Dynamics of Si–H–Si bridges in agostically stabilized silylium ions

Samat Tussupbayev, Georgii I. Nikonov, and Sergei F. Vyboishchikov*^a

^a Institut de Química Computacional, Campus de Montilivi, Universitat de Girona, 17071 Girona, Catalonia, Spain.

Fax: +34 97241 8356; Tel: +34 97241 8362; vybo@stark.udg.es

^b Chemistry Department, Brock University, 500 Glenridge Ave., St. Catharines, ON, L2S 3A1, Canada.

Fax: +1 (905) 6829020; Tel: +1 (905) 6885550 ext 3350; gnikonov@brocku.ca

Supporting materials

- Cartesian coordinates (in ångström) and absolute energies	Pages 2–8
- Vibrational dynamics spectra	Pages 9–20

- Cartesian coordinates (in ångström) and absolute energies at PBEPBE//6-311G** level (in au)

Structure **1a** E = -2445.79557

С	-0.001808	0.704280	1,180880
C	0.001808	-0.704280	1,180880
C	0 001808	1 421837	-0 037838
C	-0 001808	-1 421837	-0 037838
C	0 010070	0 714646	-1 275517
C	-0.010070	-0.714646	-1,275517
si	-0 001948	1 529664	2 882966
н Н	0.000000	0.00000	3,592241
C	1.598697	2.114385	3.684469
н	1.676255	3.211105	3,663480
H	1.631292	1.791024	4.736365
H	2.475838	1.696566	3.168534
C	-1.601289	2.115775	3.685467
H	-1.677568	3.212637	3.664655
Н	-2.479019	1.699129	3.169544
H	-1.634335	1.792361	4.737306
Si	0.001948	-1.529664	2.882966
C	1.601289	-2.115775	3.685467
H	2.479019	-1.699129	3.169544
H	1.634335	-1.792361	4.737306
H	1.677568	-3.212637	3.664655
C	-1.598697	-2.114385	3.684469
H	-2.475838	-1.696566	3.168534
H	-1.676255	-3.211105	3.663480
H	-1.631292	-1.791024	4.736365
Si	0.037762	-3.307438	0.255563
H	-0.010192	-3.193004	1.808952
C	1.667566	-4.196512	-0.057720
H	1.688530	-5.137331	0.515075
H	1.802555	-4.444767	-1.119903
H	2.521723	-3.581652	0.263292
С	-1.504333	-4.307056	-0.153321
H	-1.503552	-5.239207	0.433763
Н	-2.418879	-3.748373	0.096433
Н	-1.545193	-4.579768	-1.217520
Si	-0.157964	-1.837572	-2.822500
Н	0.176370	-3.187944	-2.241759
С	1.086765	-1.559648	-4.213076
Н	0.915721	-0.646328	-4.798970
Н	2.116518	-1.536256	-3.825712
Н	1.014080	-2.412071	-4.907936
С	-1.942562	-1.931042	-3.429660
Н	-2.307986	-0.971639	-3.821651
Н	-2.026220	-2.678926	-4.234138
Н	-2.612898	-2.238162	-2.612420
Si	-0.037762	3.307438	0.255563
Н	0.010192	3.193004	1.808952
С	-1.667566	4.196512	-0.057720
Н	-1.688530	5.137331	0.515075

Η	-1.802555	4.444767	-1.119903
Н	-2.521723	3.581652	0.263292
С	1.504333	4.307056	-0.153321
Н	1.503552	5.239207	0.433763
Н	2.418879	3.748373	0.096433
Н	1.545193	4.579768	-1.217520
Si	0.157964	1.837572	-2.822500
Η	-0.176370	3.187944	-2.241759
С	1.942562	1.931042	-3.429660
Η	2.612898	2.238162	-2.612420
Η	2.307986	0.971639	-3.821651
Н	2.026220	2.678926	-4.234138
С	-1.086765	1.559648	-4.213076
Η	-1.014080	2.412071	-4.907936
Η	-0.915721	0.646328	-4.798970
Н	-2.116518	1.536256	-3.825712

Structure **1b** E = -2445.78514

С	0.390168	1.373558	-0.130961
С	0.161554	0.685671	1.087083
С	0.228317	0.681742	-1.366869
С	-0.161554	-0.685671	1.087083
С	-0.228317	-0.681742	-1.366869
С	-0.390168	-1.373558	-0.130961
Si	0.865504	3.185662	0.238183
H	0.406382	3.166912	1.716895
С	2.701119	3.582358	0.384392
H	3.178532	3.764987	-0.587191
H	2.822317	4.492948	0.993201
Н	3.245130	2.765631	0.881673
С	-0.161554	4.547147	-0.555226
H	0.102250	4.715784	-1.609160
H	-1.235307	4.313381	-0.503554
Н	0.009387	5.492376	-0.016091
Si	0.218971	1.501060	2.794528
С	1.834918	1.885287	3.680480
H	2.665784	1.292224	3.270523
Н	2.096450	2.950214	3.598688
Н	1.736137	1.642824	4.750057
С	-1.327586	2.301315	3.511551
H	-2.213871	2.060455	2.906328
Н	-1.499467	1.940590	4.537340
H	-1.224023	3.395484	3.549854
Si	-0.218971	-1.501060	2.794528
H	0.00000	0.00000	3.510852
С	1.327586	-2.301315	3.511551
Н	1.499467	-1.940590	4.537340
H	1.224023	-3.395484	3.549854
H	2.213871	-2.060455	2.906328

