.3949060000
B	-1.1151290000	0.5509780000	-0.5206790000
B	-0.7040870000	2.1687240000	-0.4251640000
B	-0.2537270000	3.6097330000	0.2138630000
B	0.1545440000	-0.6409670000	-0.7117130000
B	0.5479850000	1.0846470000	-0.6940510000
B	2.0973960000	1.5317050000	-0.4041140000
B	1.7283030000	0.0172220000	-0.8170100000
B	1.0194870000	2.7353060000	-0.1974600000

19

energy

Al	-1.0502690000	-1.3137550000	1.0633170000
Al	-3.4826580000	-0.3213560000	0.5526110000
Al	1.4356140000	-0.4229420000	1.4792810000
B	-0.9916960000	-1.9730150000	-1.0574630000
B	-0.6086890000	0.8759960000	-1.0964840000
B	-1.6370050000	-0.5272810000	-1.2005400000
B	1.0988830000	0.6276210000	-0.9596080000
B	1.7488850000	-0.8506270000	-0.9638950000
B	0.4398870000	2.1014220000	-0.5590570000
B	2.8193380000	0.3876730000	-0.0822370000
B	2.0622230000	-2.3494970000	-0.2769550000
B	0.5250270000	-2.3732070000	-0.7582930000
B	3.0634670000	-1.2033010000	0.0065770000
B	2.1081400000	1.8026630000	0.2049860000
B	0.0873110000	-0.6706360000	-1.1625880000
B	-1.3299640000	2.2502110000	-0.3413220000
B	-2.2170440000	0.9135470000	-0.6763490000
B	1.1949860000	3.0543840000	0.5709280000

B	-0.3107350000	3.2849850000	0.3047570000
5			
energy			
Al	1.4534940000	1.3716100000	-0.0018570000
Al	1.4532560000	-1.3714610000	-0.0017940000
Al	-2.4846280000	0.0004040000	-0.0037760000
B	-0.5490220000	-0.7827480000	0.0094970000
B	-0.5484980000	0.7813120000	0.0098130000
6			
energy			
Al	-1.9410460000	-1.4592060000	-0.0000900000
Al	2.2343790000	-0.9511460000	-0.0000810000
Al	-0.2933630000	2.4105350000	-0.0000890000
B	-0.8757480000	0.3727370000	0.0002630000
B	0.1150110000	-0.9451230000	0.0002110000
B	0.7608150000	0.5719100000	0.0002040000
7			
energy			
Al	-1.8736490000	-0.5206320000	-0.4490790000
Al	-0.2361380000	1.6179500000	-0.1549480000
Al	1.6580520000	-0.3267120000	-0.8975990000
B	-0.0788390000	-1.4548880000	0.1171220000
B	0.9882260000	-0.9196670000	1.1799840000
B	-0.5609180000	-0.2546780000	1.2428450000
B	0.8260430000	0.6256600000	1.3642770000
8			
energy			
Al	1.6844230000	0.5327050000	-1.0263720000
Al	-2.3689210000	-0.3012710000	-0.2877500000
Al	-0.5154580000	1.3286090000	0.4183180000
B	1.0446850000	0.2947650000	1.4433000000
B	-0.0644700000	-0.8084710000	0.8770530000
B	1.6641950000	-1.0698970000	1.0460350000
B	-0.4873330000	-0.9606120000	-0.7516340000
B	0.9628070000	-1.5118970000	-0.2856620000
9			
energy			
Al	0.9178710000	-0.7527060000	-1.4614790000
Al	1.3100540000	1.4068190000	0.0016320000
Al	0.9169980000	-0.7564640000	1.4605770000
B	-0.2405560000	-1.7109010000	-0.0019720000
B	-2.0868560000	1.3879070000	0.0009780000
B	-0.6306650000	1.9008880000	0.0001270000
B	-2.5894750000	-0.0770540000	0.0002030000
B	-0.8818640000	0.1554860000	-0.0000910000
B	-1.7473860000	-1.3902170000	-0.0011450000
10			
energy			
Al	0.7001090000	-0.0024620000	-1.4571840000
Al	0.6981880000	0.0024940000	1.4555330000
Al	-3.3480030000	0.0000640000	-0.0000670000
B	2.3067840000	-0.7899800000	0.0027110000
B	2.3099030000	0.7837280000	0.0000180000
B	1.1413920000	1.8090410000	-0.0017520000
B	-0.3537150000	1.4006800000	-0.0021320000
B	1.1343930000	-1.8108790000	0.0041310000
B	-0.3590270000	-1.3964480000	0.0021450000
B	-1.1104940000	0.0036070000	-0.0006540000
11			
energy			
Al	1.1332230000	-0.3648210000	1.5957950000
Al	-2.3961500000	-1.0343380000	0.0887450000
Al	-1.8993320000	1.5784660000	-0.0126350000
B	0.8960550000	-1.5069280000	-0.8094800000
B	2.8082120000	0.4990570000	-0.3815790000
B	0.2034460000	1.4574490000	-0.3029910000
B	-0.3885730000	-0.0931210000	-0.5454740000

B	1.2136370000	0.2555300000	-0.9138060000
B	1.7623670000	1.6477460000	-0.1565790000
B	2.3732260000	-0.9717320000	-0.6555290000
B	-0.6464970000	-1.7541980000	-0.5815150000

12

energy

Al	0.0107120000	-1.8748980000	-0.0007770000
Al	-2.4615590000	-1.5343910000	0.0008150000
Al	2.4793600000	-1.5072560000	0.0010190000
B	2.4755070000	0.4742070000	-0.0009470000
B	0.8538380000	0.1521860000	-0.0001640000
B	-0.8558060000	0.1419260000	-0.0005980000
B	-1.7794360000	1.8505000000	-0.0000580000
B	-0.0098250000	1.6495650000	-0.0008450000
B	-0.7850360000	3.0949760000	0.0006710000
B	0.7499950000	3.1033280000	0.0005850000
B	-2.4810620000	0.4468820000	-0.0008360000
B	1.7576910000	1.8694480000	-0.0005580000

4

energy

Al	1.1407960000	-1.8477080000	0.0000000000
Al	-1.1407960000	1.8477080000	0.0000000000
Al	1.1407960000	0.8391850000	0.0000000000
Al	-1.1407960000	-0.8391850000	0.0000000000

5

energy

Al	0.2745070000	-1.9626960000	-0.0006210000
Al	-2.3875560000	-0.0024120000	0.0003190000
Al	0.2691630000	1.9631080000	0.0000660000
Al	1.9921280000	0.0022680000	0.0003340000
B	-0.3854300000	-0.0006940000	-0.0002530000

14

energy

Al	-1.8938830000	-1.9021120000	0.0320020000
Al	0.7713860000	0.7355640000	1.3794370000
Al	2.9593220000	-0.7898480000	-0.1394260000
Al	0.6288070000	-1.7947610000	0.2425370000
B	1.0210720000	0.2026900000	-1.0248600000
B	-0.2433730000	2.6091900000	0.0642780000
B	-0.3922990000	1.1632770000	-0.7893510000
B	-3.0310070000	1.1043170000	0.2392800000
B	-0.4383860000	-0.4215840000	-1.0873010000
B	-1.8631210000	0.2629420000	-0.6025680000
B	-1.7084600000	2.0279280000	0.1122560000
B	-3.2571790000	-0.3748800000	0.0703700000
B	1.1711010000	2.1210530000	-0.4405280000
B	2.3310070000	1.0580730000	-0.4794040000

15

energy

Al	1.9706910000	-2.2402850000	-0.1265960000
Al	-0.8291480000	-0.0660960000	1.3341830000
Al	-1.5143030000	-0.5258100000	-1.3734820000
Al	1.4780400000	1.0952740000	1.2503190000
B	-1.5775720000	1.7597310000	-0.2021200000
B	1.1624670000	2.4504840000	-0.7104810000
B	-2.7755360000	-0.8160290000	0.5211730000
B	-0.1713150000	-1.9361810000	0.0196830000
B	-1.6807420000	-1.9188940000	0.4365360000
B	-0.3244140000	2.7147520000	-0.4634060000
B	0.0353520000	1.0830190000	-0.6723510000
B	-2.6556680000	0.6896460000	0.2100720000
B	0.6282410000	-0.5169320000	-0.5005590000
B	2.1805110000	1.2719370000	-0.8801390000
B	2.3049460000	-0.2655470000	-0.5779070000

16

energy

Al	-0.3631600000	0.9765600000	1.2935230000
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Al	1.2286090000	0.9283260000	-1.1384860000
Al	2.6551630000	-1.2569890000	-0.5865900000
Al	-2.2837710000	-0.6873720000	0.9904230000
B	1.2867660000	2.2762590000	0.6432600000
B	1.8493350000	0.9102890000	1.1651260000
B	1.3992220000	-0.5958780000	1.2415020000
B	0.9338550000	-2.0739350000	0.8013680000
B	0.0741390000	-0.8688940000	-0.0276670000
B	-0.3427850000	-2.5322520000	0.0327260000
B	-0.9111470000	0.1415060000	-0.8837180000
B	-1.2584720000	1.9104770000	-0.8029730000
B	-2.3839710000	-0.6754500000	-1.3507270000
B	0.0028250000	2.6341900000	-0.1543350000
B	-2.3513370000	0.8688900000	-1.3044230000
B	-1.5142160000	-1.8925650000	-0.8132030000

17

energy

Al	1.6134470000	-0.8004710000	0.9301360000
Al	-1.5205650000	-1.0396250000	0.8960160000
Al	-0.0322450000	-0.0324400000	2.6976680000
Al	-0.1492320000	1.7852180000	0.9381510000
B	0.7737800000	-2.4751080000	-1.0412970000
B	1.9584750000	-1.4478470000	-1.1592230000
B	2.5351650000	0.0146390000	-1.0497370000
B	2.1545490000	1.5263780000	-0.9569550000
B	-0.7817320000	-2.4329030000	-1.0770770000
B	0.8008780000	0.5464910000	-1.0714550000
B	0.0771400000	-0.9487100000	-1.1765260000
B	0.8493100000	2.3803090000	-1.0552720000
B	-0.7242190000	2.3480070000	-1.1374320000
B	-1.9232550000	-1.3555440000	-1.2254120000
B	-2.5512330000	0.0821960000	-1.0712020000
B	-0.8570610000	0.4231860000	-1.1574070000
B	-2.0814510000	1.5659310000	-1.0221300000

18

energy

Al	-0.5107450000	-1.7206250000	2.2891240000
Al	1.2958250000	0.2463570000	-1.5844270000
Al	1.2939590000	0.2474920000	1.5826250000
Al	-0.5095840000	-1.7260710000	-2.2863530000
B	-1.7446980000	0.8409280000	-0.0012730000
B	-3.0094370000	1.8605420000	-0.0020680000
B	2.0706490000	-1.3441500000	0.0019310000
B	-3.2878760000	0.3363630000	-0.0016410000
B	-1.0079540000	-1.9180230000	0.0025760000
B	0.5524480000	-1.7757830000	0.0014690000
B	-0.4397690000	-0.2375760000	-0.0020850000
B	2.9629710000	-0.0821630000	0.0013670000
B	-0.1389090000	1.3729830000	0.0014720000
B	-0.0916370000	3.0895840000	-0.0016660000
B	1.2859110000	2.3765490000	-0.0006600000
B	2.5611190000	1.4035960000	0.0001950000
B	-1.5918670000	2.6138010000	-0.0016350000
B	-2.2015340000	-0.8592510000	-0.0005030000

19

energy

Al	-1.4366550000	1.0391420000	0.8566390000
Al	0.0016400000	1.0031030000	-1.6917450000
Al	0.0033970000	3.1205120000	-0.0626780000
Al	1.4414380000	1.0372850000	0.8554200000
B	-0.7636250000	-1.0275450000	2.4212490000
B	-2.7538600000	-0.8365080000	-1.1175530000
B	-3.0202110000	-0.8327820000	0.4136180000
B	-2.1563980000	-0.9817280000	1.6831710000
B	-1.4905310000	-1.3373140000	-0.0890150000
B	-1.4442230000	-1.0865240000	-1.9576590000
B	-0.0021100000	-1.3337400000	0.8083270000

B	2.1520740000	-0.9864880000	1.6839400000
B	0.7589290000	-1.0294080000	2.4217420000
B	1.4865270000	-1.3407010000	-0.0885850000
B	3.0172960000	-0.8405770000	0.4150220000
B	2.7518900000	-0.8439040000	-1.1163270000
B	1.4418070000	-1.0902240000	-1.9567760000
B	-0.0010410000	-1.0672480000	-2.5748040000
B	-0.0020580000	-1.4854200000	-0.8362060000

20

energy

Al	-1.4180260000	1.2479050000	-0.6761880000
Al	0.0001510000	0.6620480000	1.8411090000
Al	1.4222850000	1.2469680000	-0.6737590000
Al	0.0011090000	3.0081380000	0.6331020000
B	-0.8569010000	-1.6790180000	0.6347570000
B	-0.0010490000	-1.4946720000	2.3369500000
B	1.5272190000	-1.1755280000	2.0958030000
B	-1.5286780000	-1.1732950000	2.0966250000
B	-2.4431690000	-0.8796360000	0.8366380000
B	0.8551040000	-1.6805090000	0.6338150000
B	-2.3199960000	-0.3289020000	-1.9948630000
B	-1.5963790000	-1.3119420000	-0.8592260000
B	-3.0099400000	-0.4488200000	-0.5973970000
B	2.4422340000	-0.8828950000	0.8363140000
B	1.5936620000	-1.3139700000	-0.8606040000
B	3.0088340000	-0.4531090000	-0.5983280000
B	-0.0015090000	-1.6573270000	-0.7841800000
B	0.8046770000	-0.6095110000	-2.3520040000
B	-0.8068630000	-0.6087700000	-2.3519850000
B	2.3184040000	-0.3312520000	-1.9954010000

