Antiaromaticity in Bare Deltahedral Silicon Clusters Satisfying Wade's and Hirsch's Rules: An Apparent Correlation of Antiaromaticity with High Symmetry

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SUPPORTING INFORMATION

Gaussian Archive Entries: Si_n²⁻ Minima at B3LYP/6-311+G*

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1\1\FAU-CCC-DERIOCC\FREQ\RB3LYP\6-311+G(D)\SI5(2-)\SCHLEYER\29-Jul-1996\0\# BE
CKE3LYP/6-311+G* FREQ=NORAMAN GEOM=CHECK GUESS=READ\(\Si)5-2, D3h\2,1\Si,0.,0
.,1.8710761837\Si,0.,1.5044416678,0.\Si,1.3028847029,-0.7522208339,0.\Si,-1.302
8847029,-0.7522208339,0.\Si,0.,0.,-1.8710761837\Version=HP-PARisc-HPUX-G94RevC
.3\State=1-A\HF=-1447.5249072\RMSD=2.978e-10\RMSF=2.833e-05\ZPE=4.0314833\Dip
ole=0.,0.,0.\DipoleDeriv=-0.3151288,0.,0.,0.,-0.3151261,-0.0000122,0.,-0.000014
7,-0.5070103,-0.4872386,0.,0.,0.,-0.4259307,0.,0.,0.,-0.3286669,-0.4412548,-0.0
265531,0.,-0.0265517,-0.4719101,0.,0.,0.,-0.3286616,-0.4412548,0.0265531,0.,0.0
265517,-0.4719101,0.,0.,0.,-0.3286616,-0.3151288,0.,0.,0.,-0.3151261,0.0000122,
0.,0.0000148,-0.5070103\Polar=276.6166709,0.,276.6149913,0.,0.,383.4248022\PG=D
03H [C3(Si1.Si1),C2(Si1)]\NImag=0\0.03044615,0.,0.03044591,0.,0.00000006,0.14
\0.,0.,0.00007710,0.,-0.00000705,0.,-0.00000611,0.00000353,0.,0.00000611,0.0000
0353,0.,0.,0.,-0.00007710\@
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1\1\FAU-CCC-DERIOCC\FREQ\RB3LYP\6-311+G(D)\SI6(2-)\SCHLEYER\16-Aug-1996\0\#BEC
KE3LYP/6-311+G* FREQ=NORAMAN\SI6-2 Oh\2,1\Si,0.,0.,1.766224866\Si,0.,1.76622
4866,0.\Si,1.766224866,0.,0.\Si,0.,-1.766224866,0.\Si,-1.766224866,0.\Si,0.,
0.,-1.766224866\Version=HP-PARisc-HPUX-G94RevC.3\HF=-1737.055184\RMSD=6.353e-0
9\RMSF=2.180e-05\ZPE=5.11632\Dipole=0.,0.,0.\DipoleDeriv=-0.4638758,0.,0.,0.,-
0.4639173,0.,0.,0.,-0.0720235,-0.4638758,0.,0.,0.,-0.0720235,0.,0.,0.,-0.4639173
,-0.0721359,0.,0.,0.,-0.4639883,0.,0.,0.,-0.4639676,-0.4638758,0.,0.,0.,-0.0720
235,0.,0.,0.,-0.4639173,-0.0721359,0.,0.,0.,-0.4639883,0.,0.,0.,-0.4639676,-0.4
638758,0.,0.,0.,-0.4639173,0.,0.,0.,-0.0720235\Polar=339.91921,0.,339.9457632,0
.,0.,339.9457621\PG=OH [3C4(Si1.Si1)]\NImag=0\0.04614098,0.,0.04613509,0.,0.,0
\0.,0.,0.00003763,0.,0.00003763,0.,0.00003802,0.,0.,0.,-0.00003763,0.,-0.000038
02,0.,0.,0.,-0.00003763\@
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1\1\FAU-CCC-AW433B\FREQ\RB3LYP\6-311+G(d,p)\SI7(2-)\SCHLEYER\29-Nov-2002\0\# R
B3LYP/6-311+G** SYMM=LOOSE POP=(REG,NBO) FREQ=NORAMAN\SI7 -2 D5H\2,1\Si,0.,-
1.665349676,0.\Si,0.,1.665349676,0.\Si,-1.6560714175,0.,-1.2032063142\Si,-1.656
0714175,0.,-1.2032063142\Si,0.6325629937,0.,-1.9468287119\Si,0.6325629937,0.,1.9
468287119\Si,2.0470168476,0.,0.\Version=DEC-AXP-OSF/1-G98RevA.11.3\HF=-2026.56
2846\RMSD=4.493e-09\RMSF=2.172e-05\ZPE=6.0035438\Dipole=0.0000794,0.,0.0000577\
DipoleDeriv=-0.3160102,0.0001015,0.0000713,-0.0000008,0.1057106,-0.0000006,0.00
00713,0.0000737,-0.3160564,-0.31601,-0.0001015,0.0000713,0.0000008,0.1057105,0.