С	-1.834918	-1.885287	3.680480
Н	-1.736137	-1.642824	4.750057
Н	-2.665784	-1.292224	3.270523
Н	-2.096450	-2.950214	3.598688
Si	-0.865504	-3.185662	0.238183
Н	-0.406382	-3.166912	1.716895
С	0.161554	-4.547147	-0.555226
Н	-0.102250	-4.715784	-1.609160
Н	1.235307	-4.313381	-0.503554
Н	-0.009387	-5.492376	-0.016091
С	-2.701119	-3.582358	0.384392
Н	-3.178532	-3.764987	-0.587191
Н	-2.822317	-4.492948	0.993201
Η	-3.245130	-2.765631	0.881673
Si	0.648200	1.545904	-3.043108
Η	1.090247	0.456728	-3.969254
С	2.145811	2.698363	-2.937700
Η	2.460590	2.888854	-3.977134
Η	1.951857	3.680813	-2.486321
Η	2.996696	2.227548	-2.423563
С	-0.836399	2.469927	-3.756488
Η	-0.556371	2.937196	-4.713916
Η	-1.683675	1.795519	-3.944417
Η	-1.181848	3.267224	-3.081397
Si	-0.648200	-1.545904	-3.043108
Η	-1.090247	-0.456728	-3.969254
С	0.836399	-2.469927	-3.756488
Η	1.683675	-1.795519	-3.944417
Η	1.181848	-3.267224	-3.081397
Η	0.556371	-2.937196	-4.713916
С	-2.145811	-2.698363	-2.937700
Н	-2.460590	-2.888854	-3.977134
Н	-1.951857	-3.680813	-2.486321
Н	-2.996696	-2.227548	-2.423563

Structure **2** E = -2115.97067

С	-0.263729	-0.008255	1.229302
С	-0.962680	-0.002600	0.00000
С	1.152712	-0.011878	1.237144
С	-0.263729	-0.008255	-1.229302
С	1.851133	-0.015524	0.00000
С	1.152712	-0.011878	-1.237144
Si	-1.429678	-0.020111	2.723189
Н	-2.741810	0.021864	1.816943
С	-1.668761	-1.626767	3.667512
Н	-0.892456	-1.752237	4.436327
Н	-2.647151	-1.622664	4.173113
Н	-1.629433	-2.496172	2.994841
С	-1.614365	1.545644	3.745117
Н	-0.828318	1.609989	4.511796
Н	-1.554914	2.445255	3.114947