6

energy

Al	-1.3258980000	1.4508180000	-0.0572650000
Al	1.3245320000	1.4514000000	-0.0567200000
Al	1.9462980000	-1.1686000000	-0.1921660000
Al	-1.9451270000	-1.1701530000	-0.1918330000
B	-0.0002540000	0.0230930000	0.7869840000
B	0.0007650000	-1.4881040000	0.5077750000

7

energy

Al	2.0612150000	-0.0000410000	-0.5314560000
Al	-0.1465630000	-1.8075130000	-0.3175470000
Al	-0.1462970000	1.8075140000	-0.3174680000
Al	-2.1986920000	0.0001520000	-0.2127860000
B	0.8464940000	-0.7906070000	1.2138330000
B	0.8466650000	0.7902790000	1.2138490000
B	-0.5742820000	0.0000370000	1.1583890000

8

energy

Al	-2.0494500000	-0.0006090000	-0.7592910000
Al	0.4565410000	1.5428960000	-0.6115010000
Al	0.4523890000	-1.5423390000	-0.6110480000
Al	2.3822610000	-0.0023810000	0.2360800000
B	-0.9674800000	-1.2598220000	0.9231070000
B	0.1656320000	0.0014910000	1.0176480000
B	-1.4589830000	0.0022580000	1.6788510000
B	-0.9676940000	1.2623970000	0.9193670000

9

energy

Al	-0.0069880000	1.8650590000	0.7685460000
Al	-0.7632940000	-0.6888110000	1.3459940000
Al	-2.6303670000	-0.8408530000	-0.4464640000
Al	3.0825610000	-0.7272650000	-0.1330660000
B	1.0790680000	-0.8757390000	0.1582880000
B	0.0221780000	1.1477230000	-1.4131650000
B	1.3217640000	0.4617360000	-0.8347960000
B	-0.1573680000	-0.4179160000	-0.8375140000

B	-1.4386140000	0.7030570000	-1.0638390000
10			
energy			
Al	-2.4617010000	-1.1290380000	-0.1278320000
Al	0.0868930000	-1.4730730000	0.3583950000
Al	2.5719320000	-0.8437110000	-0.1834410000
Al	0.1289900000	1.0498490000	1.4819870000
B	-2.1154680000	0.9145080000	-0.2223600000
B	0.4703380000	1.7955070000	-0.7493500000
B	-1.0844420000	2.0344890000	-0.5311630000
B	1.8514060000	1.0404810000	-0.3688350000
B	-0.7488010000	0.3796020000	-0.9546280000
B	0.7790690000	0.0649470000	-1.1493460000
11			
energy			
Al	-1.3759950000	0.0023690000	1.6418280000
Al	2.3777770000	0.0006710000	0.7551940000
Al	1.3751730000	1.9836670000	-0.5361310000
Al	1.3764690000	-1.9838120000	-0.5351840000
B	-3.0059170000	-0.0024240000	-0.5135200000
B	-1.3026760000	-0.0018860000	-0.9292980000
B	-0.6369110000	-1.4897890000	-0.4354290000
B	-2.2172810000	-1.3400090000	-0.4054060000
B	-2.2194180000	1.3364860000	-0.4093170000
B	0.2629180000	0.0011810000	-0.3144420000
B	-0.6396200000	1.4889150000	-0.4394280000
12			
energy			
Al	-0.9013700000	-2.1910860000	0.2492100000
Al	-2.5909430000	0.0023780000	-0.5052200000
Al	0.3437010000	0.0005470000	-1.2308500000
Al	-0.8974170000	2.1908980000	0.2503520000
B	0.5876110000	0.8646860000	1.2331370000
B	1.5618810000	-1.6378980000	0.1972980000
B	0.5871010000	-0.8677770000	1.2319500000
B	1.8921820000	-0.0008190000	0.6521880000
B	-0.7901110000	-0.0008320000	1.0962110000
B	2.5597870000	0.7911920000	-0.6968540000
B	1.5614820000	1.6363610000	0.1984800000
B	2.5597440000	-0.7920300000	-0.6974880000
13			
energy			
Al	-0.2353110000	-0.7853910000	-1.2917280000
Al	-2.8296430000	0.4166790000	-0.4291380000
Al	2.1467450000	1.6404390000	0.0395620000
Al	-0.6050380000	2.1657740000	0.0040710000
B	0.7764100000	-2.4384390000	0.1829210000
B	-0.7189810000	-2.4698400000	0.6119370000
B	0.0077340000	-1.0435410000	1.2120670000
B	-1.6356590000	-1.2272390000	0.8226150000
B	-1.0309790000	0.3068860000	1.0711170000
B	1.9647870000	-1.7335450000	-0.5961750000
B	1.5590370000	-0.5929420000	0.6308140000
B	0.5654930000	0.5478730000	1.1995850000
B	2.4726010000	-0.2867160000	-0.7740740000
5			
energy			
Al	-0.0002290000	-0.8754350000	2.5152180000
Al	-0.0002290000	-0.8754350000	-2.5152180000
Al	-0.0002290000	1.4239130000	-1.2408210000
Al	-0.0002290000	1.4239130000	1.2408210000
Al	0.0009150000	-1.0969560000	-0.0000000000
6			
energy			
Al	-1.4676130000	-1.5928720000	-0.0000000000
Al	1.0614490000	-1.8878720000	0.0000000000
Al	2.1233560000	0.4261820000	0.0000000000

Al	0.2510410000	2.1511140000	0.0000000000
Al	-1.9682330000	0.9034200000	-0.0000000000
B	0.0000000000	0.0000750000	0.0000000000

15

energy

Al	0.2294300000	-1.8192230000	0.1471480000
Al	1.0134150000	0.7474980000	1.1950260000
Al	2.8164490000	-1.4171370000	0.1935460000
Al	-1.8460710000	-0.2514400000	1.7498760000
Al	-2.1338350000	-1.5516000000	-0.9880220000
B	1.9944890000	1.8611730000	-0.5088290000
B	1.4262180000	-0.0160520000	-1.0896800000
B	-0.0979270000	-0.2511850000	-1.4320290000
B	-1.3215960000	0.6815650000	-0.8989150000
B	0.6998880000	2.6872240000	-0.2107990000
B	-0.8406840000	2.3733780000	-0.1330340000
B	0.2718550000	1.2945640000	-1.0782820000
B	-2.3132610000	1.7106600000	-0.0243470000
B	2.8078570000	0.5142900000	-0.3397770000
B	-2.8332510000	0.3033260000	-0.2580040000

16

energy

Al	-0.9717050000	-1.4224680000	1.4629700000
Al	-2.5961660000	0.0584180000	-0.8196870000
Al	1.6856150000	1.2277040000	1.0739970000
Al	-0.9057150000	1.3339670000	1.4969040000
Al	1.6130860000	-1.3535000000	0.9947070000
B	-0.4542070000	-0.7557090000	-0.8281210000
B	-1.7250430000	-1.8278250000	-0.5964730000
B	-0.3289970000	-2.4423520000	-0.9943260000
B	1.1341490000	-1.8030300000	-1.2430820000
B	0.9435150000	0.0329190000	-1.1519670000
B	2.3624570000	-0.7676950000	-1.4197390000
B	-0.2763290000	2.5308960000	-0.8230080000
B	-0.4499270000	0.8549240000	-0.8845550000
B	1.1602020000	1.8543440000	-1.1359150000
B	-1.6923860000	1.9147070000	-0.5066260000
B	2.3812690000	0.8141040000	-1.3593020000

17

energy

Al	-2.8067100000	-0.5077490000	-1.2022570000
Al	0.5860480000	0.5376060000	1.4411100000
Al	-1.2870010000	1.6202070000	-0.5425300000
Al	0.2758180000	-2.4186420000	1.3992200000
Al	2.6576240000	-0.5568480000	0.1651360000
B	-0.1388740000	-2.0835450000	-1.1698180000
B	-0.2600400000	-0.5499290000	-0.4497880000
B	-1.6587520000	0.7093550000	1.6367400000
B	-1.5174880000	-0.6955700000	0.9197260000
B	-1.3422340000	-1.8490180000	-0.1848870000
B	1.0384370000	-1.2015400000	-1.7418090000
B	-0.9530600000	2.0932100000	1.6359960000
B	1.2264880000	2.2318650000	-0.3474720000
B	2.0146880000	0.0247920000	-1.9899500000
B	2.1249580000	1.4552230000	-1.4073240000
B	0.7415890000	0.6292280000	-0.9792080000
B	0.2172650000	2.6820370000	0.8000280000

18

energy

Al	-2.2877950000	-0.0019890000	-0.3143560000
Al	-0.3024540000	1.4934710000	1.0906890000
Al	-0.2982840000	-1.4917290000	1.0920830000
Al	-2.1599560000	-0.0008270000	2.3150300000
Al	3.1446720000	0.0041900000	0.9439740000
B	0.1959130000	-0.0014510000	-1.7470540000
B	0.9653050000	2.7907820000	-0.3022210000
B	0.8251120000	1.4256550000	-1.2152640000

B	1.8392440000	1.5540980000	0.2419360000
B	-0.2786060000	2.7050640000	-1.2269540000
B	-1.4649900000	-0.0036910000	-2.2849750000
B	1.2765330000	0.0009740000	-0.3245470000
B	-0.8921710000	1.4512840000	-1.9927110000
B	1.8430060000	-1.5498410000	0.2443800000
B	0.8280550000	-1.4260150000	-1.2123040000
B	0.9721800000	-2.7896730000	-0.2979650000
B	-0.2717510000	-2.7085620000	-1.2232070000
B	-0.8879040000	-1.4567270000	-1.9904050000

19

energy

Al	2.5093490000	0.0013320000	-0.0364550000
Al	-1.5819500000	-1.4590110000	0.3807990000
Al	-2.9253130000	-0.0013650000	-1.3880350000
Al	-0.2693650000	-0.0006220000	-1.6796210000
Al	-1.5828840000	1.4583660000	0.3797000000
B	1.0117080000	1.4996440000	0.6344240000
B	0.7328200000	0.0002010000	1.3384410000
B	1.0130730000	-1.4986770000	0.6338230000
B	1.3029530000	-1.9917930000	-1.1403860000
B	-0.0000250000	1.4550270000	2.2784410000
B	0.5943260000	2.9388060000	-0.1050070000
B	0.0195700000	2.7215090000	1.3227040000
B	1.7763510000	0.7718870000	-2.0265480000
B	1.3006700000	1.9930200000	-1.1400470000
B	0.0013750000	-1.4557860000	2.2784810000
B	0.5972060000	-2.9383010000	-0.1055880000
B	-0.1391560000	-0.0004450000	2.8292010000
B	0.0222050000	-2.7216990000	1.3221270000
B	1.7773490000	-0.7700130000	-2.0266730000

20

energy

Al	1.9652460000	0.0015510000	0.7229900000
Al	-0.5413980000	-1.4486110000	1.2681830000
Al	-0.5466730000	1.4428140000	1.2706870000
Al	0.7412040000	-0.0019510000	3.0419770000
Al	-2.6917110000	-0.0029760000	-0.4643420000
B	-0.8509170000	-1.4968730000	-1.2624320000
B	0.7840460000	-0.9416250000	-1.5606210000
B	0.7811280000	0.9480180000	-1.5586140000
B	1.9274460000	-2.1026430000	-1.0441430000
B	-1.0341750000	-2.9174360000	-0.3874890000
B	0.4653220000	-2.6521500000	-0.7872490000
B	-2.2241380000	-1.9356310000	-0.2857950000
B	-0.5380530000	0.0013390000	-1.7904640000
B	2.6121480000	0.7997610000	-1.3795960000
B	2.6143540000	-0.7893090000	-1.3812460000
B	0.4582120000	2.6556160000	-0.7818520000
B	1.9218520000	2.1107730000	-1.0402860000
B	-0.8551610000	1.4977050000	-1.2597010000
B	-1.0419340000	2.9156610000	-0.3810420000
B	-2.2294660000	1.9306440000	-0.2821560000

21

energy

Al	3.0347590000	0.1276570000	0.1893740000
Al	-1.5215690000	1.3847360000	-0.8600800000
Al	-2.3679410000	-0.7316370000	-2.1671020000
Al	0.1639070000	-0.8938620000	-1.4497250000
Al	-2.1459240000	-1.1353790000	0.4030310000
B	-1.5230710000	0.7067130000	2.1228070000
B	0.0074090000	-0.1993420000	2.1462040000
B	-1.4829020000	-0.8760400000	2.4029810000
B	1.1865360000	-1.1148070000	1.2347560000
B	2.1721130000	0.1496730000	-1.8590930000
B	1.1257460000	1.6050080000	0.2750220000
B	0.0454230000	1.4549430000	1.6591930000