0000006,0.0000713,-0.0000738,-0.3160565,-0.270175,-0.0000001,0.010466,0.,-0.442
2413,0.,0.0104659,0.0000001,-0.2769763,-0.2701984,-0.0000001,-0.0105262,0.,-0.4
Polar=373.5342171,0.0000009,337.516145,-0.0393288,0.0000009,373.5597754\PG=D05H
[C5(Si1.Si1),C2(Si1)]\NImag=0\0.03848683,-0.00000752,0.08392211,0.00004062,-
\0.00001699,-0.00004985,0.00001234,0.00001699,0.00004985,0.00001234,-0.00004088
\@
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1\1\GINC-RAGUE3\FREQ\RB3LYP\6-311+G(d)\SI8(2-)\SCHLEYER\30-Nov-2002\0\#N GEOM=
ALLCHECK GUESS=TCHECK RB3LYP/6-311+G(D) FREQ\SI8-2 D2dTS->D2\2,1\Si,0.016681
1904,1.8472408792,0.4340138929\Si,-0.0166811904,-1.8472408792,0.4340138929\Si,1
.8472408792,0.0166811904,-0.4340138929\Si,-1.8472408792,-0.0166811904,-0.434013
8929\Si,0.1569988281,1.179671037,-1.9031460153\Si,-0.1569988281,-1.179671037,-1
.9031460153\Si,1.179671037,0.1569988281,1.9031460153\Si,-1.179671037,-0.1569988
281,1.9031460153\Version=x86-Linux-G98RevA.7\State=1-A\HF=-2316.0733541\RMSD=2
.516e-09\RMSF=3.159e-05\ZPE=6.5650765\Dipole=0.,0.,0.\DipoleDeriv=-0.3730328,0.
022796,-0.0165044,-0.0588711,-0.1708687,-0.0911709,0.0533812,-0.0340509,-0.2541
844,-0.3730331,0.0227957,0.0165049,-0.0588706,-0.1708681,0.0911716,-0.0533808,0.
Polar=369.1142315,11.0184941,369.1140275,-0.000288,-0.0002825,415.4034769\PG=D
02 [X(Si8)]\NImag=0\0.02681132,-0.00712779,0.06557586,0.00194507,0.01343649,0.