$\begin{array}{llllllllllllllllllllllllllllllllllll$	H	-2.587957	1.546076	4.259838
C -3.856631 -1.571598 0.00000 H -3.202241 -2.455749 0.00000 H -4.502483 -1.619458 0.88961 C -3.823893 1.6626268 0.00000 H -4.4502483 -1.619458 -0.88961 C -3.823893 1.6626268 0.00000 H -4.468606 1.686651 -0.889683 H -4.468606 1.686651 0.889683 H -4.468606 1.686651 0.889683 H -4.468606 1.686651 0.889683 H -2.771810 0.021864 -1.816943 C -1.668761 -1.622664 -4.17311 H -0.892456 -1.752237 -4.436322 H -1.554914 2.445255 -3.11494 H -2.587957 1.546076 -4.259833 H -1.554914 2.445255 -3.11494 H 0.809177 -0.115923 -3.860433 C 3.114535 -1.497384 -3.254163 H 3.95608 -1.	Si	-2.846990	0.017144	0.00000
H-3.202241-2.4557490.00000H-4.502483-1.6194580.88961H-4.502483-1.619458-0.88961C-3.8238931.6262680.00000H-3.1519182.4970830.00000H-4.4686061.686651-0.88968Si-1.429678-0.020111-2.72318H-2.7418100.021864-1.81694C-1.668761-1.626767-3.667511H-2.647151-1.622664-4.17311H-0.892456-1.752237-4.43632H-1.629433-2.496172-2.99484C-1.6143651.545644-3.74511H-2.5879571.546076-4.25983H-1.5549142.445255-3.11494'H-0.8283181.609989-4.51179'Si2.008969-0.003103-2.94403H0.809177-0.115923-3.860433C3.114535-1.497384-3.254160H2.598597-2.437437-3.00739H3.395608-1.535825-4.318433C2.8640971.631818-3.341060H3.1527111.647510-4.40404H3.1527111.6475104.40404H3.1527111.6475104.40404H3.1527111.6475104.40404H3.1527111.6475104.40404H3.95608-1.5358254.318433H3.95608-1.535825	С	-3.856631	-1.571598	0.00000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-3.202241	-2.455749	0.00000
H-4.502483-1.619458-0.88961C-3.8238931.6262680.00000H-3.1519182.4970830.00000H-4.4686061.686651-0.88968Si-1.429678-0.020111-2.72318Si-1.429678-0.020111-2.72318H-2.7418100.021864-1.81694C-1.668761-1.626767-3.66751H-2.647151-1.622664-4.17311H-0.892456-1.752237-4.43632H-1.629433-2.496172-2.99484C-1.6143651.545644-3.74511H-2.5879571.546076-4.25983H-1.5549142.445255-3.11494H-0.8283181.609989-4.51179Si2.008969-0.003103-2.94403H0.809177-0.115923-3.860433C3.114535-1.497384-3.254166H4.044501-1.453447-2.668014H2.598597-2.437437-3.007394H3.395608-1.535825-4.318433C2.8640971.6318183.341066H3.1527111.647510-4.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.647510	Н	-4.502483	-1.619458	0.889616
C -3.823893 1.626268 0.00000 H -3.151918 2.497083 0.00000 H -4.468606 1.686651 -0.88968 Si -1.429678 -0.020111 -2.72318 H -2.741810 0.021864 -1.81694 C -1.668761 -1.626767 -3.667511 H -2.647151 -1.622664 -4.17311 H -0.892456 -1.752237 -4.436322 H -1.629433 -2.496172 -2.994843 C -1.614365 1.545644 -3.74511 H -2.587957 1.546076 -4.259833 H -1.554914 2.445255 -3.1149424 H -0.828318 1.609989 -4.51179 Si 2.008969 -0.003103 -2.944033 C 3.114535 -1.497384 -3.254163 H 4.044501 -1.453447 -2.668014 H 2.598597 -2.437437 -3.007393 H 3.395608 -1.535825 -4.318433 C 2.864097	Н	-4.502483	-1.619458	-0.889616
H-3.1519182.4970830.00000H-4.4686061.686651-0.88968H-4.4686061.6866510.88968Si-1.429678-0.020111-2.72318H-2.7418100.021864-1.81694C-1.668761-1.626767-3.66751H-2.647151-1.622664-4.17311H-0.892456-1.752237-4.43632C-1.6143651.545644-3.74511H-2.5879571.546076-4.25983H-1.5549142.445255-3.11494'H-0.8283181.609989-4.51179Si2.008969-0.003103-2.94403C3.114535-1.497384-3.25416H0.809177-0.115923-3.860433C3.114535-1.497384-3.25416H3.395608-1.535825-4.318433C2.8640971.631818-3.341065H3.1527111.647510-4.40404H2.1948382.486009-3.158643Si2.008969-0.0031032.944033H3.1527111.6475104.404044H3.7794381.7878092.75056H3.1527111.6475104.404044H3.7794381.7878092.75056H2.1948382.4860093.158643C3.861431.6475104.404044H3.7949470.4265370.883323H3.7949470.4265370	С	-3.823893	1.626268	0.00000
H-4.4686061.686651-0.88968H-4.4686061.6866510.88968Si-1.429678-0.020111-2.72318H-2.7418100.021864-1.81694C-1.668761-1.626767-3.66751H-2.647151-1.622664-4.17311H-0.892456-1.752237-4.43632C-1.6143651.545644-3.74511H-2.5879571.546076-4.25983H-1.5549142.445255-3.11494'H-0.8283181.609989-4.51179Si2.008969-0.003103-2.94403H0.809177-0.115923-3.860433C3.114535-1.497384-3.254163H4.044501-1.453447-2.668013H3.395608-1.535825-4.318433C2.8640971.631818-3.341063H3.1527111.647510-4.404044H2.1948382.486009-3.158643C2.8640971.6318183.341063H3.1527111.6475104.404044H3.1527111.6475104.404044H3.7794381.7878092.750566H3.1527111.6475104.404044H3.7949470.4265373.860433C3.861431.6973843.254166H3.395608-1.5358254.318433H2.598597-2.4374373.007393H3.0527111.647510	Н	-3.151918	2.497083	0.00000