B	-0.3192120000	2.6945660000	0.4421750000
B	-1.4644520000	2.1089390000	1.3887060000
B	1.5197370000	1.5554400000	-1.4664230000
B	0.5061820000	2.6080930000	-0.9190970000
B	1.3587010000	0.5006530000	1.4760780000
B	0.5768210000	-2.6289510000	0.8201760000
B	-0.3350680000	-1.8778820000	1.8802970000
B	1.6871210000	-2.1545760000	-0.1556430000
B	2.3145150000	-1.2863660000	-1.3484340000

7

energy

Al	-1.8711150000	-0.0018170000	-1.2054470000
Al	-1.2897700000	0.0099470000	1.3656380000
Al	0.4809590000	1.8392720000	0.5885740000
Al	0.4679140000	-1.8374680000	0.6004250000
Al	2.1073450000	-0.0073500000	-0.4436800000
B	0.1367710000	0.7954190000	-1.1793850000
B	0.1353640000	-0.8021400000	-1.1749430000

8

energy

Al	-1.3508610000	-0.5111670000	1.2733720000
Al	1.0268670000	-1.3910650000	0.6482330000
Al	-2.4004140000	-0.3649320000	-1.0868560000
Al	-0.1086830000	1.8898910000	0.7945600000
Al	2.8217690000	0.0174970000	-0.5456900000
B	-0.1184750000	-0.6419310000	-0.9594610000
B	-0.7196540000	0.8806620000	-1.0614780000
B	0.8675650000	0.6966870000	-0.7964690000

9

energy

Al	-0.0004940000	0.5494860000	-1.3562020000
Al	0.0001520000	0.5509210000	1.3562530000
Al	-2.3945990000	-0.9130160000	-0.0003340000
Al	0.0003240000	-1.7684610000	0.0011020000
Al	2.3950880000	-0.9122990000	-0.0005670000
B	-0.7814640000	2.2075130000	-0.0005330000
B	0.7806870000	2.2076190000	-0.0007660000
B	1.7832650000	1.0340280000	0.0001400000
B	-1.7837100000	1.0335990000	0.0005010000

10

energy

Al	-2.4643180000	-0.8591190000	-0.0585790000
Al	0.4612830000	1.3304410000	0.6570020000
Al	-2.0309040000	1.7665560000	-0.1626590000
Al	2.8753010000	0.8777180000	-0.2390870000
Al	0.2238210000	-1.3067360000	1.4062750000
B	0.7280900000	-0.3139530000	-1.0450030000
B	-0.8081860000	0.1384480000	-0.9557980000
B	-0.5511670000	-1.5100950000	-0.9653820000
B	0.9523800000	-1.9876640000	-0.8103180000
B	2.1094050000	-1.0297740000	-0.3911760000

11

energy

Al	-2.5316090000	-0.0854940000	0.4359550000
Al	-0.9280560000	-1.9836330000	-0.5235720000
Al	1.5859740000	-1.9053710000	0.4566580000
Al	-0.1104850000	0.5980100000	1.3336760000
Al	2.3154040000	0.5459130000	-0.2479770000
B	0.4974140000	-0.4547340000	-0.9489920000
B	-1.0114900000	0.1355100000	-1.2097350000
B	-1.4143810000	1.6029280000	-0.6435290000
B	-0.3196990000	2.6409730000	-0.1413250000
B	0.2206830000	1.2036190000	-0.9203940000
B	1.1662790000	2.2311990000	0.0816520000

12

energy

Al	-1.3654550000	1.8672050000	0.0395250000
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Al	1.3665180000	1.8675580000	0.0414190000
Al	2.9329750000	-0.4304300000	-0.7561650000
Al	-2.9335660000	-0.4294320000	-0.7559510000
Al	0.0014940000	-0.5594840000	-1.0739770000
B	-0.0010400000	-0.9321960000	1.3440650000
B	-0.0001530000	0.7363350000	1.3184760000
B	1.4079540000	-0.0631740000	1.0584860000
B	1.3815870000	-1.6427570000	0.6192390000
B	-0.0011010000	-2.4151010000	0.4969500000
B	-1.3833800000	-1.6411610000	0.6175340000
B	-1.4089810000	-0.0620300000	1.0586360000

13

energy

Al	0.2662630000	0.6132250000	-1.2359240000
Al	-1.4047230000	-1.7894940000	0.1433450000
Al	1.2486590000	-2.0347080000	0.0556570000
Al	3.1907420000	-0.0555060000	-0.5880940000
Al	-3.3844880000	-0.0804440000	-0.3837160000
B	-2.0748290000	1.4832330000	-0.2699100000
B	-1.2767470000	0.5207170000	0.8322750000
B	-0.7651380000	2.2807600000	0.1329830000
B	0.3125620000	1.0945320000	1.2030890000
B	0.7723040000	2.4966700000	0.3587920000
B	-0.1059100000	-0.5099630000	1.2610650000
B	1.4714440000	-0.1082010000	1.0310580000
B	1.8835370000	1.4442610000	0.6733530000

14

energy

Al	0.9606550000	0.6629430000	-1.2668740000
Al	-1.6796530000	-1.4163050000	-0.1358130000
Al	0.9741710000	-2.1029160000	-0.0925560000
Al	3.4206680000	-0.6691500000	-0.2082700000
Al	-3.9981700000	-0.2663670000	0.2128380000
B	0.0210890000	2.4955290000	-0.0464320000
B	-2.3853720000	0.8488700000	-0.6142580000
B	-1.0514480000	0.7781380000	0.5042490000
B	-1.3109860000	1.9806110000	-0.7274390000
B	1.4801250000	-0.3461830000	1.0917940000
B	0.5330060000	1.0799730000	1.1282780000
B	1.4700100000	2.3684440000	0.5095480000
B	-0.1507820000	-0.4411550000	1.0555450000
B	2.2324140000	1.0944420000	0.9744690000

6

energy

Al	-0.4527960000	1.6685750000	-0.9639210000
Al	-1.2181540000	-1.2270810000	-0.9641530000
Al	0.4520390000	-1.6671530000	0.9644930000
Al	-1.6712740000	0.4418790000	0.9628200000
Al	1.6727860000	-0.4420520000	-0.9634100000
Al	1.2174000000	1.2258330000	0.9641700000

7

energy

Al	0.1302330000	-1.8757180000	-0.3751520000
Al	-1.2192420000	0.4908520000	1.5085650000
Al	-2.0235470000	-0.4165290000	-0.8740980000
Al	1.2204940000	-0.4961120000	1.5061190000
Al	-0.1304280000	1.8765010000	-0.3692330000
Al	2.0226680000	0.4203010000	-0.8737090000
B	-0.0004610000	0.0018310000	-1.3584830000

16

energy

Al	1.8232460000	0.2454270000	-1.1386110000
Al	0.6833010000	2.6127220000	-0.8673860000
Al	-1.5775920000	1.2269730000	-0.9045590000
Al	-0.6952010000	-1.3486900000	-1.0072630000
Al	-3.2407690000	-1.2022500000	-0.0554730000
Al	1.5424030000	-2.4419560000	-0.2961260000

B	2.9252830000	-1.0800260000	0.3905930000
B	1.4888180000	-0.7242100000	1.2170880000
B	0.1555500000	0.3255230000	1.4575140000
B	1.5725340000	1.3119210000	1.1508320000
B	2.8286490000	0.3484800000	0.9609070000
B	-0.0074010000	-1.3003540000	1.1776460000
B	-2.5907720000	0.5638950000	0.8697690000
B	0.1330500000	1.9944180000	1.2868770000
B	-1.3389070000	1.3806910000	1.3954260000
B	-1.3588120000	-0.4601240000	1.1938350000

17

energy

Al	0.6458170000	1.5338270000	-2.1981880000
Al	-1.4803810000	-0.0542520000	-1.4980410000
Al	2.0300480000	-0.7806980000	1.3032490000
Al	-1.4691560000	-0.1622870000	1.4924860000
Al	2.0192080000	-0.6838160000	-1.3670770000
Al	0.6573220000	1.3709400000	2.3017180000
B	0.7502820000	2.0891710000	0.0743940000
B	1.8812460000	0.9812020000	0.0331810000
B	-2.3442810000	1.4387010000	0.0581820000
B	-0.8267130000	1.8902190000	0.0696720000
B	0.2538120000	0.3848430000	0.0126660000
B	-0.0068670000	-2.9370060000	-0.1040890000
B	0.0020140000	-1.2414360000	-0.0438630000
B	-2.7406220000	-1.3583090000	-0.0414090000
B	-1.4551380000	-2.2683030000	-0.0770790000
B	1.4061780000	-2.2951650000	-0.0844260000
B	-3.1673460000	0.1344280000	0.0139850000

18

energy

Al	1.9176900000	1.2673750000	-0.1770490000
Al	3.1475060000	-1.2399300000	-0.0402170000
Al	-1.8423300000	-0.4271410000	1.4169400000
Al	-0.9735400000	1.0380020000	-0.8589890000
Al	-1.0972480000	-1.7134020000	-1.1469190000
Al	-3.4308900000	-0.2800300000	-0.8240630000
B	0.6419340000	2.2919850000	-1.6716010000
B	-0.3291960000	1.4340500000	2.5154690000
B	-0.0517030000	2.2879560000	1.1967420000
B	0.2683450000	2.8303090000	-0.2582670000
B	0.9316110000	0.8575910000	-2.1987780000
B	1.0903020000	-0.6149350000	-1.6288990000
B	0.4153790000	0.5553370000	1.3054640000
B	0.6512630000	-0.6031210000	0.1789500000
B	-0.0767960000	-0.0618700000	2.8402970000
B	0.4275540000	-1.2982000000	1.9836280000
B	1.1127620000	-1.9608690000	-0.7786500000
B	0.8434560000	-2.1949070000	0.7544180000

19

energy

Al	0.7816890000	0.9942860000	1.5295450000
Al	1.3361980000	-1.3255890000	2.5631040000
Al	-1.7030080000	1.7901480000	0.3039180000
Al	-0.4924630000	-1.5417990000	0.6894350000
Al	2.3217490000	-0.9316270000	0.1788200000
Al	-3.3278070000	-0.1849760000	0.6607860000
B	0.3493350000	1.9866610000	-0.9240070000
B	1.5239700000	2.6087710000	0.0610450000
B	0.0491560000	2.8192200000	0.5340250000
B	-1.7453860000	-0.1373320000	-1.0468240000
B	-0.2982740000	-0.5683630000	-1.9590800000
B	0.9056800000	0.6302760000	-1.8177190000
B	1.4407560000	-1.0586730000	-2.1034560000
B	2.4894830000	0.1144750000	-1.6948280000
B	-1.1988480000	-2.0496200000	-1.4494840000
B	0.2842150000	-2.1287270000	-1.9777940000

B	-2.3753060000	-1.5569350000	-0.4912880000
B	-0.7216440000	0.9653100000	-1.6090330000
B	2.1143340000	1.4937850000	-0.9281410000

20

energy

Al	-0.8416130000	-1.1497010000	1.1590420000
Al	-1.8875830000	1.6684140000	-0.3556610000
Al	2.0386540000	-1.0573670000	0.5679370000
Al	0.5827380000	1.3712920000	1.3646770000
Al	1.0229800000	-0.6584070000	2.9660270000
Al	-3.5983090000	-0.1196200000	0.0978570000
B	-1.5583190000	-0.5021490000	-1.1466430000
B	-2.4319790000	-1.6838660000	-0.3990630000
B	0.1355840000	-1.0685840000	-1.5652510000
B	1.2957240000	0.3895910000	-1.5274570000
B	2.9702220000	0.6001290000	-1.2271570000
B	1.6965700000	-2.0747780000	-1.6137020000
B	0.3617360000	-2.7148180000	-1.2638050000
B	-1.1313840000	-2.3696570000	-0.9045020000
B	-0.3676830000	0.4796820000	-1.6411520000
B	0.3951420000	1.8162290000	-1.1227870000
B	2.6838690000	-0.8346170000	-1.6392390000
B	-0.3804830000	2.9756850000	-0.0986210000
B	1.1614990000	2.9800350000	-0.1912560000
B	2.1456420000	1.8651300000	-0.7390510000

21

energy

Al	2.7353410000	-1.4391770000	0.2741850000
Al	1.0281970000	1.4604980000	-0.7796140000
Al	-1.0633140000	-0.1466350000	-1.7691500000
Al	-1.1733640000	2.4737720000	-1.7611480000
Al	-1.6018670000	1.4715290000	0.5844900000
Al	-3.0694000000	-1.4079030000	0.2322900000
B	2.3871040000	-0.3452970000	-1.6507410000
B	3.0365270000	0.5769080000	-0.6105010000
B	0.4020040000	-1.8391110000	-0.3083260000
B	-1.2514390000	-2.1630630000	-0.6701550000
B	1.2106240000	-1.3947340000	-1.8949250000
B	-0.1492520000	-2.1636440000	-1.8284520000
B	0.2625890000	1.2465070000	2.4781110000
B	-1.2399060000	0.7158820000	2.6084060000
B	-1.8908260000	-0.4864020000	1.7937320000
B	-0.8846910000	-1.5884670000	0.9022830000
B	-0.2018110000	-0.4468070000	2.0610750000
B	1.3938330000	0.0833280000	1.6002900000
B	2.6434260000	1.1849850000	0.8168050000
B	0.8088370000	-1.3791010000	1.1966540000
B	1.6484380000	1.7275980000	1.8750060000

