Supporting information

"The Structures of Silicon Cluster Cations in the Gas Phase"

Jonathan T. Lyon, Philipp Gruene, André Fielicke, Gerard Meijer, Ewald Janssens, Pieterjan Claes, and Peter Lievens

Complete Reference 38.

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

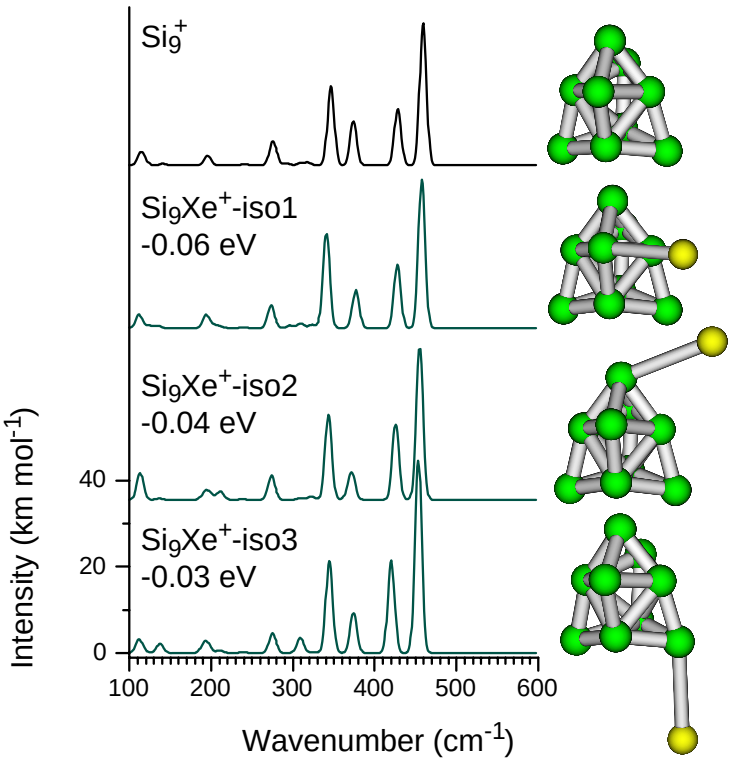


Figure S1. Comparison of the calculated IR spectra of bare Si_9^+ and different low-energy isomers of Si_9Xe^+ with the calculated Xe binding energies.

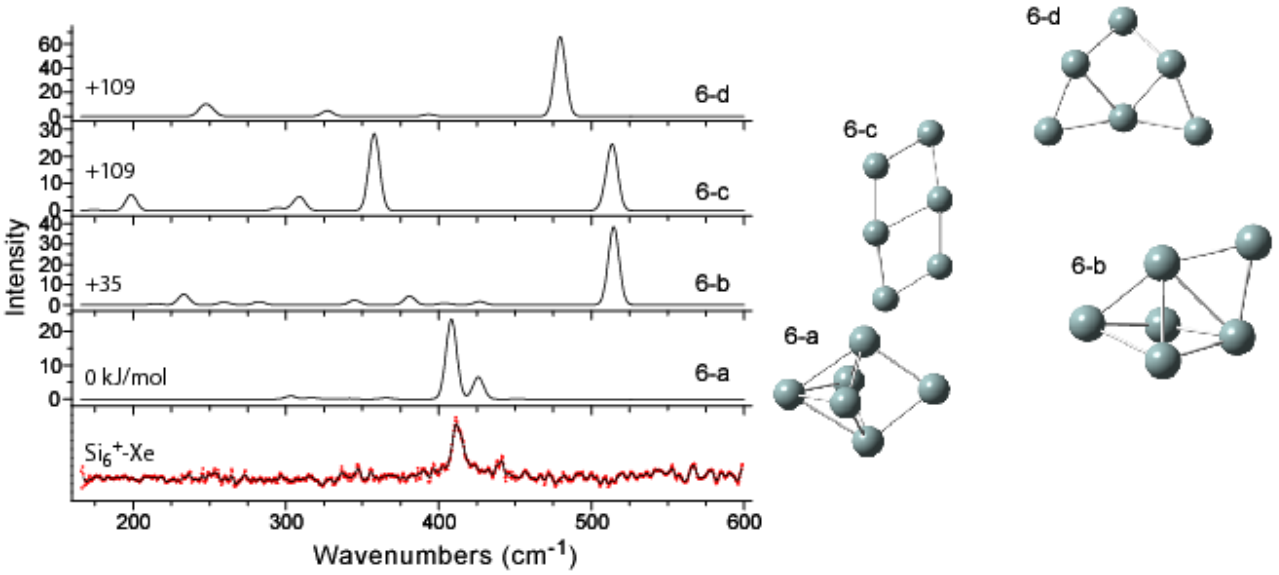


Figure S2. IR-MPD spectrum of the Si_6^+ cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