H -4.468606 1.686651 0.88968 Si -1.429678 -0.020111 -2.72318 H -2.741810 0.021864 -1.81694 C -1.668761 -1.626767 -3.667512 H -2.647151 -1.622664 -4.173112 H -0.892456 -1.752237 -4.43632^2 H -1.629433 -2.496172 -2.99484^2 C -1.614365 1.545644 -3.74511^2 H -2.587957 1.546076 -4.25983^2 H -1.554914 2.445255 -3.11494^2 H -0.828318 1.609989 -4.51179^2 Si 2.008969 -0.003103 -2.94403^2 H 0.809177 -0.115923 -3.86043^2 C 3.114535 -1.497384 -3.25416^2 H 4.044501 -1.453447 -2.66801^4 H 2.598597 -2.437437 -3.00739^2 H 3.395608 -1.535825 -4.31843^2 C 2.864097 1.631818 -3.34106^2 H 3.152711 1.647510 -4.40404^2 H 2.194838 2.486009 -3.15864^2 Si 2.008969 -0.003103 2.94403^3 H 3.152711 1.647510 4.40404^2 H 3.152711 1.647510 4.40404^2 H 3.152711 1.647510 4.40404^2 H 3.298597 -2.437437 3.00739^3 H 3.395608 -1.535825 4.31843^3 <	Н	-4.468606	1.686651	-0.889681
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-4.468606	1.686651	0.889681
H -2.741810 0.021864 -1.816943 C -1.668761 -1.622664 -4.17311 H -2.647151 -1.622664 -4.17311 H -0.892456 -1.752237 -4.43632° H -1.629433 -2.496172 -2.99484° C -1.614365 1.545644 -3.74511° H -2.587957 1.546076 -4.259833° H -1.554914 2.445255 -3.11494° H -0.828318 1.609989 -4.5179° Si 2.008969 -0.003103 -2.944033° H 0.809177 -0.115923 -3.860433° C 3.114535 -1.497384 -3.25416° H 4.044501 -1.453447° -2.66801° H 3.395608 -1.535825 -4.318433° C 2.864097 1.631818 -3.34106° H 3.152711 1.647510 -4.40404° H 2.194838 2.486009 -3.15864° Si 2.008969 -0.003103 2.94403° H 3.152711 1.647510 4.40404° H 3.152711 1.647510 4.40404° H 3.152711 1.647510 4.40404° H 3.395608 -1.535825 4.31843° H 3.395608 -1.535825 4.31843° H 3.395608 -1.535825 4.31843° H 3.395608 -1.535825 4.31843° H 3.395	Si	-1.429678	-0.020111	-2.723189
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-2.741810	0.021864	-1.816943
H -2.647151 -1.622664 -4.17311 H -0.892456 -1.752237 $-4.43632'$ H -1.629433 -2.496172 $-2.99484'$ C -1.614365 1.545644 $-3.74511'$ H -2.587957 1.546076 $-4.25983'$ H -1.554914 2.445255 $-3.11494'$ H -0.828318 1.609989 $-4.51179'$ Si 2.008969 -0.003103 $-2.94403'$ H 0.809177 -0.115923 $-3.86043'$ C 3.114535 -1.497384 $-3.25416'$ H 4.044501 -1.453447 $-2.66801'$ H 2.598597 -2.437437 $-3.00739'$ H 3.395608 -1.535825 $-4.31843'$ C 2.864097 1.631818 $-3.34106'$ H 3.152711 1.647510 $-4.40404'$ H 2.194838 2.486009 $-3.15864'$ Si 2.008969 -0.003103 $2.94403'$ H 3.152711 1.647510 $4.40404'$ H 3.152711 1.647510 $4.40404'$ H 3.779438 1.787809 $2.75056'$ H 2.194838 2.486009 $3.15864'$ C 3.114535 -1.497384 $3.25416'$ H 3.395608 -1.535825 $4.31843'$ H 2.598597 -2.437437 $3.00739'$ H 4.044501 -1.453447 $2.66801'$ C 3.363114 -0.064760 $0.00000'$ H 3.7	С	-1.668761	-1.626767	-3.667512
H -0.892456 -1.752237 $-4.43632'$ H -1.629433 -2.496172 $-2.994843'$ C -1.614365 1.545644 $-3.74511'$ H -2.587957 1.546076 $-4.25983'$ H -1.554914 2.445255 $-3.11494'$ H -0.828318 1.609989 $-4.51179'$ Si 2.008969 -0.003103 $-2.94403'$ H 0.809177 -0.115923 $-3.86043'$ C 3.114535 -1.497384 $-3.25416'$ H 4.044501 -1.453447 $-2.66801'$ H 2.598597 -2.437437 $-3.00739'$ H 3.395608 -1.535825 $-4.31843'$ C 2.864097 1.631818 $-3.34106'$ H 3.779438 1.787809 $-2.75056'$ H 3.152711 1.647510 $-4.40404'$ H 2.194838 2.486009 $-3.15864'$ Si 2.008969 -0.003103 $2.94403'$ H 3.152711 1.647510 $4.40404'$ H 3.152711 1.647510 $4.40404'$ H 3.152711 1.647510 $4.40404'$ H 3.779438 1.787809 $2.75056'$ H 2.194838 2.486009 $3.15864'$ C 3.114535 -1.497384 $3.25416'$ H 3.395608 -1.535825 $4.31843'$ H 2.598597 -2.437437 $3.00739'$ H 4.044501 -1.453447 $2.66801'$ C 3.63	Н	-2.647151	-1.622664	-4.173113
H -1.629433 -2.496172 -2.994844 C -1.614365 1.545644 -3.745117 H -2.587957 1.546076 -4.259833 H -1.554914 2.445255 -3.114944 H -0.828318 1.609989 -4.511799 Si 2.008969 -0.003103 -2.944033 H 0.809177 -0.115923 -3.860433 C 3.114535 -1.497384 -3.254163 H 4.044501 -1.453447 -2.668019 H 2.598597 -2.437437 -3.007394 H 3.395608 -1.535825 -4.318433 C 2.864097 1.631818 -3.341063 H 3.779438 1.787809 -2.750564 H 3.152711 1.647510 -4.404044 H 2.194838 2.486009 -3.158644 Si 2.008969 -0.003103 2.944033 H 0.809177 -0.115923 3.860433 C 2.864097 1.631818 3.341065 H 3.152711 1.647510 4.404044 H 3.779438 1.787809 2.750566 H 2.194838 2.486009 3.1586443 C 3.114535 -1.497384 3.254163 H 3.395608 -1.535825 4.318433 H 2.598597 -2.437437 3.0073943 H 3.395608 -1.535825 4.318433 H 2.598597 -2.437437 3.0073943 H 3.3	Н	-0.892456	-1.752237	-4.436327
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-1.629433	-2.496172	-2.994841
H -2.587957 1.546076 -4.259833 H -1.554914 2.445255 $-3.11494'$ H -0.828318 1.609989 -4.511796 Si 2.008969 -0.003103 -2.944036 H 0.809177 -0.115923 -3.860433 C 3.114535 -1.497384 -3.254166 H 4.044501 -1.453447 -2.668016 H 2.598597 -2.437437 -3.007396 H 3.395608 -1.535825 -4.318433 C 2.864097 1.631818 -3.341066 H 3.779438 1.787809 -2.750566 H 3.152711 1.647510 -4.404044 H 2.194838 2.486009 -3.15864336 Si 2.008969 -0.003103 2.9440336 H 0.809177 -0.115923 3.8604336 C 2.864097 1.631818 $3.3410663666666666666666666666666666666666$	С	-1.614365	1.545644	-3.745117