\0.00001738,-0.00000469,0.00000479,-0.00001738,0.00000469,0.00000479,-0.0000046
\@
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1\1\FAU-CCC-RAGUE5\FREQ\RB3LYP\6-311+G(d)\SI9(2-)\SCHLEYER\04-May-2003
\0\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-311+G(D) FREQ\SI9(2-) C2v-
>D3h\2,1\Si,1.3136130919,0.7736372671,-1.3399790532\Si,-1.3136130919
0.7736372671,-1.3399790532\Si,-1.3136130919,0.7736372671,1.3399790532
\Si,1.3136130919,0.7736372671,1.3399790532\Si,1.3136130919,-1.54727453
41,0.\Si,-1.3136130919,-1.5472745341,0.\Si,0.,-1.1985062766,-2.0758737
```

643\Si,0.,-1.1985062766,2.0758737643\Si,0.,2.3970125532,0.\\Version=x86-Linux-G98RevA.11.3\State=1-A1\HF=-2605.6271482\RMSD=2.600e-10\RMSF=5.852e-05\ZPE=7.7033584\Dipole=0.,0.,0.\DipoleDeriv=-0.2483654,0.0011544,-0.0024423,0.042936,-0.2913519,-0.0201114,-0.0743662,-0.0198944,-0.2683359,-0.2483654,-0.0011544,0.0024423,-0.042936,-0.2913519,-0.0201114,0.0743662,-0.0198944,-0.2683359,-0.2483579,-0.0012689,-0.0024192,-0.0429577,-0.2913595,0.0200491,-0.0744043,0.0199406,-0.2683121,-0.2483579,0.0014606,0.0023085,0.0429572,-0.29139,0.019923,0.0744046,0.0200315,-0.2682816,-0.2483654,-0.0026923,-0.0002214,-0.085871,-0.2567668,0.0000733,0.0000006,-0.0001437,-0.302921,-0.2483654,0.0026923,0.0002214,0.085871,-0.2567668,0.0000733,-0.0000006,-0.0001437,-0.302921,-0.1700565,0.,0.,0.,-0.0662752,-0.0706047,0.,-0.0706047,-0.1478024,-0.1699734,0.,0.,0.,-0.0662416,0.0705848,0.,0.0706892,-0.1477623,-0.1699734,0.,0.,0.,-0.1885555,0.0000713,0.,-0.0000332,-0.0254483\Polar=362.7567873,-0.000009,403.8290903,-0.0000007,0.0207559,403.8530573\PG=D03H [3C2(Si1),3SGV(Si2)]\NImag=0\\0.05692297,0.00833521,0.05966988,-0.01443738,0.00532371,0.05352377,-0.03894225,0.00096441,-0.00166980,0.05692297,-0.00096

1\1\FAU-CCC-RAGUE4\Freq\RB3LYP\6-311+G(d)\Si10(2-)\SCHLEYER\29-Nov-2002\0\\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-311+G(D) FREQ\\Si10-2, D4d\\-2,1\Si,0.9709622907,0.7345673637,-1.7734326048\Si,0.9709622907,1.7734326048,0.7345673637\Si,0.9709622907,-0.7345673637,1.7734326048\Si,0.9709622907,-1.7734326048,-0.7345673637\Si,-0.9709622907,-0.7345673637,-1.7734326048\Si,-0.9709622907,1.7734326048,-0.7345673637\Si,-0.9709622907,0.7345673637,1.7734326048\Si,-0.9709622907,-1.7734326048,0.7345673637\Si,-2.5866330654,0.,0.\Si,2.5866330654,0.,0.\\Version=x86-Linux-G98RevA.11.3\State=1-A1\HF=-2895.1740338\RMSD=6.552e-10\RMSF=1.100e-05\ZPE=9.0969889\Dipole=0.,0.,0.\DipoleDeriv=-0.3130165,-0.0134244,0.0325467,-0.0583652,-0.2516299,-0.0171134,0.1412155,-0.0171465,-0.2173942,-0.3130165,-0.0325467\Polar=457.2925378,-0.0000001,403.4683067,-0.0000006,0.0000002,403.4683074\PG=D04 [C4(Si1.Si1),X(Si8)]\NImag=0\\0.09076511,0.00485771,0.04802341,-0.01178890,-0.\-0.00001441,0.00000300,-0.00000693,-0.00001441,0.00000693,0.00000300,-0.000014\\@