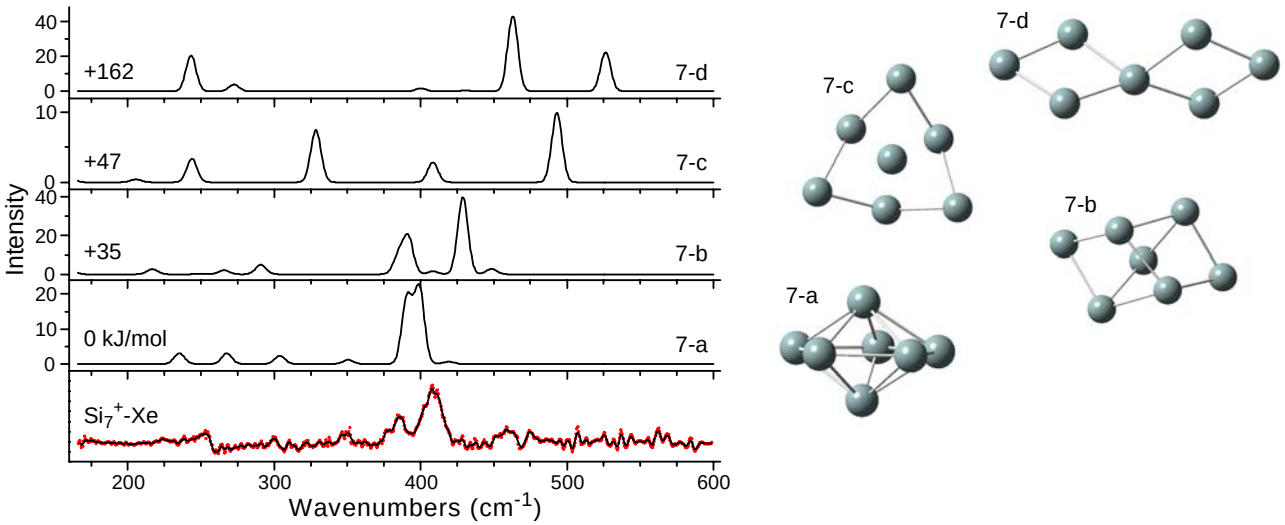


Figure S3. IR-MPD spectrum of the Si_7^+ cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