H -1.554914 2.445255 $-3.11494'$ H -0.828318 1.609989 -4.51179 Si 2.008969 -0.003103 -2.94403 H 0.809177 -0.115923 -3.86043 C 3.114535 -1.497384 -3.254163 H 4.044501 -1.453447 -2.668016 H 2.598597 -2.437437 -3.007393 H 3.395608 -1.535825 -4.318433 C 2.864097 1.631818 -3.341063 H 3.779438 1.787809 -2.750566 H 3.152711 1.647510 -4.404044 H 2.194838 2.486009 -3.158643 Si 2.008969 -0.003103 2.944033 H 0.809177 -0.115923 3.860433 C 2.864097 1.631818 3.341063 H 3.152711 1.647510 4.404044 H 3.779438 1.787809 2.750566433 H 3.79438 1.787809 2.7505664333 H 3.395608 -1.535825 $4.31843333333333333333333333333333333333$	Н	-2.587957	1.546076	-4.259838
H -0.828318 1.609989 -4.511799 Si 2.008969 -0.003103 -2.94403 H 0.809177 -0.115923 -3.860433 C 3.114535 -1.497384 -3.254163 H 4.044501 -1.453447 -2.668016 H 2.598597 -2.437437 -3.007393 H 3.395608 -1.535825 -4.318433 C 2.864097 1.631818 -3.341063 H 3.779438 1.787809 -2.750566 H 3.152711 1.647510 -4.404044 H 2.194838 2.486009 -3.158643 Si 2.008969 -0.003103 2.944033 H 0.809177 -0.115923 3.860433 C 2.864097 1.631818 3.341063 H 3.152711 1.647510 4.404044 H 3.395608 -1.535825 4.318433 H 2.598597 -2.437437 3.007393 H 4.044501 -1.453447 2.668016332 H 3.794947 0.426537 0.883323 H 3.794947 0.426537 -0.883323	Н	-1.554914	2.445255	-3.114947
Si 2.008969 -0.003103 -2.944034 H 0.809177 -0.115923 -3.860434 C 3.114535 -1.497384 -3.254164 H 4.044501 -1.453447 -2.668014 H 2.598597 -2.437437 -3.007394 H 3.395608 -1.535825 -4.318434 C 2.864097 1.631818 -3.341064 H 3.779438 1.787809 -2.750564 H 3.152711 1.647510 -4.404044 H 2.194838 2.486009 -3.158643 Si 2.008969 -0.003103 2.944034 H 0.809177 -0.115923 3.860433 C 2.864097 1.631818 3.34106536433 H 3.152711 1.647510 $4.4040444404444644444444444444444444444$	Н	-0.828318	1.609989	-4.511796
H0.809177-0.115923-3.860433C3.114535-1.497384-3.254163H4.044501-1.453447-2.668014H2.598597-2.437437-3.007393H3.395608-1.535825-4.318433C2.8640971.631818-3.341063H3.7794381.787809-2.750563H3.1527111.647510-4.404044H2.1948382.486009-3.158643Si2.008969-0.0031032.944033H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.1527111.6475104.404044H3.7794381.7878092.750563H2.1948382.4860093.1586443C3.114535-1.4973843.2541633H3.395608-1.5358254.318433H2.598597-2.4374373.0073933H4.044501-1.4534472.668014C3.363114-0.0647600.000004H3.7949470.4265370.883323H3.718348-1.1092800.000004H3.7949470.426537-0.883323	Si	2.008969	-0.003103	-2.944036
C3.114535-1.497384-3.254169H4.044501-1.453447-2.66801H2.598597-2.437437-3.007399H3.395608-1.535825-4.318439C2.8640971.631818-3.341067H3.7794381.787809-2.750567H3.1527111.647510-4.404047H2.1948382.486009-3.158643Si2.008969-0.0031032.944037H0.809177-0.1159233.860433C2.8640971.6318183.341067H3.1527111.6475104.404047H3.1527111.6475104.404047H3.1527111.6475104.404047H3.1527111.6475104.404047H3.1527111.6475104.404047H3.1527111.6475104.404047H3.1527111.6475104.404047H3.395608-1.5358254.318439C3.114535-1.4973843.254169H3.395608-1.5358254.318439H2.598597-2.4374373.007399H4.044501-1.4534472.668014C3.363114-0.0647600.000000H3.7949470.4265370.883323H3.718348-1.1092800.000000H3.7949470.426537-0.883323	Н	0.809177	-0.115923	-3.860435
H4.044501-1.453447-2.668010H2.598597-2.437437-3.007393H3.395608-1.535825-4.318433C2.8640971.631818-3.341063H3.7794381.787809-2.750563H3.1527111.647510-4.404044H2.1948382.486009-3.158643Si2.008969-0.0031032.944033C2.8640971.6318183.341063H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.7794381.7878092.750563H2.1948382.4860093.158643C3.114535-1.4973843.2541633H2.598597-2.4374373.0073933H4.044501-1.4534472.668010C3.363114-0.0647600.000003H3.7949470.4265370.883323H3.718348-1.1092800.000003H3.7949470.426537-0.883323	С	3.114535	-1.497384	-3.254169
H2.598597-2.437437-3.007393H3.395608-1.535825-4.318433C2.8640971.631818-3.341063H3.7794381.787809-2.750563H3.1527111.647510-4.404043H2.1948382.486009-3.158643Si2.008969-0.0031032.944033H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404043H3.7794381.7878092.750563H2.1948382.4860093.1586443C3.114535-1.4973843.2541633H2.598597-2.4374373.0073933H4.044501-1.4534472.6680133C3.363114-0.0647600.00000333H3.7949470.4265370.88332333333333333333333333333333333333	Н	4.044501	-1.453447	-2.668016
H3.395608-1.535825-4.318433C2.8640971.631818-3.341063H3.7794381.787809-2.750564H3.1527111.647510-4.404044H2.1948382.486009-3.158643Si2.008969-0.0031032.944033H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.1527111.6475104.404044H3.7794381.7878092.750564H2.1948382.4860093.158643C3.114535-1.4973843.254163H3.395608-1.5358254.318433H2.598597-2.4374373.007393H4.044501-1.4534472.668014C3.363114-0.0647600.000004H3.7949470.4265370.883323H3.718348-1.1092800.000004H3.7949470.426537-0.883323	Н	2.598597	-2.437437	-3.007398