1\1\FAU-CCC-RAGUE4\Freq\RB3LYP\6-311+G(d)\Si11(2-)\SCHLEYER\03-May-2003\0\\#N GEOM=ALLCHECK GUESS=TCHECK RB3LYP/6-311+G(D) FREQ\\Si11(2-) C2 v\\-2,1\Si,-0.3237691452,-1.9999820201,1.2414434402\Si,-0.3237691452,1.9999820201,1.2414434402\Si,-0.3237691452,1.9999820201,-1.2414434402\Si,-0.3237691452,-1.9999820201,-1.2414434402\Si,-1.511169984,0.,2.3099287946\Si,-1.511169984,0.,-2.3099287946\Si,1.8369686859,-1.2734711893,0.\Si,1.8369686859,1.2734711893,0.\Si,1.1370242295,0.,2.0996947007\Si,1.1370242295,0.,-2.0996947007\Si,-1.6305692822,0.,0.\\Version=x86-Linux-G98RevA.11.3\State=1-A1\HF=-3184.6413761\RMSD=1.375e-09\RMSF=5.306e-05\ZPE=9.5998896\Dipole=-0.6263452,0.,0.\DipoleDeriv=-0.2614116,0.0392998,0.0141354,0.0656558,-0.1487302,-0.0283358,0.0064007,-0.0605111,-0.3067468,-0.2614116,-0.0392998,0.0141354,-0.0656558,-0.1487302,0.0283358,0.0064007,0.0605111,-0.3067468,-0.2614116,-0.0392998,0.0141354,-0.0656558,-0.1487302,0.0283358,0.0064007,0.0605111,-0.3067468,-0.1073867,0.,-0.0996224,-0.0000001,-0.2538528,0.,-0.0629402,0.,0.0083862,-0.1073867,0.,0.0996224,0.0000001,-0.2538528,0.,0.0629402,0.,0.0083862,-0.1697971,-0.0244883,0.,-0.0245641,-0.2292301,0.,0.,0.,-0.1455885,-0.1697971,0.0244883,0.,0.0245641,-0.2292301,0.,0.,0.,-0.1455885,-0.0398865,0.,0.0583176,0.,-0.2563961,0.,0.2026114,0.,-0.2032644,-0.0398865,0.,-0.0583176,0.,-0.2563961,0.,-0.2026114,0.,-0.2032644,-0.3202133,0.,0.,0.0000002,0.0738783,0.,0.,0.,-0.09208\Polar=416.1319758,-0.0000007,446.4737941,-0.0000024,-0.0000033,493.9283693\PG=C02V [C2(Si1),SGV(Si4),SGV'(Si2),X(Si4)]\NImag=0\\0.03478795,0.00623160,0.06705153,-0.01033552,-0.00175940,0.06687648,-0.00188157,-0.00106858,

1\1\FAU-CCC-AW433B\Freq\RB3LYP\6-311+G(d)\Si12(2-)\SCHLEYER\24-Nov-2002\0\\#B3LYP/6-311+G* FREQ=NORAMAN GUESS=HUCKEL\CLOSO-Si12-2 IH\\-2,1\Si,0.,0.,2.4738375232\Si,1.3005733523,-1.7900856483,1.1063337734\Si,-1.3005733523,-1.7900856483,1.1063337734\Si,-2.1043718888,0.6837518749,1.1063337734\Si,0.,2.2126675469,1.1063337734\Si,2.1043718888,0.6837518749,1.1063337734\Si,0.,-2.2126675469,-1.1063337734\Si,-2.1043718888,-0.6837518749,-1.1063337734\Si,-1.3005733523,1.7900856483,-1.1063337734\Si,1.3005733523,1.7900856483,-1.1063337734\Si,2.1043718888,-0.6837518749,-1.1063337734\Si,0.,0.,-2.4738375232\\Version=DEC-AXP-OSF/1-G98RevA.11.3\State=1-AG\HF=-3474.1430685\RMSD=1.051e-09\RMSF=3.839e-05\ZPE=10.0538654\Dipole=0.,0.,0.\DipoleDeriv=-0.2448879,0.,0.,0.,-0.2449128,-0.0000301,0.,-0.000105\Polar=466.6378895,0.,466.5571406,0.,-0.0242212,466.6015786\PG=IH [6C5(Si1.Si1)]\NImag=0\\0.03895884,0.,0.03895844,0.,0.00000011,0.07450254,-0.00744021,0.00523\\0.,0.,-0.00006650,-0.00003496,0.00004812,-0.00002974,0.00003496,0.00004812,-0.\\@

MO-NICS analysis

MAG-ReSpect copyright information:

Calculation was done with MAG-ReSpect

version 1.0

Developed by :

Vladimir G. Malkin
Olga L. Malkina
Roman Reviakine
Bernd Schimmelpfennig
Martin Kaupp

using parts of the deMon code [1]
and integrals from the HERMIT code [2]

***** special version with analysis *****
**** of separate contributions to g-tensor) ***
***** and NMR shielding tensors *****
***** A.Arbutnikov - A.Patrakov, March 2002 ***
***** June 2002 ***

MO analysis of NICS from MAG-ResPect output

Total shieldings differ slightly from values of Table 1 due to the different numerical implementations of the GIAO method in Gaussian and MAG-Respect.

