

Supporting Information

for

Synthesis of substituted β -diketiminato gallium hydrides via oxidative addition of H–O bonds

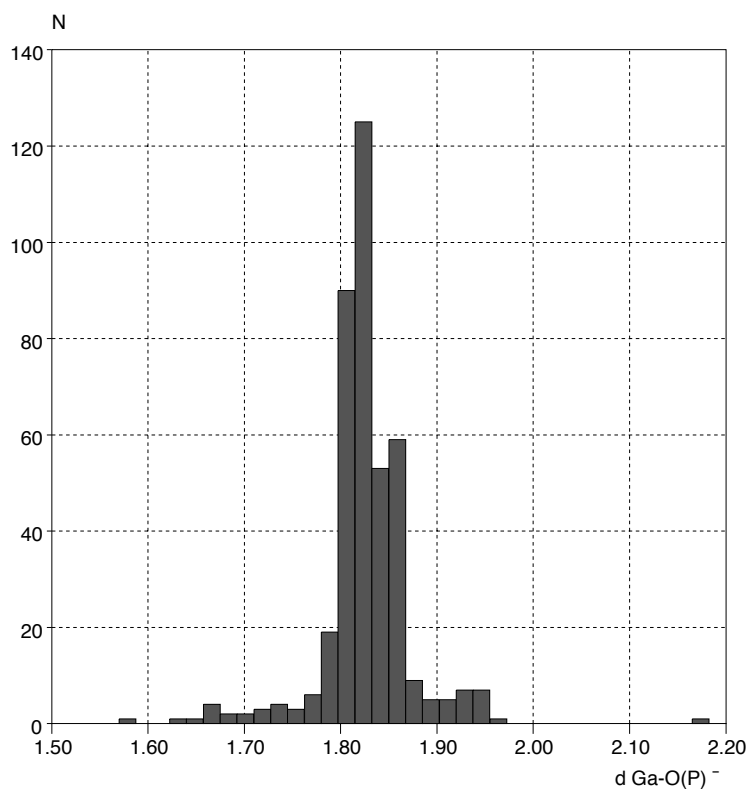
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Full reference 26:

Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Histogram of the Ga-O(P) distances reported in the CSD 2015



Plot Data

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X-axis

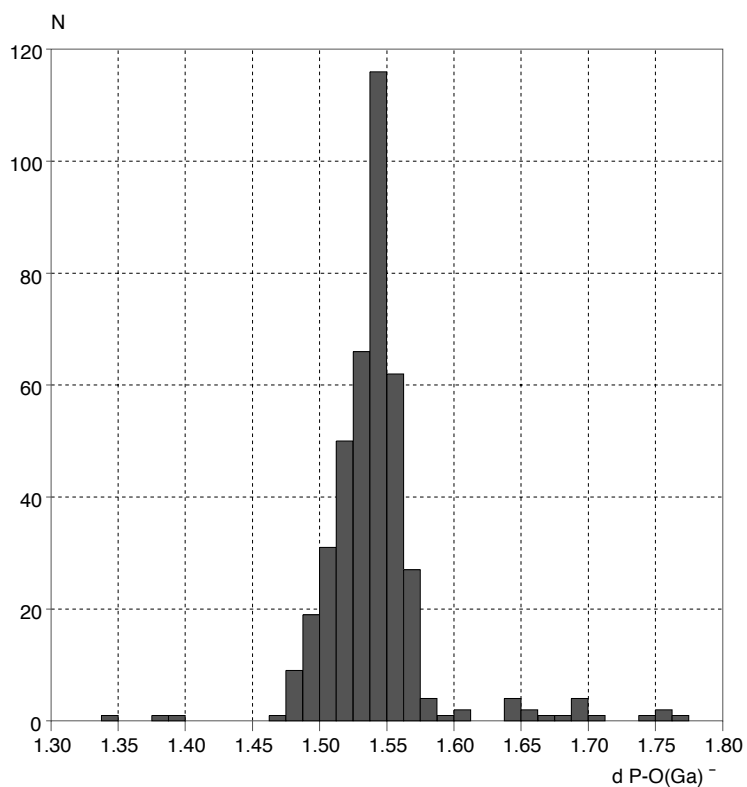
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Sample SD=0.048

Histogram

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HQ=1.865
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Figure S1: Histogram of the Ga–O(P) distances reported in the CSD 2015

Histogram of the P-O(Ga) distances reported in the CSD 2015



Plot Data

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Histogram

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Figure S2: Histogram of the P–O(Ga) distances reported in the CSD 2015