22

energy

Al	1.2058700000	2.0992390000	0.0735360000
Al	0.3025000000	-1.7169750000	1.1972800000
Al	-1.1107710000	0.9777370000	1.3081420000
Al	-0.6735900000	0.8064790000	-1.6257410000
Al	-1.2297540000	2.9999390000	-0.3557700000
Al	-3.3169390000	-0.3680110000	-0.1136550000
B	2.0457230000	-0.9288660000	-1.0417010000
B	2.6199230000	-0.5342470000	0.6774390000
B	-0.8214370000	-0.7360310000	2.6242850000
B	-1.8187450000	-1.2068980000	1.4603640000
B	1.8730460000	0.5277970000	2.0232580000
B	0.5336120000	0.0046740000	2.6751390000
B	2.8495270000	0.6588980000	-0.6141910000
B	2.8726400000	1.0512630000	0.9449570000
B	2.1565390000	0.4405970000	-2.0170330000
B	2.1796350000	-2.0137320000	0.2622890000
B	-1.6189400000	-1.8773060000	0.0110200000

B	-1.6791270000	-1.2990310000	-1.5256180000
B	-0.4710700000	-2.3602810000	-1.0816340000
B	-0.3611720000	-1.2147340000	-2.3960150000
B	1.0679670000	-0.5099220000	-2.5276700000
B	1.1108540000	-2.4780400000	-0.7327520000

8

energy

Al	-0.2153940000	-1.7811630000	-0.3046830000
Al	-2.7308270000	-0.0725050000	-0.6100410000
Al	-1.2346800000	0.4480090000	1.4181430000
Al	0.2151690000	1.7809150000	-0.3123520000
Al	1.2341320000	-0.4413820000	1.4202830000
Al	2.7314940000	0.0679560000	-0.6100350000
B	-0.7841190000	0.0848090000	-1.3021210000
B	0.7843960000	-0.0895640000	-1.3012970000

9

energy

Al	-3.3401590000	-0.2051590000	0.0000890000
Al	0.0004200000	-0.3840400000	-1.7220770000
Al	-1.3136220000	1.3423510000	0.0001180000
Al	1.3143020000	1.3416980000	0.0019300000
Al	-0.0019380000	-0.3869550000	1.7211380000
Al	3.3410770000	-0.2055750000	0.0002540000
B	0.0001590000	-1.7241900000	-0.0016130000
B	-1.4235660000	-1.0917290000	-0.0021110000
B	1.4231980000	-1.0901150000	-0.0000540000

10

energy

Al	2.1272190000	1.6212380000	-0.4039780000
Al	-0.0016320000	1.7421600000	1.1332350000
Al	-2.1292310000	1.6183690000	-0.4048910000
Al	0.0006880000	-0.9279580000	1.1797360000
Al	2.5718380000	-1.8538590000	-0.0040350000
Al	-2.5686070000	-1.8562550000	-0.0027180000
B	0.0006270000	-0.9758640000	-1.1849260000
B	1.3941300000	-0.2809580000	-0.9040900000
B	-0.0010510000	0.6459190000	-0.8972140000
B	-1.3944240000	-0.2827040000	-0.9068800000

11

energy

Al	2.9034880000	-0.0316120000	-0.1735590000
Al	1.2865440000	-2.0709440000	0.0165610000
Al	-1.2936550000	-2.0678870000	0.0170750000
Al	-0.0006970000	0.2465280000	-1.2052680000
Al	-2.9030090000	-0.0231820000	-0.1733800000
Al	0.0053900000	2.7050600000	-0.2417070000
B	1.5029710000	1.2777650000	0.6475580000
B	0.8660150000	-0.2368310000	1.0074130000
B	-0.8662990000	-0.2346760000	1.0067940000
B	0.0015020000	1.1408630000	1.2675210000
B	-1.4991470000	1.2821710000	0.6474370000

12

energy

Al	-2.6170140000	0.6226790000	-0.8826240000
Al	1.8409370000	1.7079600000	0.0706650000
Al	-0.8278670000	2.1773340000	0.2536260000
Al	-2.0711510000	-1.6733930000	0.2019210000
Al	3.0261060000	-0.7447290000	-0.6769890000
Al	0.1464090000	-0.3829370000	-1.0924320000
B	-1.3158360000	0.1976620000	1.0111490000
B	0.1720220000	0.6908170000	1.3982530000
B	-0.1048120000	-0.9534930000	1.2330080000
B	1.4476600000	-0.2354670000	1.0716250000
B	1.2610150000	-1.7745420000	0.5828180000
B	-0.1533400000	-2.3629530000	0.2303150000

13

energy

Al	2.0269660000	1.4739460000	-0.2993450000
Al	-0.0000230000	-1.0450890000	-1.1476970000
Al	3.0681220000	-1.1091260000	-0.4971830000
Al	-3.0679350000	-1.1093700000	-0.4969600000
Al	-0.0002990000	2.9353810000	0.3155690000
Al	-2.0271350000	1.4734880000	-0.2996870000
B	1.3853680000	-1.8457420000	0.7878570000
B	0.0001930000	-2.5675680000	0.8988090000
B	0.0000940000	-0.9105020000	1.3111550000
B	-1.4269890000	-0.1806530000	0.8351880000
B	1.4271070000	-0.1806140000	0.8348740000
B	0.0000690000	0.7209180000	0.8500540000
B	-1.3850490000	-1.8458380000	0.7878520000

14

energy

Al	1.2487730000	0.7858990000	-0.7085810000
Al	-0.4693500000	-2.1629920000	-0.5745880000
Al	3.1958570000	-1.2337200000	-0.9129240000
Al	-0.4681260000	3.0647310000	-0.6830010000
Al	-2.2374270000	0.7060080000	-0.7483080000
Al	-3.0191640000	-1.7292940000	0.2344900000
B	-0.8000210000	1.3541930000	0.7012520000
B	0.6485180000	2.0438670000	1.1720220000
B	0.2965250000	0.4516120000	1.6235230000
B	1.4863740000	-1.6546780000	0.2940110000
B	1.8557180000	-0.4040560000	1.3024990000
B	1.8644280000	1.1519290000	1.5765500000
B	0.2674220000	-1.1640120000	1.2488240000
B	-1.0704260000	-0.2984990000	0.9028880000

15

energy

Al	-3.6838430000	-0.3160150000	0.0172130000
Al	-1.4806150000	-2.0329370000	-0.0482810000
Al	1.0906910000	-1.8873630000	0.2616730000
Al	1.7876460000	0.3703960000	1.6353400000
Al	-1.0495280000	0.6217210000	1.2404700000
Al	3.2286310000	-0.9051080000	-0.8914470000
B	1.1011560000	0.7436170000	-0.7285400000
B	-2.2437460000	1.2956350000	-0.6767280000
B	-1.6457830000	-0.1996210000	-1.0493300000
B	-0.5463330000	1.1120860000	-1.0834990000
B	-1.2832280000	2.5002000000	-0.4418260000
B	2.7683810000	1.0249030000	-0.2316880000
B	0.2772610000	2.5373900000	-0.3561340000
B	1.8465020000	2.2252010000	-0.1915140000
B	0.0040370000	-0.4512150000	-0.9996590000

7

energy

Al	1.1043910000	0.9284240000	1.5325230000
Al	1.9164620000	-1.1296410000	0.0002430000
Al	-0.4089150000	-1.1420850000	1.3511340000
Al	-0.7819570000	1.7892400000	-0.0003760000
Al	1.1035420000	0.9274830000	-1.5337110000
Al	-0.4090650000	-1.1435210000	-1.3500070000
Al	-2.5244590000	-0.2299000000	0.0001950000

8

energy

Al	2.0869350000	1.5501980000	-0.0008080000
Al	-0.4853730000	1.3181560000	1.3883360000
Al	2.0891660000	-1.5484110000	0.0005980000
Al	-0.4857090000	1.3139040000	-1.3922400000
Al	-0.4857650000	-1.3197770000	-1.3874200000
Al	-2.4490410000	0.0007080000	0.0000310000
Al	-0.4855390000	-1.3147340000	1.3916730000
B	0.5598500000	-0.0001140000	-0.0004460000

17

energy

Al	-1.5948270000	-0.1132590000	-1.1119740000
Al	-0.8401590000	-2.2065650000	0.5814480000
Al	-0.5183790000	-2.3362390000	-2.0380270000
Al	1.4291320000	-1.2480290000	-0.6009190000
Al	0.9264040000	1.3453480000	-1.2277950000
Al	3.4136770000	0.9637910000	-0.1018640000
Al	-1.3659080000	2.7069090000	-0.6889600000
B	-1.3890650000	1.2290930000	1.0682900000
B	-0.1258880000	0.3150720000	1.7803730000
B	-1.6574590000	-0.5396020000	2.0047090000
B	-2.7559360000	1.3647630000	0.0966890000
B	-2.7676560000	0.2039280000	1.1118210000
B	0.1378870000	1.6791300000	0.8882250000
B	2.4957700000	-0.5022350000	1.1006050000
B	-0.2961390000	-1.2069670000	2.4476800000
B	1.1976080000	-0.9617830000	1.9139340000
B	1.3910360000	0.7275180000	1.0767110000

18

energy

Al	-0.8003480000	-1.4451860000	1.0290790000
Al	1.8196250000	-1.6595470000	-0.0323040000
Al	1.3934540000	-1.4684800000	2.5300500000
Al	1.1909730000	0.8442100000	1.2330070000
Al	-1.6207610000	1.2659540000	0.9069530000
Al	-0.2548700000	3.2667240000	0.0513820000
Al	-3.4713860000	-0.2375630000	-0.0770430000
B	-1.2829860000	-0.5227180000	-1.2651980000
B	0.3898410000	-0.1783580000	-1.7541660000
B	0.4085080000	-2.0070060000	-2.0346220000
B	-1.0122410000	-2.3234270000	-1.4125510000
B	-0.6970790000	0.9382610000	-1.2220760000
B	2.5153030000	1.4991530000	-0.9399920000
B	1.6906970000	-1.1977230000	-2.2527530000
B	2.2713940000	0.1504310000	-1.7282120000
B	0.8211090000	1.4207870000	-1.1985570000
B	-2.2339800000	-1.7781950000	-0.6649200000
B	1.6620520000	2.5269030000	-0.1938750000

19

energy

Al	1.5166740000	-1.8775510000	0.3787910000
Al	1.1478340000	-1.0579020000	2.8299850000
Al	-0.3237690000	2.5677780000	0.0965710000
Al	-3.4487110000	-0.9666610000	0.4076110000
Al	1.8296880000	0.8534210000	1.1024880000
Al	-0.7569930000	-0.1612600000	1.2138240000
Al	-2.6984450000	1.6049890000	-0.0707250000
B	-1.8164760000	-0.1155770000	-0.9455410000
B	2.7090160000	1.6799110000	-0.8321980000
B	-1.8099440000	-1.7712800000	-0.9370470000
B	0.8948310000	-2.1108980000	-1.8328560000
B	1.6554290000	2.6899100000	-0.3341100000
B	2.2757510000	-1.3189200000	-1.7488590000
B	-0.5439390000	-0.9513260000	-1.6440050000
B	1.0752560000	1.3890520000	-1.2760290000
B	-0.3846240000	0.6823960000	-1.3647090000
B	2.6289170000	0.1784800000	-1.3764870000
B	0.9660950000	-0.2374240000	-1.7936580000
B	-0.5426320000	-2.6176430000	-1.4067200000

20

energy

Al	-2.2760370000	0.0135950000	-0.1777180000
Al	1.5622780000	-0.0080110000	2.9000230000
Al	0.0561060000	-1.4590640000	1.2954200000
Al	0.0856370000	1.4720300000	1.2965490000
Al	2.4972090000	-0.0175700000	0.4318760000
Al	-2.6948100000	-2.4774410000	0.0227770000
Al	-2.6600900000	2.5105660000	0.0187680000

B	-0.7881040000	-1.5387330000	-1.0746580000
B	-0.7531070000	-2.9575630000	-0.2024910000
B	0.8341890000	-0.9430780000	-1.5367420000
B	0.8476860000	0.9250990000	-1.5406870000
B	2.6729150000	0.7723110000	-1.7757100000
B	2.6622510000	-0.8131600000	-1.7713580000
B	2.0397040000	-2.1214190000	-1.3312940000
B	0.6571330000	-2.6853690000	-0.8091320000
B	2.0672600000	2.0896110000	-1.3394820000
B	-0.5357050000	0.0006370000	-1.5587790000
B	-0.7662320000	1.5443160000	-1.0771270000
B	0.6922530000	2.6732310000	-0.8197660000
B	-0.7130050000	2.9654450000	-0.2107790000

21

energy

Al	1.9713980000	-0.9836490000	-1.3368150000
Al	1.8785710000	0.9915110000	0.9191500000
Al	-0.0018220000	2.8728510000	0.2458870000
Al	-1.9685020000	-0.9849830000	-1.3378940000
Al	-1.8816510000	0.9904320000	0.9191330000
Al	-0.0013500000	-0.2185180000	2.8437090000
Al	0.0019650000	-2.7978510000	-0.9080760000
B	2.9164740000	-0.9537150000	0.7257840000
B	1.4355320000	-1.4512650000	1.0232480000
B	3.6205830000	0.0632180000	-0.1796210000
B	2.8986790000	1.0409030000	-1.1223030000
B	-0.0002540000	2.0219820000	-1.8732110000
B	1.4306420000	1.4776040000	-1.5690560000
B	0.0002680000	0.5653650000	-0.9278750000
B	-1.4341750000	-1.4526210000	1.0220680000
B	-2.9155220000	-0.9567030000	0.7236280000
B	-1.4307090000	1.4761680000	-1.5698400000
B	-2.8986780000	1.0379820000	-1.1240700000
B	-3.6203910000	0.0592360000	-0.1823440000
B	0.0008320000	-2.0443300000	1.2676990000
B	0.0003380000	-0.5452860000	0.2886450000