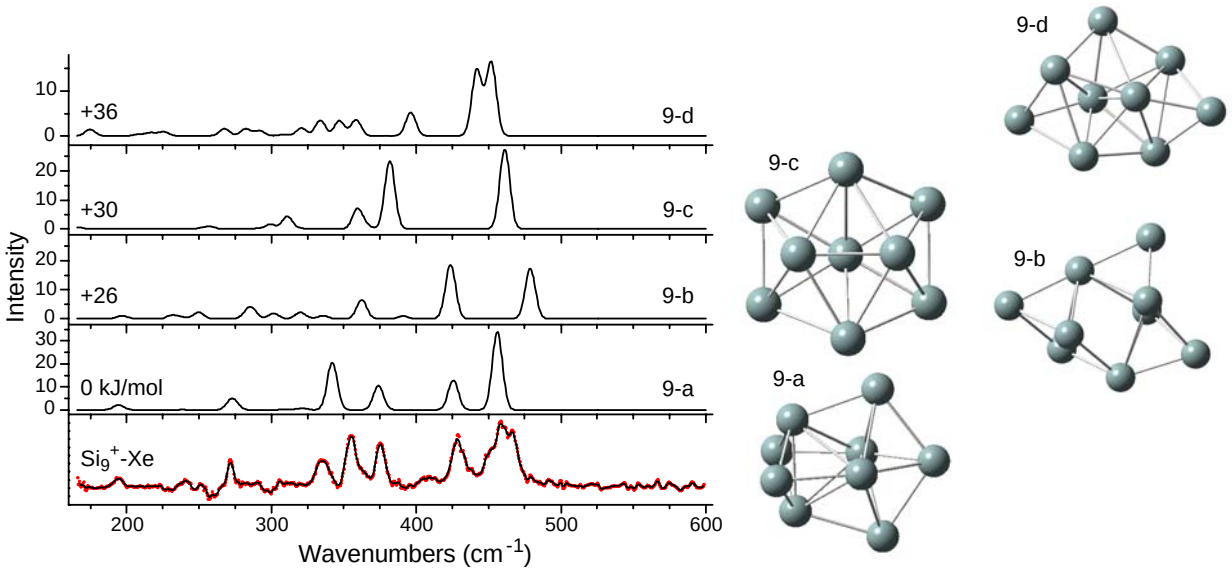


Figure S4. IR-MPD spectrum of the Si_9^+ cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

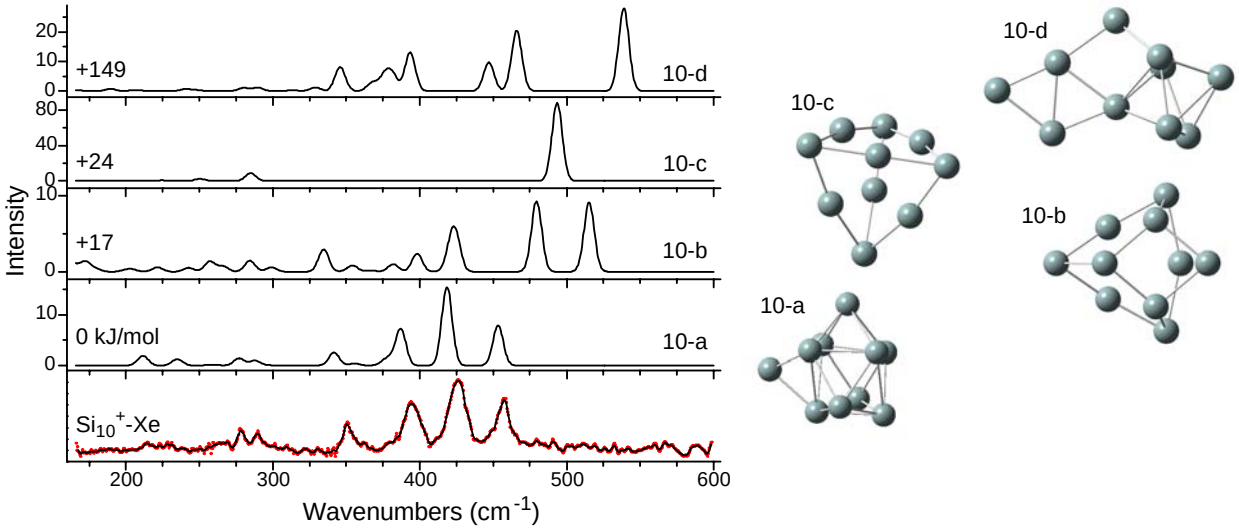


Figure S5. IR-MPD spectrum of the Si_{10}^{+} cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

