Synthesis and characterization of a germanium bismethanediide complex

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Electronic Supplementary Information

Content:

Table S1. Individual hybrid contributions, NLMO/NPA bond orders and Wiberg index of the Ge(1)–C(1), C(1)–P(2), P(2)–S(2), Ge(1)–S(2) and C(1)-P(1) bonds in compound **2**

Bond	NLMO/NPA bond order	MO(1)	Contr. %	Type (contr. %)[a]	MO(2)	Contr. %	Type (contr. %) [a]	Wiberg index
Ge(1)–C(1)	0.624	Ge	28.2	s (35.1) $p^{1.85}$ (64.8)	C	71.8	s (31.0) $p^{2.22}$ (69.0)	0.858
C(1)–P(2)	0.835	C	61.1	s (30.7) $p^{2.26}$ (69.3)	P	38.9	s (30.2) $p^{2.29}$ (69.1)	1.051
P(2)–S(2)	0.907	P	44.8	s (19.3) $p^{4.14}$ (79.6)	S	55.2	s (13.6) $p^{6.33}$ (86.0)	1.019
Ge(1)–S(2)	0.494	Ge	25.7	s (15.2) $p^{5.50}$ (83.4)	S	74.3	s (14.0) $p^{6.12}$ (85.8)	0.671
C(1)–P(1)	0.727	C	64.0	s (37.5) $p^{1.67}$ (62.5)	P	36.0	s (26.4) $p^{2.76}$ (72.8)	0.902

[a] The individual hybrid contribution may not sum up to 100% as the contribution from the d-type orbital is not listed

2. Complete citation for reference 18

18. Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

3. Carterian coordinates for compound **2**

Ge	0.000000	0.000000	0.487057
S	-1.847249	0.470372	1.910268
S	1.847249	-0.470372	1.910268
C	1.048974	1.444964	-0.127832
C	-1.048974	-1.444964	-0.127832
P	-2.461568	-1.249246	0.884003
P	2.461568	1.249246	0.884003
P	-0.711406	-2.883394	-1.111218
P	0.711406	2.883394	-1.111218
S	2.305330	3.563187	-2.103397
S	-2.305330	-3.563187	-2.103397
C	2.810696	2.603709	2.067924
C	3.502626	3.741452	1.617814
C	2.349425	2.549007	3.391291
C	3.732915	4.805953	2.490523
H	3.844664	3.803354	0.588715
C	2.593757	3.613805	4.261763
H	1.812172	1.672774	3.742222
C	3.283986	4.742855	3.812960
H	4.262373	5.685242	2.133406
H	2.243022	3.559258	5.289204

H	3.471161	5.571546	4.491199
C	-2.810696	-2.603709	2.067924
C	-3.502626	-3.741452	1.617814
C	-2.349425	-2.549007	3.391291
C	-3.732915	-4.805953	2.490523
H	-3.844664	-3.803354	0.588715
C	-2.593757	-3.613805	4.261763
H	-1.812172	-1.672774	3.742222
C	-3.283986	-4.742855	3.812960
H	-4.262373	-5.685242	2.133406
H	-2.243022	-3.559258	5.289204
H	-3.471161	-5.571546	4.491199
C	4.059652	0.913332	0.067834
C	4.112908	0.642774	-1.303914
C	5.236906	0.884266	0.834237
C	5.341512	0.367396	-1.908824
H	3.206519	0.676039	-1.896532
C	6.458564	0.594444	0.227011
H	5.204669	1.094975	1.899918
C	6.512249	0.341736	-1.148241
H	5.379960	0.179933	-2.978368
H	7.366524	0.573647	0.824075
H	7.466443	0.129363	-1.624116
C	-4.059652	-0.913332	0.067834
C	-4.112908	-0.642774	-1.303914
C	-5.236906	-0.884266	0.834237
C	-5.341512	-0.367396	-1.908824
H	-3.206519	-0.676039	-1.896532
C	-6.458564	-0.594444	0.227011
H	-5.204669	-1.094975	1.899918
C	-6.512249	-0.341736	-1.148241
H	-5.379960	-0.179933	-2.978368
H	-7.366524	-0.573647	0.824075
H	-7.466443	-0.129363	-1.624116
C	0.000000	4.218971	-0.047664
C	-0.005885	5.539452	-0.523943
C	-0.547433	3.946636	1.211707
C	-0.561081	6.564582	0.243394
H	0.444293	5.761153	-1.487609
C	-1.100230	4.973723	1.982575
H	-0.543624	2.932186	1.593496
C	-1.111776	6.283325	1.498450
H	-0.559171	7.583359	-0.136361
H	-1.519969	4.746255	2.959382
H	-1.540810	7.082645	2.097858
C	0.000000	-4.218971	-0.047664
C	0.005885	-5.539452	-0.523943
C	0.547433	-3.946636	1.211707
C	0.561081	-6.564582	0.243394
H	-0.444293	-5.761153	-1.487609
C	1.100230	-4.973723	1.982575
H	0.543624	-2.932186	1.593496
C	1.111776	-6.283325	1.498450
H	0.559171	-7.583359	-0.136361
H	1.519969	-4.746255	2.959382
H	1.540810	-7.082645	2.097858