22

energy

Al	1.1936610000	2.3299740000	-0.3000330000
Al	-3.0422440000	-0.8792990000	-0.5221660000
Al	-1.1752220000	-0.6052780000	1.6145630000
Al	1.7980930000	-0.0875880000	1.0663400000
Al	0.7721450000	-0.0731460000	-1.7411380000
Al	3.1534140000	0.7432480000	-1.0420170000
Al	1.8450870000	-2.6359730000	-0.1283650000
B	-1.9105790000	1.0834020000	-0.6740150000
B	-1.6893820000	1.8935010000	0.9011070000
B	0.5798170000	-0.8362250000	2.7187730000
B	0.5181050000	-2.0215000000	1.6540470000
B	-0.0806980000	2.0200110000	1.9742870000
B	0.3968890000	0.6967780000	2.6853230000
B	-1.0342080000	2.6777590000	-0.5979430000
B	-0.4901460000	3.0243050000	0.8591410000
B	-1.0152830000	1.8011620000	-1.9130180000
B	-2.6040250000	0.6041560000	0.7760470000
B	-0.3896300000	-2.4496520000	0.3998610000
B	0.0048820000	-2.1734860000	-1.2395950000
B	-1.5648450000	-2.2711460000	-0.6958420000
B	-1.1175440000	-1.2366550000	-1.9342240000
B	-1.4201810000	0.3285500000	-2.1766280000

23

energy

Al	2.1506560000	1.6311650000	-0.0001760000
Al	-1.9112940000	-0.2438280000	1.3931070000
Al	1.2984400000	-0.8211480000	1.3121340000
Al	1.4021290000	-0.5725000000	-1.5617540000
Al	3.5226360000	-0.5950310000	-0.0746130000

Al	0.6023270000	-3.2197160000	-0.2838650000
Al	-3.7896600000	0.0067290000	-0.3760840000
B	-0.7372300000	2.0568320000	-0.9377640000
B	-0.7769750000	2.2784120000	0.7966490000
B	-0.4314010000	-1.1927110000	2.5782700000
B	-0.6066440000	-2.1165430000	1.2904830000
B	0.2654250000	1.7314480000	2.2346620000
B	-0.0757740000	0.2868520000	2.7972720000
B	0.5265810000	3.0690010000	-0.2933200000
B	0.7062050000	2.8674210000	1.2813990000
B	0.6968660000	2.4076020000	-1.7275220000
B	-1.9757120000	1.5329350000	0.0546160000
B	-1.2582510000	-1.9093250000	-0.1618030000
B	-0.4853680000	-1.7827010000	-1.6338760000
B	-1.8902830000	-0.9267760000	-1.3328340000
B	-0.6669000000	-0.3185810000	-2.3428470000
B	-0.1310080000	1.1991570000	-2.3359540000
B	-1.6751420000	0.7342320000	-1.3301790000

9

energy

Al	2.8595380000	0.0009060000	0.3894710000
Al	1.0051840000	1.5287870000	-0.9406250000
Al	1.0039880000	-1.5337420000	-0.9337200000
Al	-1.2859580000	1.9117640000	0.4550880000
Al	-0.7261800000	0.0062870000	2.2680780000
Al	-1.2848480000	-1.9087050000	0.4668850000
Al	-1.7204860000	-0.0061110000	-1.9276930000
B	0.8012690000	0.0021320000	0.8063130000
B	-0.4144870000	-0.0000140000	-0.2277730000

10

energy

Al	0.0350980000	0.1968910000	1.6152570000
Al	-2.0393840000	-1.1683480000	0.8756420000
Al	-2.9860140000	0.7979840000	-0.6941900000
Al	2.5470370000	1.2188090000	-0.5111140000
Al	0.2283410000	2.4841510000	0.0739320000
Al	2.3016720000	-1.1831040000	0.3783530000
Al	0.3916810000	-2.3596620000	-0.8777880000
B	-0.8632850000	0.8429280000	-0.6472970000
B	-0.9289890000	-0.7379560000	-0.9403600000
B	0.5483500000	-0.0704440000	-0.6485830000

11

energy

Al	0.1454190000	0.1158820000	1.2834430000
Al	2.9698010000	0.5845100000	-0.0038040000
Al	1.9628290000	-1.7597300000	-0.0124950000
Al	-0.1401430000	2.6509700000	0.4723930000
Al	-2.5855250000	-1.1632690000	0.4054840000
Al	-2.2956590000	1.2440250000	-0.5224410000
Al	-0.4871510000	-2.4540610000	-0.1767800000
B	1.2627730000	1.4985400000	-0.7565350000
B	-0.2356900000	1.0665720000	-1.1693100000
B	-0.8103350000	-0.4240020000	-0.8744110000
B	0.9023720000	-0.1087620000	-0.9588230000

12

energy

Al	3.0781450000	-0.4926680000	-0.5377940000
Al	-2.0977270000	-1.4571270000	0.2420820000
Al	1.8259500000	2.0106370000	0.0086290000
Al	0.1404420000	-0.0466730000	-1.0715840000
Al	-0.8363930000	2.3932220000	0.1717130000
Al	-2.7555160000	0.8374060000	-0.7157060000
Al	0.0107060000	-2.8436660000	-0.1073440000
B	1.4684800000	0.0478300000	1.0622380000
B	-0.0376540000	-0.8046610000	1.1808420000
B	0.1496720000	0.8745050000	1.3759710000
B	1.3712080000	-1.4934390000	0.5965680000

B	-1.3022840000	0.3328220000	1.0103910000
13			
energy			
Al	2.9733490000	-0.0001200000	-1.0085360000
Al	1.1065000000	1.8555650000	-0.6165290000
Al	-1.4478450000	2.3754860000	-0.4245890000
Al	1.7410740000	-0.0000760000	1.4270060000
Al	1.1063110000	-1.8555860000	-0.6165570000
Al	-2.6226560000	0.0000910000	-0.8388620000
Al	-1.4480530000	-2.3754130000	-0.4245750000
B	-0.2512300000	0.0000170000	0.0463100000
B	0.0150620000	1.4424270000	1.1714930000
B	-0.3163480000	0.0000040000	1.9077470000
B	0.0149280000	-1.4424490000	1.1714920000
B	-1.5625230000	-0.8334860000	1.1048980000
B	-1.5624550000	0.8336240000	1.1049290000
14			
energy			
Al	1.2181750000	-0.1907870000	1.6605820000
Al	-1.1441500000	1.9125780000	1.4224620000
Al	1.2131340000	-1.3434270000	-0.9967940000
Al	-1.1403350000	-2.1877480000	0.9473930000
Al	1.2111530000	1.5363560000	-0.6658670000
Al	-1.1522470000	0.2734160000	-2.3661300000
Al	3.4955210000	0.0021500000	-0.0062510000
B	-0.8301730000	-0.2197490000	1.8946870000
B	-0.6103910000	0.0000490000	-0.0002020000
B	-2.1716270000	0.8889530000	-0.3817200000
B	-2.1674900000	-0.1134610000	0.9679490000
B	-2.1706200000	-0.7810510000	-0.5751430000
B	-0.8352680000	-1.5306000000	-1.1366420000
B	-0.8376810000	1.7492570000	-0.7569560000
15			
energy			
Al	-0.3949100000	2.7894160000	-0.6648290000
Al	-2.6604790000	1.3656710000	-0.4720970000
Al	-3.4502460000	-1.3071730000	0.3894510000
Al	1.8230230000	-1.6550190000	-0.8315990000
Al	1.5785970000	1.0674850000	-1.1256760000
Al	-0.8500000000	-2.2771070000	-1.0567420000
Al	3.7309360000	-0.3665380000	0.5584780000
B	-0.2431730000	-0.0375050000	1.2583650000
B	-0.8707650000	1.4894490000	1.0622630000
B	-1.8972690000	0.2100350000	1.1439400000
B	-1.2645490000	-1.3273620000	0.8951900000
B	0.3526770000	-1.5113030000	0.8105140000
B	1.4295650000	-0.3181510000	1.0750120000
B	0.7550480000	1.4132180000	1.1278310000
B	2.3184710000	1.0781100000	0.9547190000
16			
energy			
Al	-3.5487430000	-1.3249650000	0.3463810000
Al	-1.2754250000	-1.7596040000	-0.9118340000
Al	1.2752220000	-1.7573670000	-0.9128910000
Al	1.7824480000	0.9405680000	-1.0550360000
Al	-1.7837920000	0.9371810000	-1.0561200000
Al	-0.0026640000	2.9209620000	-0.7574060000
Al	3.5501910000	-1.3248730000	0.3441790000
B	1.4434720000	-0.5605040000	1.1428990000
B	-2.7214040000	0.4651980000	0.8911880000
B	-1.4418180000	-0.5614440000	1.1424000000
B	0.0005590000	0.3299990000	1.3946430000
B	-1.4451510000	1.3413860000	1.2863260000
B	2.7229240000	0.4654250000	0.8900900000
B	0.0008900000	2.0017430000	1.3724240000
B	1.4467400000	1.3406840000	1.2877740000
B	0.0009720000	-1.2654340000	0.9993450000

8

energy

Al	3.2268790000	-0.0004050000	-0.1195960000
Al	-1.2313560000	-1.6685670000	0.5188440000
Al	-1.2299940000	1.6679350000	0.5211020000
Al	0.2507380000	-0.0019700000	1.9203420000
Al	1.1743270000	1.5548860000	-0.3501420000
Al	-2.9242720000	0.0009710000	-0.4302390000
Al	-0.4395720000	0.0015320000	-1.7079110000
Al	1.1732510000	-1.5543820000	-0.3523990000

9

energy

Al	-1.5792530000	-0.0867020000	-1.8785190000
Al	1.0002770000	-0.7414720000	1.4704740000
Al	1.0001920000	-0.7692380000	-1.4562390000
Al	-1.1837550000	-2.0062350000	0.0205720000
Al	3.1533070000	0.0886790000	-0.0013290000
Al	-1.7131180000	1.8023710000	-0.0184330000
Al	1.0098930000	1.7252820000	-0.0167380000
Al	-1.5778020000	-0.0474430000	1.8806360000
B	-0.2853240000	0.0903720000	-0.0011050000

18

energy

Al	-0.9563610000	-1.3313320000	-1.6347230000
Al	-0.9200410000	-1.4693850000	1.2760100000
Al	-1.8148290000	0.8159860000	-0.1647920000
Al	-3.3221490000	-1.6597610000	-0.2021160000
Al	2.7564840000	0.6590580000	-0.8319560000
Al	0.7865640000	2.2562730000	-0.1276690000
Al	1.8170430000	-2.2202040000	-0.7733850000
Al	2.0223230000	-1.0815530000	1.4698800000
B	-0.1941580000	0.8466390000	2.8685880000
B	0.5533770000	-0.4899140000	2.7335040000
B	-1.2385830000	2.8594050000	0.6842020000
B	-0.6829980000	1.9335190000	1.8234770000
B	-1.2455060000	2.9043200000	-0.8643140000
B	0.3594690000	0.7364890000	-2.0536370000
B	-0.6160830000	1.9661200000	-1.9019950000
B	0.3555250000	0.5303710000	1.2598260000
B	1.1684450000	-0.5644220000	-1.8014520000
B	0.5810270000	-0.2421450000	-0.1774440000

19

energy

Al	0.8955510000	0.1572550000	1.3101940000
Al	0.2869750000	-2.5141570000	0.3098470000
Al	-0.2528280000	-1.7708480000	2.7442670000
Al	-1.8561740000	-0.7156870000	0.9193690000
Al	-0.4717130000	2.3095690000	0.3415140000
Al	2.0319290000	2.5823660000	-0.1100740000
Al	-3.0188580000	2.1570540000	0.1843280000
Al	3.5618740000	0.4446910000	0.2202650000
B	2.3718510000	-0.8856490000	-1.0357350000
B	0.8729780000	-0.6124610000	-1.7241890000
B	-0.8135230000	-0.5826170000	-1.7904180000
B	1.5481780000	-2.1581880000	-1.5886910000
B	0.0103890000	-2.2159500000	-1.9990040000
B	0.0327220000	0.7859530000	-1.3514570000
B	-2.5286800000	-0.9349850000	-1.3933010000
B	-3.1102760000	0.3273990000	-0.6294040000
B	-1.5638230000	0.8275840000	-1.0721540000
B	1.6789080000	0.6473730000	-0.9685330000
B	-1.5582900000	-2.0890910000	-1.8383640000

20

energy

Al	-0.4283280000	-2.2193420000	-1.3332350000
Al	-3.6532580000	1.1385760000	-0.7723730000
Al	2.0390240000	1.8305470000	-0.4435330000