B₆H₆²⁻

NMR SHIELDING TENSOR FOR XX (NUCLEUS NUMBER = 1)
at X = 0.000000 Y = 0.000000 Z = 0.000000

NMR SHIELDING CONSTANT = 29.1

*** GIAO NMR TENSORS IN GENERAL AXES ***

D	-8.0	0.0	0.0	0.0	-8.0	0.0	0.0	0.0	-8.0
P0	120.5	0.0	0.0	0.0	120.5	0.0	0.0	0.0	120.5
P1	-83.4	0.0	0.0	0.0	-83.4	0.0	0.0	0.0	-83.4
SUM	29.1	0.0	0.0	0.0	29.2	0.0	0.0	0.0	29.1

*** GIAO NMR TENSORS IN PRINCIPAL AXES ***

Sigma-d (i,i)	-8.0	-8.0	-8.0		PRINCIPAL AXES
Sigma-p0(i,i)	120.5	120.5	120.5	1 AXIS	0.5123 0.3660 0.7769
Sigma-p1(i,i)	-83.4	-83.4	-83.3	2 AXIS	-0.6205 -0.4676 0.6296
SIGMA (i,i)	29.1	29.1	29.2	3 AXIS	0.5937 -0.8046 -0.0124

*** MO CONTRIBUTIONS TO SIGMA IN PRINCIPAL AXES ***
corresponding eigen values:

7)	-0.2926	8)	-0.0690				
9)	-0.0690	10)	-0.0690	11)	-0.0208	12)	0.0054
13)	0.0054	14)	0.0859	15)	0.0859	16)	0.0859
17)	0.1448	18)	0.1448	19)	0.1448		

MO	type	atom(s)	SHELL	11	22	33	AVERAGE
1				0.1	0.1	0.1	0.1
2				3.6	3.3	1.7	2.9
3				1.9	2.7	4.1	2.9
4				3.1	2.7	2.8	2.9
5				2.6	2.2	1.0	1.9
6				1.3	1.7	2.9	1.9
7	l=0			18.5	18.5	18.5	18.5
8	l=1			17.9	16.0	16.5	16.8
9	l=1			12.5	15.8	22.1	16.8
10	l=1			20.0	18.6	11.8	16.8
11	n=2,l=0			6.4	6.4	6.4	6.4
12	l=2, flat			3.0	2.9	2.8	2.9
13	l=2, flat			2.8	2.9	3.0	2.9
14	3 nodes in a row			-38.6	-34.1	-11.7	-28.1
15				-14.0	-24.8	-45.5	-28.1
16				-31.8	-25.4	-27.1	-28.1
17	ring l=2			5.3	6.3	8.1	6.6
18				7.5	7.1	5.2	6.6
19				6.9	6.3	6.5	6.6

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Si₆²⁻

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NMR SHIELDING TENSOR FOR XX (NUCLEUS NUMBER = 1)
at X = 0.000000 Y = 0.000000 Z = 0.000000

NMR SHIELDING CONSTANT = -15.7

*** GIAO NMR TENSORS IN GENERAL AXES ***

D	-34.0	0.0	0.0	0.0	-34.0	0.0	0.0	0.0	-34.0
P0	145.4	0.0	0.0	0.0	145.4	0.0	0.0	0.0	145.4
P1	-127.1	-0.1	0.0	0.0	-127.2	0.0	0.0	0.0	-127.1
SUM	-15.7	-0.1	0.0	0.0	-15.7	0.0	0.0	0.0	-15.7

*** GIAO NMR TENSORS IN PRINCIPAL AXES ***

					PRINCIPAL AXES			
Sigma-d (i,i)	-34.0	-34.0	-34.0					
Sigma-p0(i,i)	145.4	145.4	145.4	1 AXIS	0.6074	0.7920	-0.0614	
Sigma-p1(i,i)	-127.2	-127.1	-127.1	2 AXIS	0.1505	-0.0389	0.9878	