C2.8640971.631818-3.341063H3.7794381.787809-2.750564H3.1527111.647510-4.404044H2.1948382.486009-3.158643Si2.008969-0.0031032.944034H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.7794381.7878092.750564H2.1948382.4860093.158643C3.114535-1.4973843.254163H3.395608-1.5358254.318433H2.598597-2.4374373.007393H4.044501-1.4534472.668014C3.363114-0.0647600.000004H3.7949470.4265370.883323H3.7949470.426537-0.883323	Н	3.395608	-1.535825	-4.318439
H3.7794381.787809-2.75056H3.1527111.647510-4.40404H2.1948382.486009-3.158643Si2.008969-0.0031032.94403H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.1527111.6475104.404044H3.7794381.7878092.750564H2.1948382.4860093.158643C3.114535-1.4973843.254163H3.395608-1.5358254.318433H2.598597-2.4374373.007393H4.046501-1.4534472.668016C3.363114-0.0647600.000006H3.7949470.4265370.883323H3.7949470.426537-0.883323	С	2.864097	1.631818	-3.341062
H3.1527111.647510-4.40404H2.1948382.486009-3.158643Si2.008969-0.0031032.94403H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404043H3.7794381.7878092.750563H2.1948382.4860093.1586433C3.114535-1.4973843.2541633H3.395608-1.5358254.31843333H2.598597-2.4374373.007393333H3.7949470.4265370.88332333333333333333333333333333333333	Н	3.779438	1.787809	-2.750564
H2.1948382.486009-3.158648Si2.008969-0.0031032.944039H0.809177-0.1159233.860439C2.8640971.6318183.341063H3.1527111.6475104.404049H3.7794381.7878092.750569H2.1948382.4860093.158648C3.114535-1.4973843.254169H3.395608-1.5358254.318439H2.598597-2.4374373.007398H4.044501-1.4534472.668019C3.363114-0.0647600.000009H3.7949470.4265370.883328H3.718348-1.1092800.000009H3.7949470.426537-0.883328	Н	3.152711	1.647510	-4.404044
Si2.008969-0.0031032.944036H0.809177-0.1159233.860439C2.8640971.6318183.341063H3.1527111.6475104.404046H3.7794381.7878092.750566H2.1948382.4860093.158649C3.114535-1.4973843.254163H3.395608-1.5358254.318439H2.598597-2.4374373.007393H4.044501-1.4534472.668016C3.363114-0.0647600.000006H3.7949470.4265370.883323H3.718348-1.1092800.000006H3.7949470.426537-0.883323	Н	2.194838	2.486009	-3.158648
H0.809177-0.1159233.860433C2.8640971.6318183.341063H3.1527111.6475104.404044H3.7794381.7878092.750564H2.1948382.4860093.158643C3.114535-1.4973843.254163H3.395608-1.5358254.318433H2.598597-2.4374373.007393H4.044501-1.4534472.668013C3.363114-0.0647600.000003H3.7949470.4265370.883323H3.7949470.426537-0.883323	Si	2.008969	-0.003103	2.944036
C2.8640971.6318183.341063H3.1527111.6475104.40404H3.7794381.7878092.750564H2.1948382.4860093.158643C3.114535-1.4973843.254163H3.395608-1.5358254.318433H2.598597-2.4374373.007393H4.044501-1.4534472.668016C3.363114-0.0647600.000006H3.7949470.4265370.883323H3.7949470.426537-0.883323	Н	0.809177	-0.115923	3.860435
H3.1527111.6475104.40404H3.7794381.7878092.75056H2.1948382.4860093.15864C3.114535-1.4973843.25416H3.395608-1.5358254.31843H2.598597-2.4374373.00739H4.044501-1.4534472.66801C3.363114-0.0647600.00000H3.7949470.4265370.883323H3.7949470.426537-0.883323	С	2.864097	1.631818	3.341062
H3.7794381.7878092.750564H2.1948382.4860093.158648C3.114535-1.4973843.254168H3.395608-1.5358254.318438H2.598597-2.4374373.007398H4.044501-1.4534472.668018C3.363114-0.0647600.000008H3.7949470.4265370.883328H3.718348-1.1092800.000008H3.7949470.426537-0.883328	Η	3.152711	1.647510	4.404044
H2.1948382.4860093.158648C3.114535-1.4973843.254169H3.395608-1.5358254.318439H2.598597-2.4374373.007398H4.044501-1.4534472.668019C3.363114-0.0647600.000009H3.7949470.4265370.883328H3.718348-1.1092800.000009H3.7949470.426537-0.883328	Н	3.779438	1.787809	2.750564
C3.114535-1.4973843.254169H3.395608-1.5358254.318439H2.598597-2.4374373.007399H4.044501-1.4534472.668019C3.363114-0.0647600.000009H3.7949470.4265370.883329H3.718348-1.1092800.000009H3.7949470.426537-0.883329	Н	2.194838	2.486009	3.158648
H3.395608-1.5358254.318439H2.598597-2.4374373.007399H4.044501-1.4534472.668019C3.363114-0.0647600.000009H3.7949470.4265370.883329H3.718348-1.1092800.000009H3.7949470.426537-0.883329	С	3.114535	-1.497384	3.254169
H2.598597-2.4374373.007393H4.044501-1.4534472.668016C3.363114-0.0647600.000006H3.7949470.4265370.883323H3.718348-1.1092800.000006H3.7949470.426537-0.883323	Н	3.395608	-1.535825	4.318439
H4.044501-1.4534472.66801C3.363114-0.0647600.00000H3.7949470.4265370.883323H3.718348-1.1092800.00000H3.7949470.426537-0.883323	Н	2.598597	-2.437437	3.007398
C3.363114-0.0647600.00000H3.7949470.4265370.883323H3.718348-1.1092800.00000H3.7949470.426537-0.883323	Н	4.044501	-1.453447	2.668016
H3.7949470.4265370.883323H3.718348-1.1092800.00000H3.7949470.426537-0.883323	С	3.363114	-0.064760	0.00000
H3.718348-1.1092800.00000H3.7949470.426537-0.883323	Н	3.794947	0.426537	0.883328
Н 3.794947 0.426537 -0.88332	Н	3.718348	-1.109280	0.00000
	Н	3.794947	0.426537	-0.883328