Al	-0.1213620000	3.1108530000	0.0826730000
Al	1.8968240000	-0.8274230000	-1.4041110000
Al	-0.6626970000	0.5891710000	-0.9349560000
Al	4.1253690000	0.1215540000	-0.0199790000
Al	-2.8000750000	-1.2517810000	0.2092160000
B	-1.5882910000	-2.8634290000	0.5519920000
B	-0.9120940000	1.5362180000	1.4072910000
B	-2.1906840000	0.6321800000	0.9155980000
B	-0.1045800000	-3.2665200000	0.6952790000
B	1.1892570000	-2.3289220000	0.8189980000
B	-0.8085860000	-0.1464050000	1.4921500000
B	2.0982020000	0.3819670000	1.1826540000
B	0.6148000000	1.0597670000	1.4034770000
B	-0.4998550000	-1.7635290000	1.3154720000
B	2.3499550000	-1.1848230000	0.8191190000
B	0.7916870000	-0.6603120000	1.1679310000
B	-1.9681050000	2.1242040000	0.2324150000

21

energy

Al	-0.4889050000	3.1027190000	-0.4149900000
Al	-2.4157080000	1.7083730000	0.4140050000
Al	-1.6491720000	-1.5690580000	1.3206570000
Al	1.9038380000	2.3195760000	0.1434170000
Al	2.5889230000	-0.2675970000	1.5336990000
Al	0.0267330000	0.5786970000	1.1630760000
Al	0.8833960000	-2.3581500000	0.9010150000
Al	-4.2294300000	-0.2052190000	-0.0085030000
B	-0.8791120000	1.0348870000	-1.1118370000
B	3.5695370000	1.1639710000	-0.1148320000
B	-1.9577110000	-0.2439220000	-0.9582290000
B	0.1261030000	-2.3200200000	-1.4180700000
B	-0.3977860000	-0.5217530000	-1.4939540000
B	2.2871750000	0.3645480000	-0.9840220000
B	0.7371900000	0.6861770000	-1.2869120000
B	-1.4117800000	-1.9368360000	-1.1600860000
B	2.8254650000	-1.4996450000	-0.9185800000
B	1.2507830000	-0.9240940000	-1.4628860000
B	3.7934010000	-0.3015530000	-0.4638960000
B	-2.8292690000	-1.5735140000	-0.5102600000
B	1.6748470000	-2.5325330000	-1.2526110000

22

energy

Al	1.7452110000	-0.6626560000	1.1909950000
Al	0.7941770000	-1.0807930000	-1.8550960000
Al	-1.5194110000	1.0966130000	1.5320880000
Al	-2.6982060000	0.6133410000	-1.1719310000
Al	-1.7756580000	-1.8900400000	-1.7433270000
Al	-0.5551200000	-1.2680600000	2.5435500000
Al	2.3663760000	2.2548860000	-0.1062690000
Al	4.1994160000	0.3703440000	0.6805790000
B	-1.0625840000	2.4654350000	-0.5788400000
B	0.3955530000	2.3384970000	-1.1570590000
B	2.5130360000	0.2034820000	-1.0314660000
B	1.2006670000	1.0470800000	-1.5661270000
B	2.7491940000	-1.3356590000	-0.7441180000
B	1.6812190000	-2.3168170000	-0.2909300000
B	-0.2659450000	0.8222660000	-0.6534530000
B	-2.4914280000	2.5362310000	0.0813980000
B	-2.3989910000	-1.0418370000	0.7360630000
B	-3.4757040000	0.1108100000	0.8927340000
B	-1.3899360000	-2.2178460000	0.4741590000
B	0.1765430000	-2.1779340000	0.2512800000
B	-0.6991790000	-0.5768810000	0.1178380000
B	-3.5800890000	1.6157270000	0.6849920000

23

energy

Al	-0.6828390000	-2.4897940000	-0.6953660000
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Al	2.0250290000	2.2568070000	-1.3770250000
Al	0.9932160000	0.9627970000	1.1943430000
Al	-1.5641630000	-0.7839140000	1.3949700000
Al	-1.5532480000	0.0698460000	-1.4809110000
Al	-3.1827440000	-1.7217720000	-0.4745040000
Al	-2.9408870000	1.6936140000	1.0068160000
Al	3.7580500000	-0.5863150000	1.4338740000
B	1.5743210000	-0.0506530000	-1.4951410000
B	1.9844720000	-1.1396670000	-0.2157840000
B	-0.1103740000	0.0673070000	2.7654690000
B	-0.9340980000	1.2970900000	2.1836610000
B	1.1849940000	-2.1419180000	1.1032520000
B	1.3235800000	-1.8678860000	-1.6965290000
B	1.4342020000	-2.6992160000	-0.3356600000
B	0.6229160000	-0.8295720000	-2.6633780000
B	2.4444400000	0.4085740000	-0.1720520000
B	-0.7200320000	2.2934610000	0.9336880000
B	-1.4117510000	2.1823060000	-0.5824550000
B	0.1920750000	2.6593200000	-0.3533200000
B	-0.3395320000	1.8980280000	-1.7544600000
B	0.3675540000	0.6924040000	-2.5479240000
B	0.5709560000	-1.2128770000	2.2249260000

24

energy

Al	-0.1412200000	2.7778760000	0.6484230000
Al	-2.5661260000	-2.2694900000	-0.5485500000
Al	-2.5047410000	1.4480940000	1.3330630000
Al	2.4217650000	1.6283100000	0.4461240000
Al	-0.0450750000	-2.5646200000	-0.2908390000
Al	-0.0488130000	-0.0216650000	0.8726150000
Al	2.2197420000	-0.1277660000	2.5936620000
Al	1.9958300000	-2.0064880000	-1.7499200000
B	1.0437180000	0.2443670000	-1.8324750000
B	-0.4120980000	1.0232170000	-1.4092710000
B	-1.8511850000	0.0961020000	-1.3153310000
B	-3.1397340000	-0.2639840000	-0.0994940000
B	-1.9108560000	1.9706110000	-1.3699370000
B	-3.1177660000	1.1092520000	-0.8469830000
B	0.8971970000	2.1098100000	-1.8838910000
B	-0.5269490000	2.7260150000	-1.5572960000
B	2.2997330000	1.3948290000	-1.7944930000
B	-0.3419200000	-0.6339020000	-1.4430990000
B	2.6981830000	-0.0143870000	-1.2362250000
B	1.6326700000	-1.7225810000	1.0253120000
B	2.5171060000	-0.6230660000	0.2970250000
B	-1.2120230000	-1.7245930000	1.7343190000
B	0.3196510000	-2.0046030000	1.8250840000
B	-2.3572670000	-0.7341430000	1.3148510000

10

energy

Al	0.0016260000	-2.5971630000	0.0002720000
Al	-2.2966620000	-1.1306250000	0.0001460000
Al	-0.0012210000	-0.5581910000	-1.7941800000
Al	-2.7114970000	1.4647810000	-0.0000950000
Al	-0.0002780000	2.6422970000	-0.0000970000
Al	2.7102230000	1.4665230000	-0.0000860000
Al	2.2978290000	-1.1293130000	-0.0008400000
Al	0.0001390000	-0.5577350000	1.7948660000
B	-0.8057090000	0.5194380000	0.0003400000
B	0.8052930000	0.5190740000	-0.0003000000

11

energy

Al	-1.1829970000	2.3354880000	-0.1478480000
Al	-2.9559950000	0.6307930000	0.3151020000
Al	-2.0262790000	-1.5845230000	-0.6154700000
Al	-0.0112610000	0.0483130000	1.3383140000
Al	0.0231490000	-2.5775210000	0.7239950000

Al	2.8046690000	0.5139330000	0.4991440000
Al	1.3533410000	2.3806830000	-0.2929080000
Al	2.0142920000	-1.5839430000	-0.7529160000
B	-0.8965560000	0.2994810000	-0.8635250000
B	0.8554970000	0.3169040000	-0.8518480000
B	-0.0081330000	-1.0407630000	-1.0599020000

12

energy

Al	-0.0005950000	-0.1073450000	-1.1327310000
Al	2.9705120000	-0.5449570000	-0.8081520000
Al	2.1388950000	1.6873120000	0.4658880000
Al	1.3154560000	-2.3241350000	0.2755570000
Al	-2.1388820000	1.6871730000	0.4651620000
Al	-1.3147750000	-2.3242480000	0.2752210000
Al	0.0000640000	2.6228710000	-0.4026770000
Al	-2.9708040000	-0.5452500000	-0.8071600000
B	1.3887290000	-0.1925590000	0.9510990000
B	0.0002180000	0.8296700000	1.0752230000
B	-1.3886230000	-0.1921750000	0.9515850000
B	0.0000120000	-0.8386350000	1.3612120000

13

energy

Al	1.4657980000	-2.4729990000	-0.3473020000
Al	-1.3159390000	-2.3267780000	-0.3279090000
Al	2.8807970000	0.0002300000	-0.5681040000
Al	-2.6909670000	-0.0006760000	-1.1462090000
Al	1.4652640000	2.4734840000	-0.3473450000
Al	-1.3169640000	2.3263070000	-0.3281320000
Al	-1.8129370000	0.0000990000	1.3799030000
Al	0.1621520000	0.0001190000	-0.7840150000
B	-0.0761460000	-1.4772290000	1.1968200000
B	1.4754170000	-0.8367860000	1.0992130000
B	1.4753790000	0.8371030000	1.0988960000
B	-0.0763700000	1.4773260000	1.1964200000
B	0.2249950000	0.0001460000	1.8283470000

14

energy

Al	1.4146820000	-2.3524040000	-0.2219730000
Al	2.6964910000	0.0000060000	-0.5575340000
Al	1.4146520000	2.3523930000	-0.2219520000
Al	-1.2080630000	-1.7852800000	-0.3485300000
Al	-3.4889160000	-0.0000330000	-0.7446340000
Al	-1.2081020000	1.7853070000	-0.3484400000
Al	0.3529290000	0.0000700000	-2.2307820000
Al	-1.6536090000	-0.0000320000	1.6549220000
B	0.0925790000	-1.4382340000	1.3865720000
B	1.6804940000	-0.8282830000	1.3270030000
B	1.6804920000	0.8282600000	1.3270290000
B	0.3855320000	0.0000030000	0.2631770000
B	0.4361540000	-0.0000240000	2.1588090000
B	0.0925830000	1.4382070000	1.3866130000

15

energy

Al	-0.1807660000	-3.1029260000	-0.6091760000
Al	2.5594530000	-1.9076520000	-0.0610880000
Al	-3.1062710000	-1.7428460000	-0.1054920000
Al	-3.4989690000	1.3900710000	0.4485690000
Al	-0.6643160000	3.0237690000	-0.6286720000
Al	-0.2911540000	-0.0660730000	-1.2831460000
Al	3.7223250000	0.3546060000	0.5813530000
Al	2.0941870000	2.1186060000	-0.5198080000
B	0.6766890000	-1.3866580000	0.7421990000
B	-0.9593050000	-1.4841860000	0.6918740000
B	-1.9132500000	-0.1463520000	0.8964540000
B	1.4698930000	0.0946780000	0.7882120000
B	-1.1745990000	1.3268570000	0.7085220000
B	-0.2106400000	-0.0151440000	1.1909360000

B	0.461540000	1.435162000	0.643199000
16			
energy			
Al	0.634861000	0.665103000	1.755815000
Al	2.465124000	-1.129650000	0.642100000
Al	0.826353000	2.628966000	-0.237795000
Al	-2.606973000	-1.041817000	0.928598000
Al	-0.114316000	-1.814981000	1.172306000
Al	-1.809175000	1.583716000	0.912819000
Al	1.158969000	-2.245145000	-1.282237000
Al	2.801323000	1.089710000	-0.473398000
B	0.775284000	0.080608000	-0.578458000
B	-1.022653000	2.619122000	-1.052623000
B	-2.105147000	1.615503000	-1.461111000
B	-2.249398000	0.040113000	-1.432168000
B	-0.516977000	0.980295000	-1.104608000
B	-0.625555000	-0.708128000	-1.022292000
B	-2.088865000	-1.524809000	-1.348713000
B	-0.892726000	-2.416045000	-0.887369000
17			
energy			
Al	-2.676982000	1.151671000	-0.143028000
Al	-0.409170000	0.881609000	1.329257000
Al	-1.901210000	-1.484759000	-0.285299000
Al	0.568345000	-1.686635000	1.037177000
Al	-1.891398000	-1.156020000	2.315799000
Al	2.175945000	0.898856000	0.746192000
Al	1.134332000	3.204706000	0.074737000
Al	3.341165000	-1.255029000	-0.080290000
B	1.257033000	-0.404197000	-0.905830000
B	0.336586000	-1.931727000	-1.742545000
B	1.675108000	-2.062128000	-0.895058000
B	-0.625582000	2.274913000	-0.492067000
B	-1.064945000	-1.457920000	-2.344169000
B	-0.146402000	-0.167099000	-1.819879000
B	0.525994000	1.054000000	-0.878865000
B	-1.076739000	1.311458000	-1.695576000
B	-1.767724000	-0.058737000	-2.211827000
9			
energy			
Al	0.740300000	2.462552000	0.000084000
Al	-2.137816000	-0.565878000	1.276113000
Al	-1.748430000	1.802366000	-0.000809000
Al	-0.352499000	-2.226434000	0.000359000
Al	0.317389000	0.071833000	1.373296000
Al	-2.137266000	-0.567575000	-1.276728000
Al	2.235305000	-1.839801000	-0.000037000
Al	0.317665000	0.071883000	-1.371532000
Al	2.765352000	0.791056000	-0.000746000
10			
energy			
Al	-0.206141000	0.082323000	-1.312637000
Al	-2.862416000	-0.703050000	-0.299939000
Al	-2.212438000	1.830500000	-0.196914000
Al	-0.679514000	-2.374905000	-0.454153000
Al	0.415112000	2.428591000	0.246968000
Al	2.108833000	-1.129935000	-0.901130000
Al	2.799125000	1.289120000	-0.218656000
Al	1.096353000	-1.655578000	1.444213000
Al	-0.845309000	0.114587000	1.484908000
B	1.004628000	0.307701000	0.539083000
19			
energy			
Al	-1.132763000	-2.131858000	0.760961000
Al	-0.895416000	0.716832000	1.305173000
Al	3.741142000	-0.941264000	-0.935353000
Al	1.456946000	-1.059982000	0.820807000