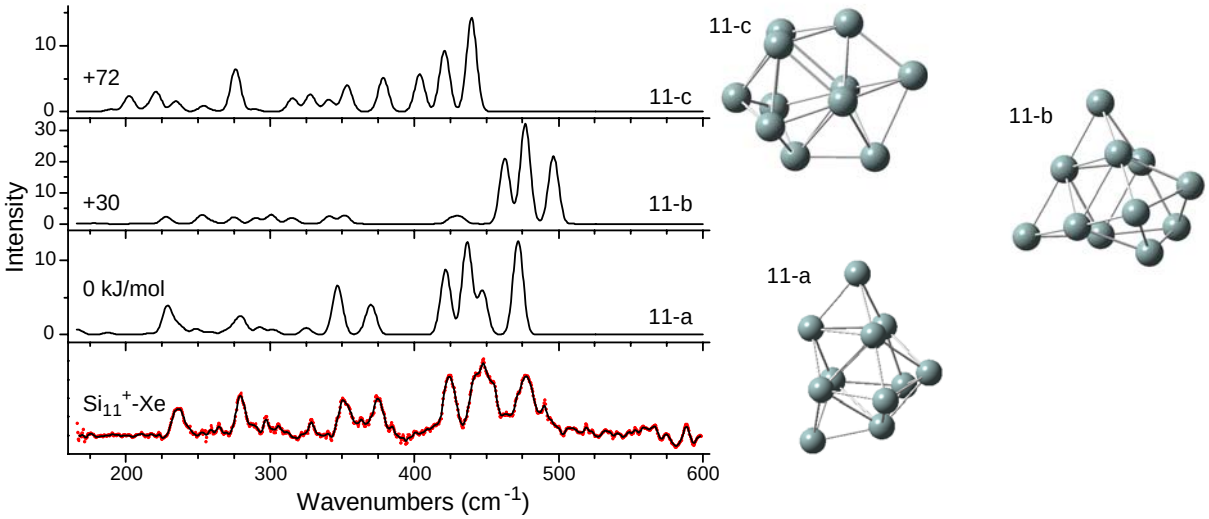


Figure S6. IR-MPD spectrum of the Si_{11}^{+} cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