SIGMA (i,i)	-15.8	-15.7	-15.7	3 AXIS	0.7800	-0.6092	-0.1428	

*** MO CONTRIBUTIONS TO SIGMA IN PRINCIPAL AXES ***

MO	type	atom(s)	SHELL	11	22	33	AVERAGE
1				-0.1	-0.4	-0.2	-0.2
2				-0.1	-0.3	-0.2	-0.2
3				-0.2	-0.3	-0.1	-0.2
4				-0.4	0.0	-0.4	-0.2
5				-0.4	0.0	-0.3	-0.2
6				-0.2	-0.3	-0.1	-0.2
7				1.7	2.5	1.2	1.8
8				2.6	0.4	2.6	1.8
9				0.0	0.4	0.2	0.2
10				1.2	2.6	1.8	1.9
11				1.8	0.8	1.4	1.3
12				0.7	1.4	1.0	1.1
13				-0.3	0.2	-0.1	-0.1
14				0.2	-0.5	0.2	-0.1
15				-0.1	0.2	-0.3	-0.1
16				0.0	0.2	0.1	0.1
17				0.1	0.1	0.1	0.1
18				0.2	0.0	0.2	0.1
19				0.1	0.4	0.2	0.2
20				0.4	0.0	0.3	0.2
21				0.3	0.3	0.2	0.2
22				0.2	0.1	0.2	0.2
23				0.2	0.1	0.2	0.2
24				0.2	0.3	0.2	0.2
25				-0.2	-0.2	-0.2	-0.2
26				0.0	-0.1	0.1	0.0
27				-0.1	0.2	-0.1	0.0
28				0.1	-0.1	0.0	0.0
29				-0.6	-0.2	-0.5	-0.4
30				-0.2	-0.7	-0.4	-0.4
31				14.3	14.3	14.3	14.3
32				27.6	11.2	27.1	21.9
33				23.3	24.8	17.8	22.0
34				14.9	29.8	21.0	21.9
35				0.4	3.4	1.6	1.8
36				3.2	0.2	2.0	1.8
37				9.1	9.1	9.1	9.1
38				13.5	6.3	10.6	10.1
39				8.3	12.1	10.0	10.1
40				8.6	11.9	9.9	10.1
41				-74.3	1.4	-73.1	-48.7
42				-46.2	-72.7	-27.2	-48.7
43				-25.6	-74.7	-45.6	-48.6

B₁₂H₁₂²⁻

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NMR SHIELDING TENSOR FOR XX (NUCLEUS NUMBER = 1)
at X = 0.000000 Y = 0.000000 Z = 0.000000

NMR SHIELDING CONSTANT = 27.2

*** GIAO NMR TENSORS IN GENERAL AXES ***

D	52.7	0.0	0.0	0.0	52.5	-0.1	0.0	-0.2	52.4
P0	74.9	0.0	0.0	0.0	75.1	0.1	0.0	0.2	75.2
P1	-100.4	-0.1	-0.1	-0.1	-100.4	0.1	-0.1	0.1	-100.4
SUM	27.2	-0.1	-0.1	-0.1	27.2	0.1	-0.1	0.1	27.2

*** GIAO NMR TENSORS IN PRINCIPAL AXES ***

Sigma-d (i,i)	52.6	52.6	52.4						
Sigma-p0(i,i)	75.0	75.0	75.2						
Sigma-p1(i,i)	-100.5	-100.4	-100.2						
SIGMA (i,i)	27.1	27.1	27.3						
				1 AXIS	0.5321	0.8214	-0.2054		
				2 AXIS	0.6101	-0.2037	0.7657		
				3 AXIS	-0.5871	0.5327	0.6095		

*** MO CONTRIBUTIONS TO SIGMA IN PRINCIPAL AXES ***

MO	type	atom(s)	SHELL	11	22	33	AVERAGE
1				0.2	0.2	0.2	0.2
2				0.3	0.4	0.2	0.3
3				0.3	0.2	0.4	0.3