Al	2.9607860000	1.4390150000	0.0688420000
Al	0.8532780000	2.9079150000	0.7353640000
Al	-0.0607620000	-1.2059780000	3.0217760000
Al	-3.1016800000	-0.1972080000	-0.2303010000
Al	-2.7961020000	2.3014050000	-0.7411960000
B	-2.6087030000	-1.9922600000	-1.0411350000
B	-1.2940080000	-2.6346730000	-1.5101430000
B	-1.3181740000	-0.9039970000	-1.4752790000
B	0.5476930000	1.3227780000	-0.9459760000
B	1.8017860000	0.2783960000	-1.2527610000
B	1.6128150000	-1.3442570000	-1.5084330000
B	0.2501000000	-0.2980580000	-1.5305910000
B	-0.7529150000	2.1880800000	-0.4805830000
B	-1.0931800000	0.6972110000	-1.1483030000
B	0.1884710000	-2.0683040000	-1.6025850000

20

energy

Al	0.2829550000	-2.2213920000	1.0183120000
Al	-1.9502100000	-0.4711910000	1.0196990000
Al	0.7887270000	0.6173300000	1.1278720000
Al	-4.0535880000	0.5115250000	-0.5203210000
Al	-0.3593160000	-0.7454380000	3.1362580000
Al	3.2119850000	0.8446290000	-0.3695930000
Al	2.7064820000	-1.5792660000	-0.6772080000
Al	2.1176480000	3.0962720000	0.4164610000
Al	-1.9124490000	2.3906270000	-0.2819790000
B	-2.3175770000	-0.9791630000	-1.2459900000
B	-0.1164750000	-3.2410070000	-1.0304350000
B	1.3969560000	-3.0966320000	-0.8112640000
B	0.5725450000	-1.7102490000	-1.4593930000
B	-0.3142680000	1.1083940000	-1.2436910000
B	1.3201050000	1.4707580000	-1.0718020000
B	0.9919100000	-0.1260980000	-1.3807620000
B	-1.8957620000	0.5597970000	-1.3623670000
B	-0.6797570000	-0.5814590000	-1.4748060000
B	-1.3214590000	-2.2215980000	-1.1810590000
B	0.1999730000	2.4652060000	-0.3991320000

21

energy

Al	4.0037470000	-1.4420930000	-0.3049610000
Al	1.4509510000	-1.3241940000	-1.2702360000
Al	3.0280260000	1.1125620000	-0.5690440000
Al	-1.2004270000	-2.0358470000	-1.1930090000
Al	1.3931090000	3.1225550000	0.1190490000
Al	-0.2762570000	0.8946610000	-1.1211930000
Al	-3.8117620000	-1.5320500000	-0.4256050000
Al	-3.1037590000	1.0923030000	-0.4565070000
Al	-1.4359600000	3.2226160000	-0.0290650000
B	1.2516230000	0.8821530000	1.1070830000
B	2.4177630000	-0.2980240000	0.9029830000
B	2.1215080000	-1.9138550000	0.8768830000
B	0.6757370000	-2.5955680000	1.0975280000
B	0.9723180000	-0.8392290000	1.5002730000
B	-0.8690960000	-2.9689280000	1.0281700000
B	-1.9488220000	-0.3411260000	0.9933650000
B	-1.5894320000	1.2861850000	1.0649850000
B	-0.0640760000	1.8648920000	1.1614780000
B	-0.3374920000	0.2436650000	1.4195550000
B	-2.1189620000	-2.0035200000	1.0046110000
B	-0.6350040000	-1.4039740000	1.4945700000

22

energy

Al	3.9138700000	-1.9538360000	-0.5111800000
Al	1.4556500000	2.0029940000	-0.7099560000
Al	1.5623360000	-0.9676420000	-1.3357610000
Al	3.8618450000	0.8602530000	-0.2935070000
Al	-2.9284440000	-3.0480900000	-0.2618110000

Al	-3.8830120000	-0.6080750000	-0.2251280000
Al	-2.5094960000	1.4735600000	-0.5994210000
Al	-1.1117410000	-0.8471390000	-1.1994050000
Al	-1.4593440000	3.7708510000	-0.3970750000
B	0.8908680000	2.0672440000	1.4785390000
B	1.8055150000	0.7438800000	1.3887570000
B	2.6839890000	-0.5754850000	0.8669210000
B	0.1197630000	3.1739500000	0.6655750000
B	-0.8618040000	1.8850230000	1.0460770000
B	0.1044630000	0.5470700000	1.5468440000
B	1.1172060000	-0.8404500000	1.3888370000
B	0.4542970000	-2.3854790000	0.9768840000
B	-2.1708420000	-1.1836820000	0.9505650000
B	-1.5478290000	0.3819140000	1.1843800000
B	-0.5808680000	-1.0107430000	1.4238250000
B	2.0090210000	-2.0845920000	0.6497500000
B	-1.1681030000	-2.4941260000	0.8194810000

23

energy

Al	0.9545470000	0.0004520000	-1.2583300000
Al	-1.8880830000	-0.0006200000	-0.9047780000
Al	0.0456880000	-2.7255420000	-0.6790800000
Al	-3.0776030000	2.4177040000	-0.9284660000
Al	2.6492290000	2.5693570000	-0.3433820000
Al	0.0436900000	2.7255240000	-0.6792360000
Al	3.6277720000	0.0010250000	-0.6166370000
Al	2.6511530000	-2.5676790000	-0.3443420000
Al	-3.0766660000	-2.4192520000	-0.9280540000
B	-0.5677280000	2.4711200000	1.4448690000
B	0.8582980000	1.7029470000	1.3654290000
B	2.1827260000	0.8126470000	0.9408740000
B	2.1831090000	-0.8116760000	0.9408440000
B	0.8347930000	0.0000990000	1.4691780000
B	-2.1189640000	-0.0006720000	1.4645180000
B	-2.0179920000	-1.5648320000	1.1010650000
B	-0.5662720000	-2.4715240000	1.4449090000
B	0.8593500000	-1.7026650000	1.3657530000
B	-0.6174270000	-0.8314560000	1.8957000000
B	-2.0191630000	1.5635120000	1.1009680000
B	-0.6176840000	0.8309660000	1.8952030000
B	-1.7042050000	-3.0448940000	0.4722040000
B	-1.7061320000	3.0439100000	0.4724810000

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energy

Al	-2.3144010000	-2.1159810000	1.6323120000
Al	0.3076010000	-1.9096240000	1.0032480000
Al	-1.6796650000	-1.5233520000	-1.1701010000
Al	-1.9808350000	2.4583460000	1.2033740000
Al	-1.8587860000	1.4956640000	-1.3192820000
Al	1.7936700000	-0.1163220000	-2.4262420000
Al	0.6738280000	2.0987620000	0.9570580000
Al	3.1153570000	2.0034040000	-0.2300370000
Al	2.7471780000	-2.3077640000	-0.1290700000
B	-2.1808310000	0.2926330000	1.9652850000
B	-2.9362700000	-0.0236300000	0.6105420000
B	-1.1423080000	0.0422790000	0.5666400000
B	-3.5455840000	-0.1109340000	-0.8643710000
B	2.1503460000	-0.9202190000	1.6010860000
B	-0.6267660000	0.0609320000	2.2122090000
B	1.0055370000	0.0546830000	2.2930110000
B	0.0259340000	0.0999110000	-0.6626710000
B	-0.2577070000	0.0047100000	-2.3643220000
B	-1.7390650000	-0.0764830000	-2.9268240000
B	-3.1600000000	-0.1296650000	-2.3444460000
B	2.2748220000	0.8131210000	1.5484660000
B	3.1680070000	-0.1629470000	-0.9781790000
B	3.2556540000	-0.1706250000	0.6034620000

B	1.6179670000	0.0100940000	-0.0151640000
25			
energy			
Al	-2.1641100000	-0.5305410000	1.3690030000
Al	-1.7108720000	2.0611080000	0.0472610000
Al	1.7185720000	1.7862020000	-0.8361160000
Al	-1.6551920000	-0.3403770000	-1.5681790000
Al	-3.7801840000	0.5109960000	-0.3527260000
Al	3.1845320000	-1.6157530000	1.1477920000
Al	1.8470590000	-1.0045130000	-1.3311360000
Al	-1.8373600000	-3.1005480000	-0.6021660000
Al	3.7890610000	0.4775720000	-0.2712140000
B	-0.0807160000	2.1391540000	-2.1786570000
B	0.7383870000	1.5626880000	1.3016520000
B	0.5319980000	0.0295860000	2.0499920000
B	-0.5450500000	-2.3677670000	1.1352800000
B	-0.3937130000	-1.4580670000	2.4247710000
B	0.2514410000	-2.2427630000	-0.2444820000
B	-0.5516060000	1.3593130000	2.6869960000
B	-0.7794340000	-0.1304440000	3.1244650000
B	0.1798490000	3.1418770000	0.5586160000
B	-0.4216140000	2.7087010000	1.9077580000
B	0.0099960000	0.7017630000	-2.8144020000
B	-0.1038140000	-2.0309940000	-1.7944680000
B	0.1091770000	-0.8357350000	-2.7763200000
B	1.6218960000	0.2545320000	0.8280350000
B	0.9582080000	-1.4048560000	1.0513560000
B	0.0570770000	3.1382330000	-1.0271370000
11			
energy			
Al	2.5346460000	-1.6112760000	-0.4404790000
Al	1.1618920000	-0.1291110000	1.4804690000
Al	2.5036640000	0.9477270000	-0.6207040000
Al	0.7303810000	2.4694510000	0.6044070000
Al	0.1553560000	-2.4191080000	0.2338870000
Al	-0.0335750000	-0.0026610000	-1.1683860000
Al	-2.3112080000	-2.0787280000	-0.3649730000
Al	-2.7441440000	0.4129720000	0.3517470000
Al	-1.3970030000	2.3278650000	-0.7988060000
B	-0.9112310000	-0.6738300000	0.9105710000
B	-0.6487930000	0.8892870000	0.9688070000
12			
energy			
Al	-0.1285900000	-0.0006290000	-0.9094420000
Al	2.4958980000	1.2643970000	-0.9152060000
Al	0.5564650000	2.4649250000	0.2755690000
Al	-1.9784270000	1.9997730000	0.2341390000
Al	2.4994670000	-1.2638790000	-0.9124770000
Al	1.7552320000	0.0007110000	1.3813970000
Al	0.5570450000	-2.4640360000	0.2737100000
Al	-3.0370170000	-0.0008250000	-1.1429630000
Al	-1.9780620000	-2.0002800000	0.2356680000
B	-0.1883730000	0.8311040000	1.4034040000
B	-1.5530660000	-0.0003910000	1.0399810000
B	-0.1877860000	-0.8311210000	1.4035900000
13			
energy			
Al	-2.7710650000	0.9689220000	-0.5114420000
Al	-0.8345370000	2.7713620000	-0.1914220000
Al	-2.6343190000	-1.7289730000	-0.8116280000
Al	1.6119260000	-2.2847940000	-0.7273230000
Al	2.8275900000	0.0349680000	-1.1938560000
Al	-0.4837120000	-2.2250410000	0.9731180000
Al	1.7927720000	-0.3936430000	1.3427670000
Al	1.6952590000	2.1403350000	-0.0620070000
Al	-0.1304830000	0.0656620000	-0.8015120000
B	-1.7322730000	-0.4679650000	0.8968440000

B	0.4016580000	1.2921920000	1.3784930000
B	-0.2602980000	-0.2038380000	1.6916730000
B	-1.2000060000	1.0727320000	1.1895850000

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energy

Al	1.5040470000	-1.9432600000	0.4493370000
Al	-3.3555470000	-0.3429890000	-0.2729330000
Al	-1.1886130000	-2.2245800000	0.3609990000
Al	2.1882690000	-0.5090270000	-1.9009670000
Al	1.0321750000	-0.1480240000	2.3758260000
Al	-1.4167330000	0.4821540000	1.5106170000
Al	2.3802010000	0.8944620000	0.3309940000
Al	0.2569440000	2.5295490000	0.5764280000
Al	-1.4965180000	1.5159040000	-1.1976540000
B	0.2745730000	-1.4409250000	-1.2838600000
B	-1.2107780000	-0.6642790000	-1.1681050000
B	0.0890970000	0.0934250000	-1.9729060000
B	0.7771600000	1.3672690000	-1.2177880000
B	0.3189630000	-0.0163820000	-0.1622210000