Structure from **Figure 3(a)** E = -2445.78299

~	1 210620	0 200120	0 010000
Ċ	1.312639	-0.309130	-0.019823
С	0.306086	-1.289038	-0.111242
С	0.978001	1.069188	0.038833
С	-1.051856	-0.919807	-0.024869
С	-0.397428	1.465490	0.015048

С	-1.414152	0.454930	0.048247
Si	3.062771	-1.031559	0.088879
Н	2.479275	-2.532200	-0.255882
С	4.279965	-0.912015	-1.341953
Н	4.979962	-0.074623	-1.208772
н	4.870072	-1.840151	-1.398568
н	3 758885	-0 780270	-2 301771
C	3 813367	-1 431635	1 770046
с ц	4 579241	-0 694799	2 051630
и П	3 044087	-1 444066	2.051050
и 11	1 201052	-2 422227	1 727964
л с¦	4.291000		1.737004
SI	0.043305	-3.000/55	-0.321184
C	1.013101		-2.042300
H 	0.928227	-3.055//3	-2.816494
Н	1.992956	-4.322380	-2.149584
H	0.233764	-4.587273	-2.222892
С	1.056727	-4.276519	1.125880
Н	0.992758	-3.751248	2.090318
Н	0.284563	-5.059584	1.108791
Н	2.040143	-4.767714	1.067523
Si	-2.182059	-2.452913	0.041162
Н	-1.011895	-3.440608	-0.346148
С	-3.428528	-2.772910	-1.331124
Н	-3.626530	-3.854829	-1.393110
Н	-4.385858	-2.267408	-1.140128
Н	-3.046694	-2.440779	-2.307924
С	-2.682252	-3.114155	1.732717
Н	-2.841761	-4.202253	1.667556
Н	-1.899069	-2.926285	2.482086
н	-3 614906	-2 655399	2 089616
si	-3 304134	0 668654	0 324720
ы ц	-3 635124	-0 745144	0.756848
C	-4 350181	0.913515	-1 229451
U U	-1 262201	1 005520	_1 600/02
п тт	4.001000	1.905528	-1.000402
п 11	-4.001902	0.104201	-1.969/6/
Н	-5.409013	0./5042/	-0.966050
C	-3./65426	1.751009	1.799483
Н	-3.494626	2.810152	1.6940/8
H	-4.854023	1.696031	1.960184
Η.	-3.273824	1.369053	2.707293
Si	2.575364	2.101656	0.265860
Η	3.497549	0.915906	0.596429
С	2.642121	3.187588	1.803308
Н	3.670439	3.553818	1.950454
Н	1.978275	4.062034	1.752754
H	2.357986	2.603356	2.691524
С	3.397894	2.816288	-1.274014
Н	4.463748	2.987351	-1.051252
Н	3.339589	2.104478	-2.111413
Н	2.969028	3.769009	-1.607186
Si	-0.858256	3.342410	0.011827
Н	-0.974479	3.762906	1.451755
С	0.424487	4.437921	-0.845577

Н	1.370396	4.582805	-0.311216
Н	0.640999	4.086685	-1.865949
Н	-0.034732	5.435930	-0.936184
С	-2.454709	3.769119	-0.907358
Н	-2.489102	4.868767	-0.974214
Н	-2.438817	3.380508	-1.937188
Н	-3.386665	3.453779	-0.425548