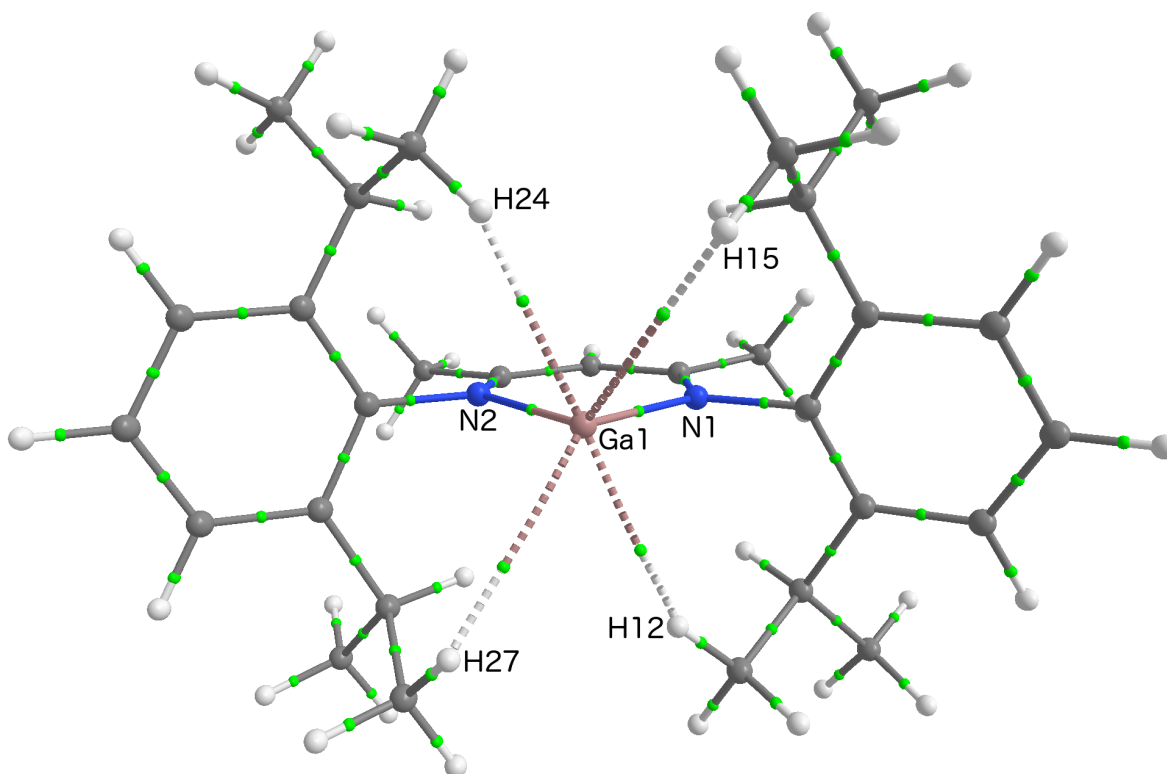


Figure S3: Molecular graph of **1** showing the Ga $\cdots$ H weak interactions. The green spheres are bond critical points (BCP).

Table S1: Topological properties of the bond critical points (BCP) of the Ga–N bonds and Ga $\cdots$ H interactions in **1**.

	Ga–N	Ga $\cdots$ H15	Ga $\cdots$ H12	Ga $\cdots$ H27	Ga $\cdots$ H24
$\rho(r_{\text{BCP}})/\text{e}\cdot\text{\AA}^{-3}$	0.513	0.054	0.074	0.054	0.074
$\nabla^2\rho(r_{\text{BCP}})/\text{e}\cdot\text{\AA}^{-5}$	7.471	0.361	0.506	0.361	0.506
ϵ	0.078	0.049	0.171	0.047	0.169
h	-0.017	0.0004	0.0002	0.0004	0.0002
DI/e	0.469	0.054	0.078	0.054	0.068
$d\text{BP}/\text{\AA}$	2.043	2.994	2.648	2.990	2.649