C	0.681084	-2.434279	-2.232393
C	0.378950	-1.821064	-3.456999
C	2.014597	-2.742258	-1.926694
C	1.395759	-1.520116	-4.363200
H	-0.656535	-1.607014	-3.704367
C	3.029953	-2.450208	-2.842272
H	2.266793	-3.229030	-0.989777
C	2.723244	-1.840529	-4.060398
H	1.151056	-1.050096	-5.312615
H	4.058916	-2.701399	-2.599383
H	3.512491	-1.621268	-4.775593
C	-0.681084	2.434279	-2.232393
C	-0.378950	1.821064	-3.456999
C	-2.014597	2.742258	-1.926694
C	-1.395759	1.520116	-4.363200
H	0.656535	1.607014	-3.704367
C	-3.029953	2.450208	-2.842272
H	-2.266793	3.229030	-0.989777
C	-2.723244	1.840529	-4.060398
H	-1.151056	1.050096	-5.312615
H	-4.058916	2.701399	-2.599383
H	-3.512491	1.621268	-4.775593

4. Carterian coordinates for compound **2A**

Ge	0.000000	0.000000	0.538749
S	1.217306	1.512274	1.900323
S	-1.217306	-1.512274	1.900323
C	0.789799	-1.533309	-0.201040
C	-0.789799	1.533309	-0.201040
P	0.000000	2.753041	0.732784
H	-0.777814	3.580879	1.569603
H	0.792674	3.697615	0.050491
P	0.000000	-2.753041	0.732784
H	0.777814	-3.580879	1.569603
H	-0.792674	-3.697615	0.050491
P	-1.994236	1.953672	-1.409731
H	-1.666066	1.256681	-2.599710
H	-3.202893	1.289590	-1.080692
P	1.994236	-1.953672	-1.409731
H	1.666066	-1.256681	-2.599710
H	3.202893	-1.289590	-1.080692
S	2.160495	-3.925252	-1.600276
S	-2.160495	3.925252	-1.600276

5. Carterian coordinates for compound **2B**

Ge	0.000000	0.000000	0.000101
S	2.517844	0.373135	-0.003338
S	-2.517844	-0.373135	-0.003338
P	1.696738	2.253548	-0.002641
H	2.133784	3.020605	-1.099758
H	2.138009	3.021179	1.092367
P	-1.696738	-2.253548	-0.002641
H	-2.138009	-3.021179	1.092367
H	-2.133784	-3.020605	-1.099758

C	0.000000	1.852380	0.000776
C	0.000000	-1.852380	0.000776
P	-1.274954	3.085613	0.003980
H	-2.140909	2.795396	-1.077258
H	-2.134807	2.795819	1.090149
P	1.274954	-3.085613	0.003980
H	2.140909	-2.795396	-1.077258
H	2.134807	-2.795819	1.090149
S	-0.492235	4.908776	0.001346
S	0.492235	-4.908776	0.001346