Structure from **Figure 6(a)** E = -2445.78126

a	1 200142	0 605560	0 040000
C	1.327143	-0.635563	0.048237
C	1.071231	0.758727	0.041892
C	0.231235	-1.548614	0.033117
С	-0.242903	1.251903	-0.100852
С	-1.104571	-1.032716	0.132965
С	-1.343721	0.363882	-0.033519
Si	3.193053	-0.945472	0.285956
Н	3.530597	0.538143	0.642365
С	3.668442	-1.899980	1.834155
Н	3.409546	-2.966673	1.760784
Н	4.753729	-1.828974	2.005688
Н	3.150727	-1.490934	2.714450
С	4.314296	-1.223543	-1.201768
Н	4.443753	-2.285921	-1.445449
Н	3.931542	-0.709730	-2.096120
Н	5.309652	-0.810055	-0.971984
Si	2.432735	2.050484	0.257520
С	2.872003	2.708023	1.967047
Н	2.175998	2.326748	2.728666
н	3.891461	2,407765	2.250736
н	2.827507	3.807779	1,975413
C	3.570585	2.574557	-1.147894
ч	3 196435	2 220051	-2 119663
н	3 636004	3 672887	-1 185648
н	4 587703	2 181327	-1 004007
ri Si	-0 352358	3 131251	-0 294342
ы ц	1 269221	3 275665	
		1 225247	
с u	-0.900404	F 102/01	1 10/001
п тт		J.IZJ401 4 EEEED	1 001041
н т	-1.949073	4.000004	1.001041
н	-0.832582	3.095241	2.093/91
	-0.445085	3.899591	-2.008623
н	0.10/24/	4.851/06	-2.023143
Н	-0.005719	3.232467	-2.764584
Н	-1.486093	4.108185	-2.297199
Si	-2.991560	1.258457	-0.397357
H	-2.422220	2.677626	-0.505363
С	-4.325006	1.374102	0.928780
Η	-4.829768	0.417920	1.125473
Η	-3.914022	1.745468	1.879531
Н	-5.091226	2.090367	0.590453
С	-3.660300	0.849698	-2.109111

Η	-4.023516	-0.185992	-2.172852
Н	-4.498736	1.518496	-2.359132
Н	-2.878235	0.979202	-2.872283
Si	0.475874	-3.441506	-0.288826
Н	0.334878	-4.209894	0.991574
С	2.179359	-3.853147	-1.003220
Н	2.141283	-4.921789	-1.273774
Н	2.394395	-3.296780	-1.927442
Н	3.024028	-3.746769	-0.309668
С	-0.737285	-4.020663	-1.619720
Н	-0.556119	-5.087613	-1.826243
Н	-1.796307	-3.913352	-1.354216
Н	-0.558724	-3.466566	-2.555049
Si	-2.499908	-2.153190	0.847259
Η	-1.920112	-3.523828	0.990563
С	-2.848789	-1.527604	2.596425
Η	-1.943680	-1.629275	3.214655
Н	-3.163437	-0.475497	2.628662
Н	-3.640452	-2.135877	3.061895
С	-4.070331	-2.305187	-0.196860
Η	-4.707846	-3.077541	0.263333
Н	-4.669447	-1.385798	-0.251721
Н	-3.848350	-2.630450	-1.224480



Figure S1. Calculated vibrational dynamics spectrum of the internal coordinate $r(Si^{\alpha 2}-H^{\alpha})-r(H^{\alpha}-Si^{\alpha 1})$ at 15 K.



Figure S2. Calculated vibrational dynamics spectrum of the internal coordinate $r(Si^{\alpha 2}-H^{\alpha}) + r(H^{\alpha}-Si^{\alpha 1})$ at 15 K.



Figure S3. Calculated vibrational dynamics spectrum of the internal coordinate $r(Si^{\beta_1}-H^{\beta_1}) - r(Si^{\beta_2}-H^{\beta_2})$ at 15 K.



Figure S4. Calculated vibrational dynamics spectrum of the internal coordinate $r(\text{Si}^{\beta_1}-\text{H}^{\beta_1}) + r(\text{Si}^{\beta_2}-\text{H}^{\beta_2})$ at 15 K.



Figure 13. Calculated vibrational dynamics spectrum of the internal coordinate $r(\text{Si}^{\gamma 1}-\text{H}^{\gamma 1}) - r(\text{Si}^{\gamma 2}-\text{H}^{\gamma 2})$ at 15 K.



Figure S5. Calculated vibrational dynamics spectrum of the internal coordinate $r(Si^{\gamma 1}-H^{\gamma 1}) + r(Si^{\gamma 2}-H^{\gamma 2})$ at 15 K.



Figure S6. Calculated vibrational dynamics spectrum of the internal coordinate r(7–8)-r(8–17) at 304 K.



Figure S7. Calculated vibrational dynamics spectrum of the internal coordinate r(7-8)+r(8-17) at 304 K.



Figure S8. Calculated vibrational dynamics spectrum of the internal coordinate r(26-27) – r(46-47) at 304 K.



Figure S9. Calculated vibrational dynamics spectrum of the internal coordinate r(26-27) + r(46-47) at 304 K.



Figure S10. Calculated vibrational dynamics spectrum of the internal coordinate r(36-37) – r(56-57) at 304 K.



Figure S11. Calculated vibrational dynamics spectrum of the internal coordinate r(36-37) + r(56-57) at 304 K.