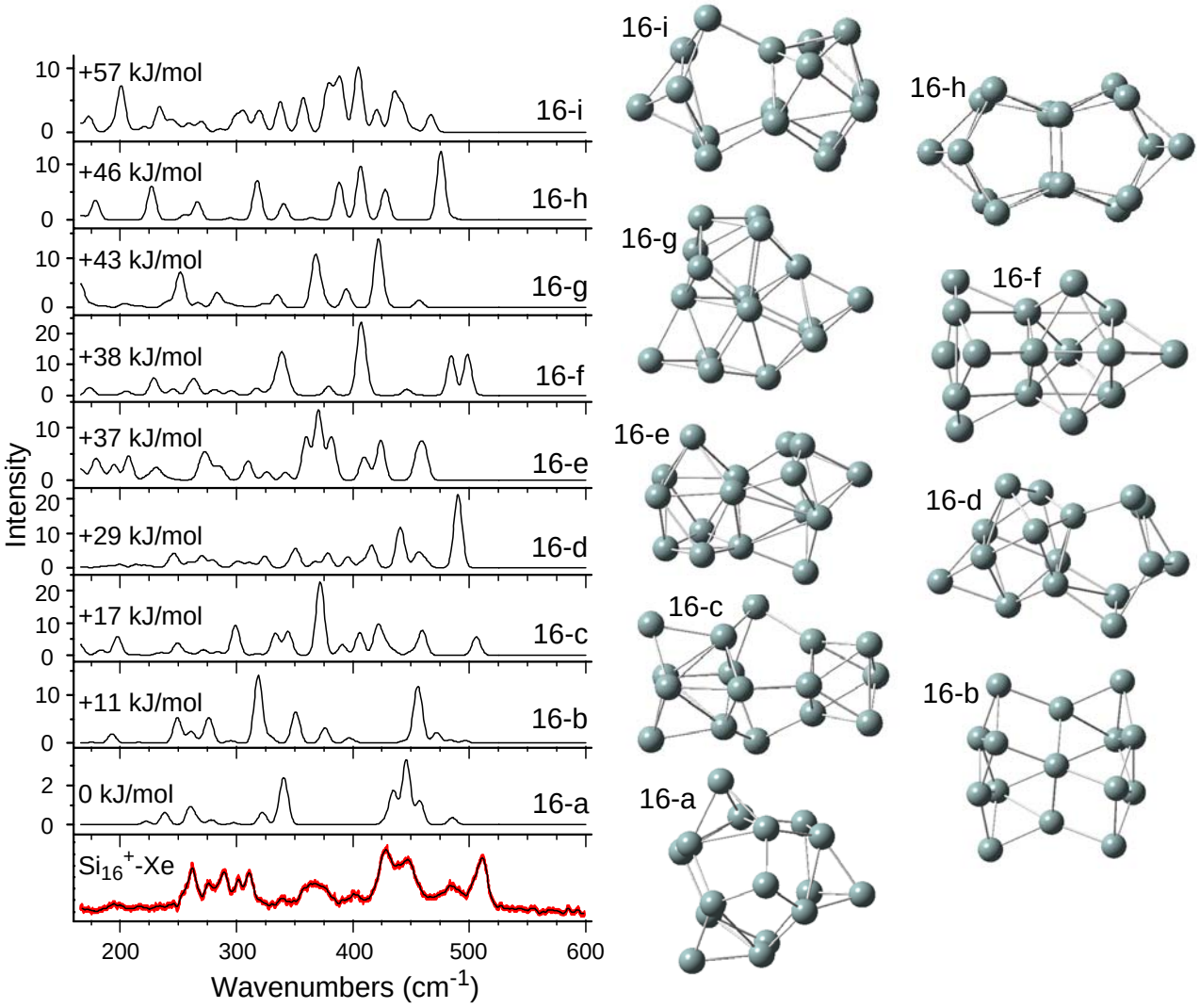


Figure S7. IR-MPD spectrum of the Si_{16}^{+} cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

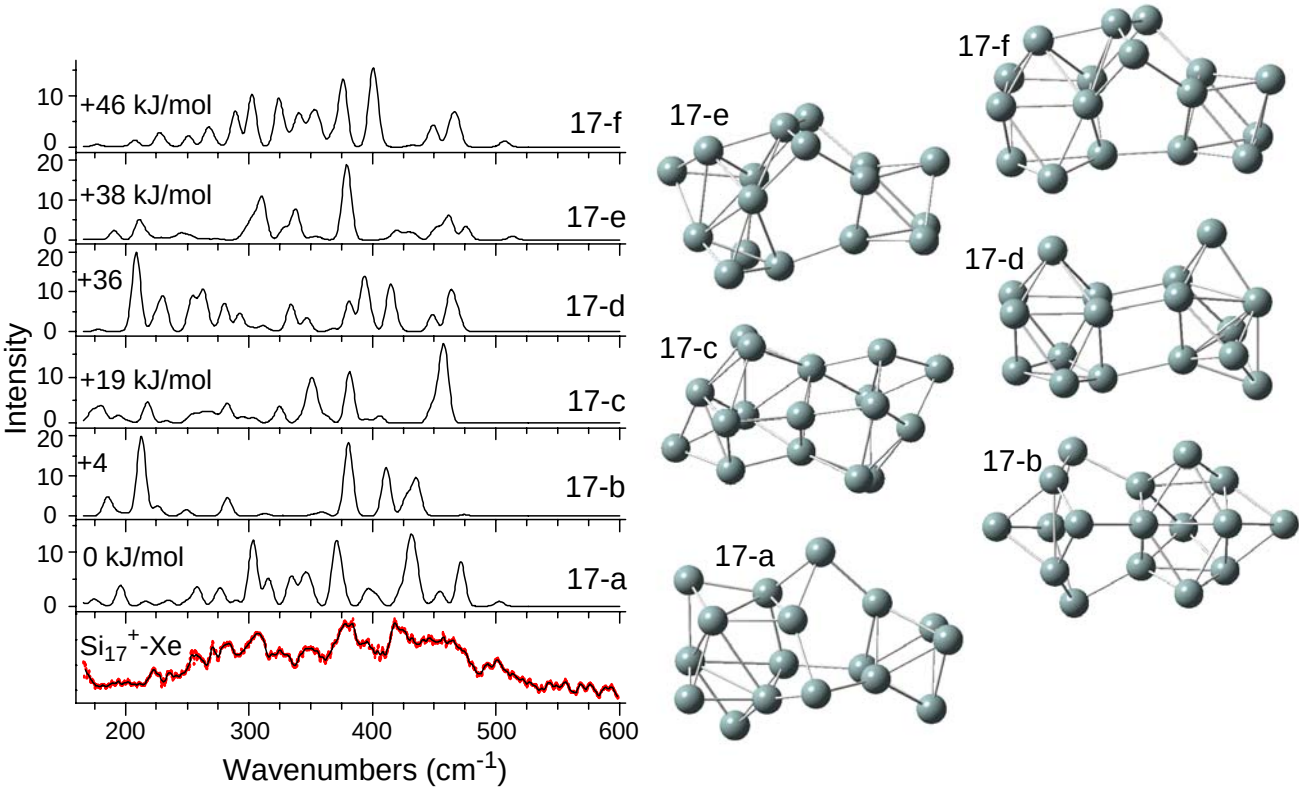


Figure S8. IR-MPD spectrum of the Si_{17}^{+} cluster tagged with a xenon atom compared to the predicted infrared spectra of multiple structural isomers with the lowest energy isomer at the bottom. The Y-axis is in km/mol for the theoretical infrared intensities (arbitrary units for experiment).

