

Supplementary Material

1,2-Disilabicyclo[1.1.1]pentan-4-ones from a disilenide and acryloyl chlorides

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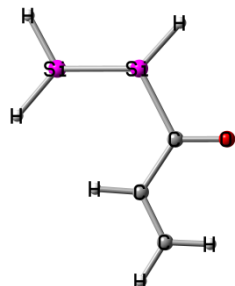
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Details of DFT calculations

All structures were optimized with Gaussian03^[S1] at the MP2/6-31g(d,p) level of theory. All compounds are local minima as verified by frequency calculations. Three different conformers of 4u were optimized.

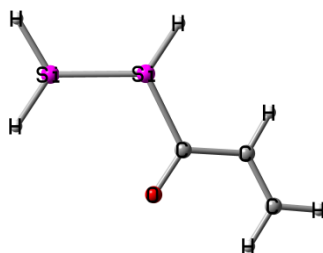
4u (*trans/cis*)



ΔG_{298} [kcal mol⁻¹]

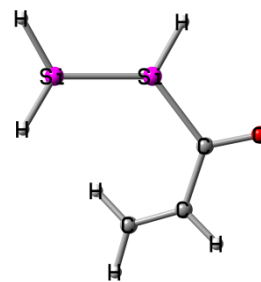
+ 20.68

4u* (*cis/cis*)



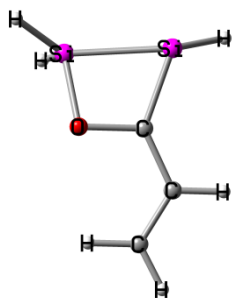
+ 21.22

4u** (*trans/trans*)



+ 21.20

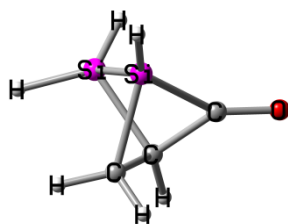
5u



ΔG_{298} [kcal mol⁻¹]

+ 3.81

6u



0.00

XYZ-COORDINATES

4u

Si	-0.88821100	0.88769500	0.17809000
Si	-2.35583300	-0.68060500	-0.13228200
O	1.76889900	1.43454900	-0.15788000
C	0.97953800	0.49527100	0.00704000
C	1.44424900	-0.91581400	0.10678600
C	2.74410500	-1.21707700	-0.02718100
H	-1.20961100	2.27737900	-0.18114400
H	-3.79927100	-0.41138300	-0.03709400
H	-2.00136100	-2.07025700	0.19960300
H	3.46088800	-0.42753000	-0.20677800
H	3.10460800	-2.23329800	0.03818600
H	0.70281300	-1.68484400	0.28908600

4u*

Si	0.77686400	-0.83404700	0.23188800
Si	2.57495700	0.30022100	-0.20628000
O	-0.82258000	1.38808900	0.21023500
C	-0.86357100	0.15577900	0.10078100
C	-2.14821700	-0.57016600	-0.10596100
C	-3.30600600	0.10185700	-0.18963500
H	0.70741000	-2.25648900	-0.15833900
H	3.88700500	-0.36667200	-0.16129000
H	2.63876100	1.73858200	0.08623500
H	-3.30622900	1.17986300	-0.10325400
H	-4.24957700	-0.40149300	-0.34257000
H	-2.11546000	-1.64975400	-0.19228600

4u**

Si	-0.54409000	-0.96064700	0.11607800
Si	-2.28265500	0.31584800	-0.09146400
O	2.10587600	-1.38613000	-0.12467300
C	1.30137900	-0.44586200	-0.04473600
C	1.77630100	0.95053600	-0.15601900
C	1.06952600	2.01065500	0.26525000
H	-0.66454300	-2.23512400	0.83847000
H	-3.62978000	-0.27547500	-0.06745300
H	-2.19519000	1.56747900	-0.85837200
H	0.09407500	1.89261500	0.71705100
H	1.46296700	3.01458300	0.19592300
H	2.77665700	1.06017500	-0.55980500

5u

Si	0.97455800	1.35976500	-0.13043700
Si	1.55449400	-0.85944700	0.15065100
O	-0.09194300	-1.01206500	-0.36158800
C	-0.48561000	0.30119000	-0.06918500
C	-1.91029700	0.50611100	0.08209800
C	-2.80845200	-0.49755500	0.08695200
H	0.97832800	2.48941500	0.82489600
H	-2.48874600	-1.52260200	-0.03243600
H	-3.86467000	-0.30316900	0.20742500
H	-2.23219300	1.53329300	0.21151800
H	1.71198900	-1.33921500	1.53371200
H	2.45025400	-1.62412900	-0.73460400

6u

Si	-0.12892700	1.10086200	-0.68044800
Si	-1.28042200	-0.87117400	-0.30876800
O	2.28199600	-0.70142300	-0.25371500
C	-0.30898100	0.97305300	1.23461500
C	0.10462700	-0.51083800	0.98781100
C	1.18885300	-0.21323800	-0.06424200
H	0.36453400	-1.15711400	1.82291900
H	0.42253400	1.52068400	1.82652400
H	-1.30552000	1.09265200	1.65620900
H	-0.15076000	2.28928600	-1.55766200
H	-1.14890000	-2.08932500	-1.12786200
H	-2.61398300	-0.75430000	0.30951400

[S1] Gaussian 98, g03 Revision B.04, 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, 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, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.