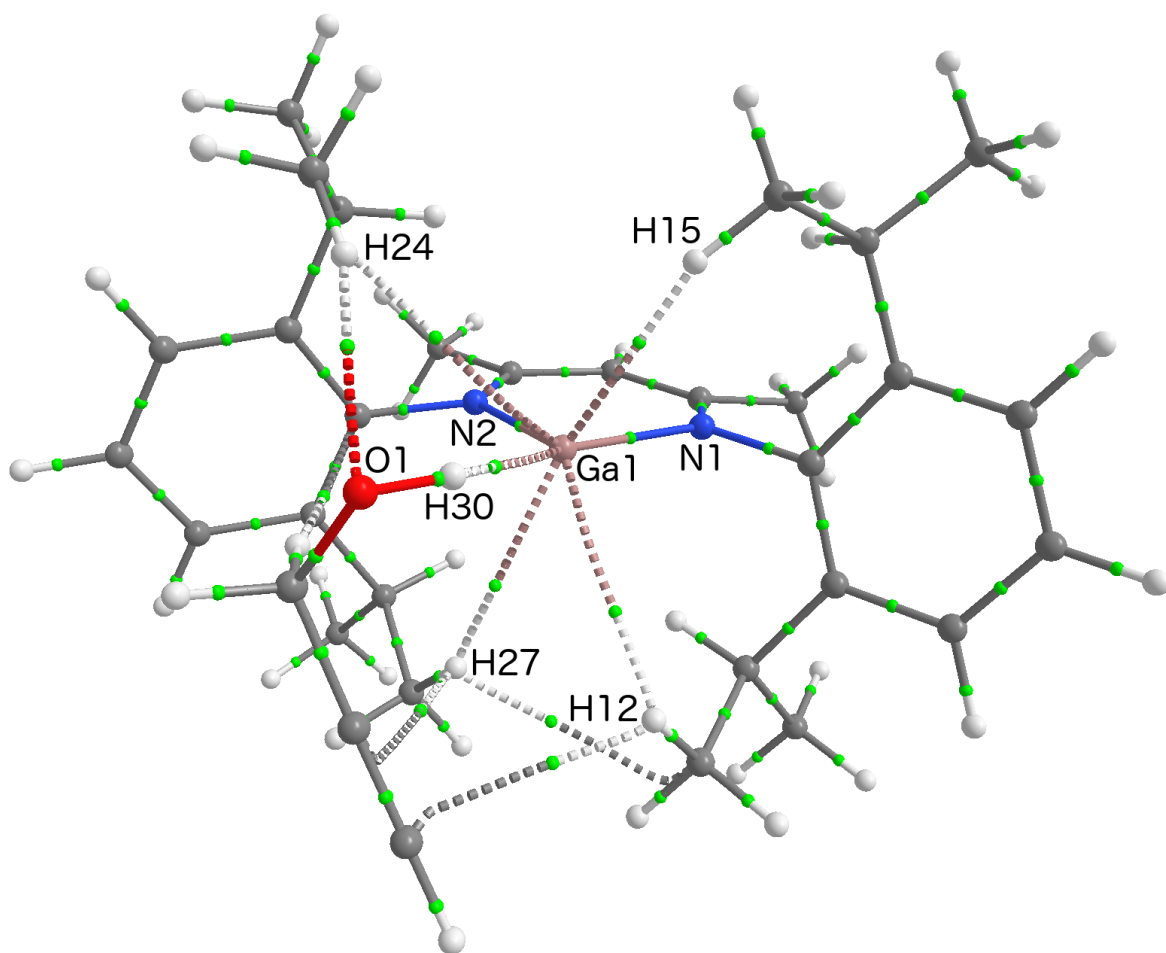


Figure S4: Molecular graph of the reacting complex **1+P** showing the Ga $\cdots$ H weak interactions. The green spheres are bond critical points (BCP).

Table S2: Topological properties of the bond critical points (BCP) of the Ga–N bonds and Ga $\cdots$ H interactions in the reacting complex **1+P**.

	Ga–N1	Ga–N2	Ga $\cdots$ H15	Ga $\cdots$ H12	Ga $\cdots$ H27	Ga $\cdots$ H24	Ga $\cdots$ H30
$\rho(r_{\text{BCP}})/\text{e}\cdot\text{\AA}^{-3}$	0.526	0.526	0.013	0.007	0.008	0.005	0.017
$\nabla^2\rho(r_{\text{BCP}})/\text{e}\cdot\text{\AA}^{-5}$	7.615	8.314	0.189	0.094	0.101	0.074	0.175
ϵ	0.073	0.079	11.664	4.000	1.615	15.953	0.217
h	-0.018	-0.018	0.0002	0.0004	0.0003	0.0004	-0.0009
DI/e	0.464	0.486	0.075	0.038	0.043	0.021	0.091
$d_{\text{BP}}/\text{\AA}$	2.036	2.014	2.522	3.108	2.879	3.385	2.565