15

energy

Al	3.1482080000	-0.9499230000	0.2141430000
Al	0.5453110000	-2.0741980000	1.0384250000
Al	2.1006100000	1.1186510000	-1.6175680000
Al	1.1822940000	-1.3879030000	-1.6140100000
Al	-3.8825850000	-0.5216230000	-0.6907190000
Al	-1.8926360000	-0.6275340000	1.4167790000
Al	-1.3228880000	-1.0144690000	-1.3880640000
Al	-2.1565530000	1.5301330000	-0.1634510000
Al	0.4871670000	2.6046190000	-0.0737590000
B	2.1381190000	1.0129250000	0.5706060000
B	1.6683290000	-0.2143740000	1.6488500000
B	0.0833900000	-0.1148190000	2.0410740000
B	0.9423980000	1.3187930000	1.6731840000
B	0.4838990000	0.1885160000	0.2418840000
B	-0.6593450000	1.2467990000	1.3077860000

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energy

Al	2.7250470000	0.9864840000	-0.5560080000
Al	2.3917610000	-1.5098320000	-0.9107050000
Al	0.5138250000	2.4171370000	1.0425070000
Al	1.4280740000	-0.0536900000	1.6633810000
Al	0.9073590000	-2.5918100000	0.8451130000
Al	-1.0871090000	-0.9280570000	1.4526590000
Al	-2.0900790000	1.4851550000	1.0414500000
Al	-3.0236110000	-0.9864210000	-0.5397720000
Al	-0.7672540000	-2.2258930000	-1.1629070000
B	-0.0137970000	2.7418780000	-1.3982480000
B	0.4473610000	-0.4352920000	-0.4699970000
B	1.4630660000	2.4522360000	-1.1540910000
B	0.4447480000	1.1033750000	-1.0810830000
B	-1.0361170000	0.1599450000	-0.9179280000
B	-1.3796790000	1.9321940000	-1.3477780000
B	-2.5204160000	0.9036720000	-1.1077420000

17

energy

Al	0.8241290000	-1.2613130000	1.2450430000
Al	-1.4504610000	-2.1175410000	0.1656680000
Al	-2.2632190000	-0.7561010000	2.3406750000
Al	2.8947490000	-1.9743120000	-0.7084280000
Al	-0.3280490000	1.0567570000	1.6170240000
Al	-2.4577060000	0.4511230000	-0.1907740000
Al	2.7240850000	0.4221500000	0.4848300000
Al	1.6302290000	2.6751920000	0.6797230000
Al	-0.2579410000	2.7445070000	-0.9383300000
B	0.4222480000	-0.7872330000	-1.1047970000
B	0.8203300000	0.7366100000	-0.5654590000

B	-0.4318770000	0.5842470000	-1.6128390000
B	-1.6935570000	1.7235510000	-1.9505870000
B	-1.9020720000	0.2968000000	-2.4737200000
B	-1.1945100000	-1.0770170000	-2.1430610000
B	-0.2625250000	-2.2706670000	-1.7341380000
B	0.8208420000	-2.4314900000	-0.6235220000

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energy

Al	-1.3358100000	2.5616260000	-0.0894090000
Al	-1.3790080000	-0.2001790000	-1.1732310000
Al	-3.5475370000	1.2428700000	-0.1303100000
Al	-3.7226370000	-1.7053880000	-0.6996620000
Al	1.3360400000	2.5593700000	-0.0895750000
Al	1.3737560000	-0.2016890000	-1.1680110000
Al	3.7214380000	-1.7031190000	-0.7025790000
Al	0.0009940000	-2.6443020000	0.6280460000
Al	3.5485260000	1.2416500000	-0.1339940000
B	0.0014790000	0.8798240000	1.2836280000
B	-0.8852550000	-0.6193160000	1.3005440000
B	-2.4988720000	-0.3978600000	0.9039820000
B	-1.6062610000	0.9229950000	1.2064160000
B	1.8658380000	-1.8420850000	0.5714110000
B	2.5008030000	-0.3976670000	0.9036700000
B	0.8881670000	-0.6195870000	1.3046470000
B	1.6088640000	0.9230500000	1.2096180000
B	-1.8637470000	-1.8415350000	0.5687700000

2

energy

Al	0.0000000000	0.0000000000	0.5811780000
B	0.0000000000	0.0000000000	-1.5110620000

11

energy

Al	-0.0027320000	0.0077600000	1.6842490000
B	1.5630290000	1.3942160000	-0.2906810000
B	2.2880270000	-0.0009770000	-0.2042380000
B	1.5634630000	-1.3970390000	-0.2808420000
B	0.0009560000	-1.6200220000	-0.4952800000
B	0.8112730000	-0.0037620000	-0.9081990000
B	0.0006340000	1.6157220000	-0.5065670000
B	-2.2868760000	-0.0013580000	-0.2073400000
B	-1.5619900000	1.3940140000	-0.2926330000
B	-0.8095660000	-0.0038330000	-0.9101190000
B	-1.5618480000	-1.3971360000	-0.2831480000

12

energy

Al	2.2937100000	-0.0007860000	-0.0281860000
B	0.0541730000	-2.4859830000	-0.0364500000
B	0.1912240000	-0.8444740000	0.1122670000
B	-1.2640940000	0.0004670000	0.1027170000
B	-2.6796580000	-0.7740520000	-0.0551720000
B	-2.6790190000	0.7759030000	-0.0552400000
B	-1.3872390000	-1.7623460000	-0.0116390000
B	-1.3856050000	1.7626950000	-0.0117840000
B	1.4683220000	-1.8717070000	-0.0236980000
B	1.4699020000	1.8710620000	-0.0235680000
B	0.1924470000	0.8445290000	0.1122890000
B	0.0559000000	2.4859490000	-0.0364390000

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energy

Al	-3.5405020000	0.0005090000	-0.2874920000
B	-1.5320670000	-0.8213770000	0.4710430000
B	1.2772840000	-2.3611310000	0.2110090000
B	-0.2531820000	0.0006990000	-0.1443730000
B	-0.2121820000	-1.7476150000	0.2885230000
B	2.6031250000	-1.5943330000	-0.0271510000
B	2.7938440000	-0.0013370000	-0.2018210000
B	1.1896730000	-0.8448760000	-0.3967750000

B	1.2807790000	2.3604240000	0.2104000000
B	1.1909780000	0.8446000000	-0.3989220000
B	-0.2094400000	1.7487230000	0.2882740000
B	2.6054390000	1.5915330000	-0.0273820000
B	-1.5289450000	0.8233670000	0.4746530000

14

energy

Al	-1.2283060000	-0.0020910000	1.6729880000
B	3.3631700000	-0.0003330000	0.2288310000
B	1.8833830000	0.0002560000	-0.5053410000
B	2.6005170000	-1.3574280000	0.1693460000
B	1.0524570000	-1.5624790000	-0.2668050000
B	0.2465620000	0.0004680000	-0.4872450000
B	-0.5547970000	-1.5506560000	-0.4808920000
B	2.6009600000	1.3570390000	0.1708790000
B	-0.5545100000	1.5518170000	-0.4781290000
B	1.0529610000	1.5631550000	-0.2647300000
B	-2.1502590000	1.3585900000	-0.4471510000
B	-1.2906880000	0.0011380000	-0.9982810000
B	-2.9055980000	0.0009240000	-0.5408570000
B	-2.1505620000	-1.3570530000	-0.4493950000

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energy

Al	-1.7672410000	0.0010030000	1.6501650000
B	2.3370560000	1.7649060000	0.0392540000
B	0.8134390000	1.6545680000	-0.2054670000
B	3.4814490000	0.7649870000	0.1227540000
B	1.8846880000	0.0014470000	-0.1461950000
B	0.1166660000	-0.0005010000	-0.2341310000
B	2.3339350000	-1.7646850000	0.0391640000
B	3.4793930000	-0.7663220000	0.1230320000
B	0.8100540000	-1.6598410000	-0.2050820000
B	-2.3332540000	1.3614230000	-0.6036650000
B	-0.7584680000	1.5187360000	-0.4552170000
B	-3.0762000000	0.0015290000	-0.7659100000
B	-2.3355190000	-1.3593290000	-0.6028660000
B	-1.3976290000	-0.0000760000	-0.9417480000
B	-0.7607850000	-1.5194490000	-0.4543510000

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energy

Al	-3.4903500000	-1.2388460000	-0.1623660000
B	3.7149470000	1.1269370000	0.0709740000
B	2.7425270000	-0.1743880000	-0.3548120000
B	-0.4068470000	0.2023580000	-0.1146070000
B	0.5717390000	1.6782760000	-0.1106150000
B	0.2073160000	-1.4406510000	0.0746440000
B	4.3065720000	-0.3339290000	0.1324260000
B	-3.6106070000	0.8079510000	0.1990750000
B	1.1597980000	0.0697540000	-0.0830950000
B	-2.0200690000	0.3629030000	0.2727140000
B	-2.5912130000	1.9529880000	0.0660840000
B	3.3919880000	-1.6115370000	0.2060220000
B	-1.0132280000	1.9253600000	0.0307850000
B	1.8120720000	-1.6520050000	0.0186830000
B	-1.3685190000	-1.2069060000	0.1487520000
B	2.1784330000	1.5138870000	-0.1348780000

17

energy

Al	-3.2066070000	0.6326680000	1.0640350000
B	-1.6190580000	1.6127540000	-0.4583290000
B	-2.0586670000	0.1317720000	-0.8200270000
B	-0.4172210000	0.5471010000	-0.9253330000
B	-1.3967030000	-2.4830990000	-0.0069420000
B	-2.4396610000	-1.3449800000	-0.2610270000
B	-0.8502550000	-1.0830620000	-0.6367120000
B	0.7688390000	-0.7246820000	-0.6290500000
B	0.2112870000	-2.2841480000	-0.0565390000

B	1.7827980000	-1.8536550000	0.2599970000
B	2.2382080000	-0.2262150000	-0.0435960000
B	3.6098920000	0.2375050000	0.7046770000
B	2.6907180000	1.4926050000	0.2786000000
B	3.2057720000	-1.2543300000	0.7454340000
B	1.4746820000	2.4747560000	0.0345780000
B	-0.0509780000	2.1256130000	-0.3174560000
B	1.1875220000	0.9871270000	-0.6347650000

3

energy			
Al	0.0000000000	0.8127590000	0.0000000000
B	0.7766290000	-1.0565710000	0.0000000000
B	-0.7766290000	-1.0566030000	0.0000000000

4

energy			
Al	1.6569770000	0.0000010000	-0.0000210000
B	-1.8887240000	0.7579140000	-0.0000430000
B	-1.8887680000	-0.7578850000	-0.0000430000
B	-0.5306490000	-0.0000310000	0.0001390000

5

energy			
Al	-1.4039340000	-0.6677250000	0.0000000000
B	0.0000000000	0.8576890000	-0.0000000000
B	1.3235380000	1.6532240000	-0.0000000000
B	1.7084430000	0.1682600000	-0.0000000000
B	0.6182470000	-0.9430900000	-0.0000000000

6

energy			
Al	2.5461510000	0.1096390000	-0.0000990000
B	0.3597820000	-0.1912490000	0.0003060000
B	-2.4151750000	-0.5841840000	-0.0002100000
B	-2.5701960000	0.9503680000	-0.0001330000
B	-0.9491190000	-1.1033020000	0.0000570000
B	-1.0452840000	0.6433070000	0.0002390000

7

energy			
Al	1.7108420000	-0.0000270000	-0.1141420000
B	0.2521920000	-1.5093450000	0.1243870000
B	-1.2713090000	-1.4073980000	-0.0712940000
B	-1.9985730000	0.0000210000	-0.2154820000
B	-1.2712270000	1.4074320000	-0.0714070000
B	0.2522570000	1.5093440000	0.1244870000
B	-0.4115290000	0.0000160000	0.4060780000

8

energy			
Al	1.9282300000	0.0000940000	-0.0000330000
B	-0.8817270000	1.8193820000	0.0003370000
B	0.5893330000	1.5278170000	-0.0004390000
B	-0.4021970000	-0.0000670000	-0.0000580000
B	-2.0134250000	0.7908030000	0.0002240000
B	-0.8815260000	-1.8193200000	0.0000530000
B	0.5895600000	-1.5278980000	-0.0000360000
B	-2.0134150000	-0.7909620000	0.0000050000

9

energy			
Al	0.0008820000	-0.0006770000	1.3070810000
B	-0.6083400000	-1.6706800000	-0.3692150000
B	0.9270620000	-1.5169980000	-0.3697860000
B	-0.0004890000	0.0003590000	-0.8146530000
B	-1.6859990000	-0.5662360000	-0.3688370000
B	1.7643850000	-0.2208100000	-0.3700610000
B	1.2727650000	1.2419310000	-0.3690540000
B	-0.1773990000	1.7692510000	-0.3685920000
B	-1.4942770000	0.9649430000	-0.3682120000

10

energy			
Al	-0.0000000000	0.0000000000	0.0007440000

B	0.000000000	2.219212000	-0.391663000
B	0.000000000	0.770925000	2.118176000
B	-0.000000000	-0.770925000	2.118176000
B	-0.000000000	-2.219212000	-0.391663000
B	0.000000000	0.000000000	-2.254486000
B	0.000000000	1.448603000	-1.726961000
B	0.000000000	1.951708000	1.126725000
B	-0.000000000	-1.951708000	1.126725000
B	-0.000000000	-1.448603000	-1.726961000