Supporting Information for

The Binding Energy and Bonding in Dialane

By

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Contents: Full author list for reference 37, comparison of AlH_4^- and CH_3O^- cross sections, competitive modeling fits and fitting parameters.

Figures S1 and S2

Table S1

Reference 37, full citation:

- (37) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; G. E. Scuseria; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision B.05; Gaussian, Inc.: Pittsburgh, PA, 2003.

Figure S1. Energy- resolved cross sections for formation of HCO_2^- in the reaction of the m/z 31 ion generated from methoxide or dimethylethylamine-alane (DMEAA) with CO_2 .

Figure S2. Energy-resolved cross sections for the reaction of Al_2H_7^- with CO_2 , along with fits to the data that take into account the competitive reaction processes.

Table S1. Single Data Set Fitting Parameters of Two Channel Competitive Modeling

Scaling Factor ^a	$\Delta S^\ddagger(1)^b$	$\Delta S^\ddagger(2)^b$	$E_0(1)^c$	$E_0(2)^c$	n	χ^2 ^d
0.90	1.73	3.22	1.31	1.40	1.51	6.717e-3
0.95	1.71	2.42	1.33	1.40	1.45	4.773e-3
1.00	1.69	1.69	1.35	1.41	1.41	3.486e-3
1.05	1.69	0.99	1.35	1.41	1.40	3.409e-3
1.10	1.69	0.36	1.34	1.37	1.40	3.489e-3

^a Scaling factor applied to frequencies of the transition state for channel 2 (hydride transfer)

^b Activation entropies for reaction transition states, in cal/mol·K

^c Dissociation energies obtained from modeling

^d χ^2 of fit obtained using the corresponding fitting parameters