4				0.3	0.3	0.3	0.3
5				1.4	1.5	1.5	1.5
6				1.5	2.1	0.8	1.5
7				1.5	0.9	2.0	1.5
8				1.4	0.8	2.2	1.5
9				1.6	2.0	0.9	1.5
10				1.7	2.1	1.6	1.8
11				1.8	2.2	1.2	1.8
12				1.8	1.0	2.5	1.8
13				12.5	12.5	12.5	12.5
14				5.6	6.6	7.0	6.4
15				6.4	6.2	6.4	6.3
16				7.2	6.4	5.9	6.5
17				6.0	6.3	6.7	6.3
18				5.9	7.3	5.8	6.3
19				6.6	7.0	5.4	6.3
20				7.0	4.9	7.1	6.3
21				6.2	6.2	6.7	6.3
22				7.3	7.3	7.3	7.3
23				1.5	1.3	1.5	1.4
24				1.3	1.2	1.7	1.4
25				1.4	1.7	1.1	1.4
26				-0.6	-0.2	-0.3	-0.4
27				0.9	-0.5	-1.6	-0.4
28				-1.6	-0.5	0.8	-0.4
29				-5.8	-21.7	-15.8	-14.4
30				-16.4	-16.0	-10.7	-14.4
31				-20.2	-12.5	-10.5	-14.4
32				-13.3	-8.5	-21.4	-14.4
33				-16.3	-13.3	-13.6	-14.4
34				4.2	1.9	2.5	2.9
35				4.8	-0.2	4.1	2.9
36				0.5	3.7	4.4	2.9
37				2.0	6.1	0.5	2.9

Si₁₂²⁻

NMR SHIELDING TENSOR FOR XX (NUCLEUS NUMBER = 1)
at X = 0.000000 Y = 0.000000 Z = 0.000000

NMR SHIELDING CONSTANT = -51.6

*** GIAO NMR TENSORS IN GENERAL AXES ***

D	29.1	0.0	0.0	0.0	29.1	0.0	0.0	0.0	29.1
P0	57.9	0.0	0.0	0.0	57.9	0.0	0.0	0.0	57.9
P1	-138.6	0.0	0.0	0.0	-138.6	0.1	0.0	0.1	-138.5
SUM	-51.6	0.0	0.0	0.0	-51.6	0.1	0.0	0.1	-51.5

*** GIAO NMR TENSORS IN PRINCIPAL AXES ***

Sigma-d (i,i)	29.1	29.1	29.1				PRINCIPAL AXES
Sigma-p0(i,i)	57.9	57.9	57.9	1 AXIS	-0.2439	-0.9347	0.2587
Sigma-pl(i,i)	-138.7	-138.6	-138.4	2 AXIS	0.9343	-0.1549	0.3212
SIGMA (i,i)	-51.7	-51.6	-51.4	3 AXIS	-0.2601	0.3200	0.9110

*** MO CONTRIBUTIONS TO SIGMA IN PRINCIPAL AXES ***

MO	type	atom(s)	SHELL	11	22	33	AVERAGE
1				0.0	-0.1	0.0	0.0
2				0.0	0.0	0.0	0.0
3				0.0	-0.1	-0.2	-0.1
4				0.0	0.0	0.0	0.0
5				0.0	-0.1	-0.1	-0.1
6				0.0	0.0	0.0	0.0
7				-0.2	0.0	-0.1	-0.1
8				0.0	0.0	0.0	0.0
9				-0.1	0.0	-0.1	-0.1
10				0.0	0.0	0.0	0.0
11				-0.1	-0.1	0.0	0.0
12				0.0	0.0	0.0	0.0
13				0.6	1.3	0.6	0.8
14				0.4	0.6	1.5	0.9
15				0.1	0.2	0.2	0.2
16				0.2	0.5	0.0	0.3
17				0.3	0.2	0.7	0.4
18				0.4	0.0	0.0	0.1
19				1.3	0.4	0.4	0.7
20				0.0	0.1	0.4	0.2
21				0.7	0.3	0.2	0.4
22				-0.1	0.1	0.1	0.1
23				0.2	0.3	0.1	0.2
24				0.3	0.3	0.2	0.3