Nuclear Coordinates for 1

73

-3161.77842683

31	0.0009200	-0.0047950	-0.9041150
7	1.3927530	-0.0344400	0.5904860
6	1.2468840	-0.0756870	1.9104110
7	-1.3896750	0.0299570	0.5919410
6	0.0025880	-0.0004960	2.5481420
1	0.0031700	0.0006220	3.6296360
6	-1.2424010	0.0742020	1.9115510
6	2.4733550	-0.2098080	2.7817130
1	3.0229450	-1.1184140	2.5163740
1	2.2027580	-0.2513610	3.8365850
1	3.1590470	0.6277650	2.6207720
6	-2.4676470	0.2123680	2.7839600
1	-3.1554530	-0.6239050	2.6253980
1	-3.0154900	1.1217250	2.5175570
1	-2.1957630	0.2553300	3.8384420
6	2.7079560	-0.0891490	0.0300190
6	3.1930650	-1.3138530	-0.4574170
6	4.4410960	-1.3289140	-1.0857330
1	4.8302130	-2.2668840	-1.4731120
6	5.1855600	-0.1671620	-1.2265730
1	6.1535340	-0.1970750	-1.7166920
6	4.6866160	1.0394460	-0.7448980
1	5.2743100	1.9441220	-0.8654490
6	3.4431110	1.1037180	-0.1186840
6	2.8623620	2.4310180	0.3487480
1	2.2064420	2.2290960	1.2031120
6	1.9883940	3.0447950	-0.7537240
1	1.1752820	2.3662860	-1.0314030
1	2.5826600	3.2308820	-1.6541410
1	1.5500520	3.9916800	-0.4219750
6	3.9275040	3.4289040	0.8062880
1	4.6092210	2.9838420	1.5373170
1	3.4508540	4.2994700	1.2652370
1	4.5246660	3.7934830	-0.0354790
6	2.3933850	-2.6023860	-0.3367420
1	1.4992210	-2.3989020	0.2632640
6	1.9361270	-3.0956910	-1.7156640
1	1.3361910	-2.3331280	-2.2218420
1	1.3341930	-4.0049490	-1.6174370
1	2.7993560	-3.3261310	-2.3490720
6	3.1899380	-3.6937300	0.3879780
1	3.5360610	-3.3539350	1.3684860
1	4.0693720	-3.9929710	-0.1912000
1	2.5704740	-4.5840020	0.5322250
6	-2.7053450	0.0866980	0.0327760
6	-3.4442530	-1.1044350	-0.1114680
6	-4.6887060	-1.0381550	-0.7355660
1	-5.2794340	-1.9413320	-0.8523620
6	-5.1849420	0.1686360	-1.2196400
1	-6.1537990	0.2001540	-1.7079070
6	-4.4366890	1.3284890	-1.0835250

1	-4.8237410	2.2665370	-1.4728000
6	-3.1875210	1.3114480	-0.4574800
6	-2.3837830	2.5979960	-0.3422700
1	-1.4878600	2.3932830	0.2546940
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1	-3.5172280	3.3562640	1.3662360
1	-4.0559670	3.9925650	-0.1927320
1	-2.5525770	4.5820950	0.5226890
6	-1.9304620	3.0875830	-1.7238220
1	-1.3251750	3.9950240	-1.6294900
1	-2.7954230	3.3199320	-2.3541400
1	-1.3350160	2.3223180	-2.2312050
6	-2.8664100	-2.4321480	0.3584530
1	-2.2106550	-2.2301600	1.2129370
6	-1.9928930	-3.0491870	-0.7425630
1	-1.1786580	-2.3724130	-1.0210600
1	-2.5870950	-3.2358170	-1.6429070
1	-1.5561690	-3.9961870	-0.4090690
6	-3.9335800	-3.4274500	0.8167780
1	-3.4587320	-4.2981130	1.2773990
1	-4.5307160	-3.7923090	-0.0248880
1	-4.6150640	-2.9801250	1.5466470

Nuclear Coordinates for the reacting complex 1+P

81
-3353.58300394

31	-0.1101330	0.3628100	-0.8790610
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1	-0.0471960	-0.0666520	3.6051800
6	1.1694050	0.0909110	1.8754020
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1	-3.2436260	0.6226920	2.7167100
1	-2.2369690	-0.3321070	3.8304520
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6	2.4167800	-0.0057410	2.7187930
1	3.1230890	0.7845740	2.4507320
1	2.9242730	-0.9582780	2.5311760
1	2.1794080	0.0628910	3.7802810
6	-2.8188900	0.1555800	0.0612490
6	-3.6224020	1.3149320	0.0806270
6	-4.8913400	1.2464600	-0.4895870
1	-5.5323400	2.1217110	-0.4803140
6	-5.3505890	0.0712480	-1.0786420
1	-6.3416150	0.0373860	-1.5198360
6	-4.5371180	-1.0507400	-1.1103070
1	-4.8954620	-1.9612960	-1.5832030
6	-3.2589610	-1.0320750	-0.5439230
6	-2.3904750	-2.2798850	-0.6157930
1	-1.4499310	-2.0869450	-0.0852670
6	-2.0556530	-2.6341470	-2.0703690
1	-1.5406120	-1.8121780	-2.5774090

1	-2.9679920	-2.8621090	-2.6321810
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6	-3.0626910	-3.4687540	0.0823820
1	-3.3016720	-3.2408360	1.1253270
1	-2.4031240	-4.3416780	0.0650650
1	-3.9941580	-3.7453740	-0.4217550
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1	-1.6544580	4.1601810	0.0464270
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6	-4.1561360	3.6005690	1.0920580
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