Cartesian Coordinates and Un-scaled Predicted Frequencies (IR intensities):

Si_6^+
Si,0,-2.1480482222,0.0016701825,-0.0000000149
Si,0,1.9629470422,-0.0015971499,0.
Si,0,0.3109105559,-1.8185881877,-0.0000003885
Si,0,0.3138567611,1.818115082,0.0000003933
Si,0,-0.2198330803,0.0001997378,1.4362209101
Si,0,-0.2198330568,0.0002003353,-1.4362209001

Frequency	IR intensities
69.6480026	0.34830001
104.979301	0.
133.243195	0.0944999978
294.300415	0.98269999
307.558807	0.445300013
317.030792	0.114799999
331.651886	0.179900005
354.839294	0.380699992
387.068298	0.
396.453094	25.1011009
413.530396	6.90910006
438.416412	0.0639000013

Si_7^+
Si,0,2.077916097,0.7364620606,0.0000003976
Si,0,1.4375556544,-1.6442204471,0.0000001215
Si,0,-1.4717239667,-1.6137098086,-0.0000006017
Si,0,0.0206356454,1.9674934866,0.0000004026
Si,0,-2.0620125417,0.7798828828,-0.0000007454
Si,0,-0.0011850939,-0.1129539089,-1.3265711642
Si,0,-0.0011857945,-0.1129542655,1.3265715895

Frequency	IR intensities
121.807404	0.136700004
123.975899	0.
135.547699	0.274399996
228.303406	2.94099998
228.901596	0.332899988
240.720306	0.00549999997
259.790894	3.17689991
294.967499	2.49410009
316.014587	0.
322.562500	0.0027999999
340.238800	1.21889997

379.348694 20.1727009
387.347198 15.7007999
387.834808 7.38520002
406.939209 0.72420001

Si_8^+
Si,0,-1.3510116576,-0.4508366576,0.2357662196
Si,0,-0.010668761,0.0549798751,2.3609682731
Si,0,-0.0115980567,-2.2631559335,1.2069617435
Si,0,0.0022150524,-1.9300068268,-1.3610296944
Si,0,0.0087455228,0.4866804307,-1.66487973
Si,0,0.0148976493,2.9061244471,-1.5497155744
Si,0,0.0013734397,1.6536293979,0.5233694859
Si,0,1.3460468111,-0.4574147328,0.2485592767

Frequency IR intensities
79.6682968 0.0719000027
110.037598 0.188600004
138.752502 0.61589998
142.855194 9.99999975E-05
171.582199 0.118799999
223.248596 0.0825000033
235.320404 0.
249.545700 0.865100026
256.799408 7.10270023
286.283691 0.552600026
311.972900 4.27820015
322.400391 0.00879999995
323.341003 0.437900007
328.630493 14.4998999
381.499908 5.5770998
393.127899 5.6335001
411.090210 20.5494003
439.992889 16.1909008

Si_9^+
Si,0,-1.261861051,0.0001456499,-1.2887492557
Si,0,0.5969328883,1.4704206596,0.0001099739
Si,0,-1.7323542736,2.0429866942,0.0001206101
Si,0,1.1084986479,-0.000199574,2.0751192356
Si,0,-1.2618771232,-0.0000219474,1.2887322792
Si,0,1.108524176,0.0000604949,-2.0751054644
Si,0,-1.7325280768,-2.0428282893,-0.0001404313
Si,0,2.5778649086,-0.0001090767,0.0000148063
Si,0,0.5967999039,-1.4704546112,-0.0001017538

Frequency IR intensities
82.8962021 0.
109.113602 3.3750999
112.424797 0.759800017
130.614197 0.389999986
186.936203 0.681299984
189.344604 0.933600008
189.414505 0.794499993
200.231201 0.
203.480392 0.0498000011
231.509598 0.122699998
264.225189 3.96869993
267.059204 1.78750002
283.525513 0.0307
300.856415 0.293500006
311.861511 0.744700015
323.910004 0.
332.090607 21.7408009
357.991913 0.0254999995
363.080200 11.1764002
413.255096 13.7312002
442.844391 35.9826012