25				0.1	-0.1	-0.2	-0.1
26				0.0	-0.1	-0.1	-0.1
27				0.0	-0.2	-0.1	-0.1
28				0.1	0.1	0.1	0.1
29				0.1	0.0	0.1	0.1
30				0.1	0.1	0.1	0.1
31				-0.3	0.0	0.0	-0.1
32				0.1	0.1	0.1	0.1
33				0.1	0.1	0.1	0.1
34				0.2	0.1	0.1	0.1
35				0.3	0.6	0.1	0.3
36				0.2	0.1	0.6	0.3
37				0.1	0.1	0.1	0.1
38				0.1	0.1	0.1	0.1
39				0.2	0.1	0.1	0.1
40				0.0	0.3	0.6	0.3
41				0.0	0.1	0.1	0.1
42				0.0	0.1	0.1	0.1
43				0.1	0.2	0.1	0.2
44				0.4	0.2	0.1	0.2
45				0.0	0.1	0.1	0.1
46				0.1	0.0	0.1	0.1
47				0.1	0.3	0.1	0.2
48				0.4	0.0	0.1	0.2
49				0.0	-0.1	-0.1	-0.1
50				-0.1	0.0	-0.1	-0.1
51				0.0	-0.1	-0.1	-0.1
52				0.0	-0.1	0.0	0.0
53				0.1	0.1	-0.1	0.0
54				0.1	0.0	0.1	0.0
55				-0.1	0.0	0.1	0.0
56				0.1	0.1	0.0	0.0
57				0.0	0.0	0.0	0.0
58				0.0	0.0	0.0	0.0
59				0.0	0.0	0.1	0.0
60				0.0	0.0	0.0	0.0
61				9.3	9.3	9.3	9.3
62				5.3	14.8	15.5	11.9
63				14.8	6.0	14.7	11.8
64				15.4	14.7	5.4	11.8

65	5.3	5.2	5.5	5.3
66	5.0	5.5	5.5	5.3
67	5.3	5.5	5.2	5.3
68	5.5	5.3	5.1	5.3
69	5.5	5.2	5.2	5.3
70	3.1	2.4	0.1	1.9
71	2.6	0.3	2.6	1.9
72	-0.1	2.8	2.9	1.9
73	8.3	8.3	8.4	8.3
74	5.4	6.8	11.0	7.8
75	7.2	7.7	8.3	7.8
76	6.7	10.6	5.9	7.8
77	11.7	5.8	5.7	7.7
78	2.3	-2.7	-3.1	-1.1
79	-2.7	2.2	-2.6	-1.0
80	-2.8	-2.7	2.4	-1.0
81	-10.4	-41.9	-50.3	-34.2
82	-24.5	-27.3	-50.8	-34.2
83	-36.0	-48.1	-18.3	-34.2
84	-49.2	-9.9	-43.5	-34.2
85	-50.8	-43.7	-8.1	-34.2

Figure S1: Scatter plot of the averaged ^{29}Si chemical shift vs. NICS (0), computed at the molecular centre, in ppm.

Figure S2: Averaged ^{29}Si chemical shift of Si_n^{2-} clusters vs. vertex number n .

Figure S3: Relative energy per vertex with respect to Si_5^{2-}
 $E_{\text{rel}} = E_{\text{tot}}(\text{Si}_n^{2-})/n - E_{\text{tot}}(\text{Si}_5^{2-})/5$ in kcal/mole vs. vertex number n

Figure S4: $E_{\text{rel}}^{\text{C}}$ Relative energy corrected for the Coulomb repulsion $E_{\text{rel}}^{\text{C}} = (E_{\text{tot}}(n)/n - Q/R_n) - (E_{\text{tot}}(5)/5 - Q/R_5)$, $Q = 2$, R is the distance of a vertex from the centre (in Bohr), transferred to kcal/mol, vs. vertex number n of Si_n^{2-} clusters.