Si_{10}^{+}
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Si,0,1.8156790077,1.4327684827,0.0210007774
Si,0,1.8022196227,-1.4496517724,0.0096720815
Si,0,-1.6143283202,0.0115983135,-1.0628928415
Si,0,-0.519581987,1.4026812351,1.0580625068
Si,0,-0.5327490661,-1.4060506276,1.0471860334
Si,0,-0.3239232098,2.1788865047,-1.2423944644
Si,0,-0.3440593303,-2.1660480448,-1.2592729359
Si,0,1.338706177,-0.0140406852,1.9856867531
Si,0,-2.4362038509,0.0067734388,1.18633327

Frequency IR intensities
92.3851013 0.277500004
93.6645966 0.350600004
119.162399 0.312999994
124.102097 0.241999999
177.318298 0.00300000003
202.413498 0.187900007
205.590393 1.8829
227.569000 0.98150003
229.526901 0.381799996
247.539093 0.0438000001

250.907303 0.102200001
256.735504 0.0388999991
268.870087 1.51719999
279.307709 0.980700016
280.922089 0.0289999992
287.136597 0.0838000029
325.351990 0.00659999996
331.645508 2.70160007
345.448395 0.40990001
364.161285 0.480100006
367.957703 1.26049995
375.731903 7.65439987
406.365814 16.4155998
440.126312 8.37110043

Si_{11}^{+}
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Si,0,0.6884260167,-1.1915070419,1.3373425635
Si,0,0.7008031042,1.1743975896,-2.2217089357
Si,0,-1.3690374251,0.4143403119,1.2519996154
Si,0,-1.1895626042,-1.9204084132,-0.0002082267
Si,0,-1.3690334536,0.4146034238,-1.2519631813
Si,0,0.7007563208,1.1739246225,2.2219812166
Si,0,-0.1365590917,2.2841318974,0.000236827
Si,0,0.6884373354,-1.1912172596,-1.3375785624
Si,0,-3.2491571726,-0.5044559706,-0.0000686785

Frequency IR intensities
102.237900 0.0922000036
113.832298 0.311300009
129.493195 1.26970005
140.779800 0.0273000002
154.744095 0.0908000022
161.883698 0.705500007
181.979599 0.304199994
209.618896 0.179499999
222.041504 3.96149993
224.718002 0.196999997
230.241394 1.245
241.342804 0.805599988
250.811493 0.388099998
262.026489 0.566299975
268.374695 1.21449995
272.579315 1.94879997
284.128113 1.05809999

293.398590 0.720799983
315.592804 0.971599996
336.379211 3.04139996
336.883087 3.95770001
356.040802 0.833500028
359.612305 3.77950001
409.429199 9.32520008
423.892914 13.1238003
434.318298 6.20219994
458.236389 13.3493996

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Si,0,0.0003917609,-1.6515500719,-1.5097558464
Si,0,0.000718902,-3.1856101843,0.263946415
Si,0,1.4486108532,-1.2747573923,0.7478976385
Si,0,1.7356998377,-0.0000042827,-1.5787749494
Si,0,1.4480164337,1.2757823167,0.7472518856
Si,0,-0.0007245726,3.1857442397,0.2623371998
Si,0,-1.448623473,1.2751345253,0.7472257501
Si,0,-0.0000258712,0.0005979945,2.3827092544
Si,0,-1.4480362029,-1.2754051289,0.7478608644
Si,0,-1.7356656423,-0.0007933009,-1.5788125005
Si,0,-0.0003589421,1.6507863188,-1.5105881413
Si,0,3.4268637636,0.0008206437,0.1393881584
Si,0,-3.4268668469,-0.0007456776,0.1393142714

Frequency IR intensities
104.995796 0.0621999986
118.946404 0.00139999995
144.071594 0.
157.555695 0.0760999992
164.120804 0.
168.820099 0.
169.700607 0.00989999995
178.647003 0.0160000008
186.310898 0.685800016
188.892395 0.0142000001
197.171600 0.0764999986
199.975906 0.58859998
213.929703 1.31500006
219.362701 0.204500005
227.455795 1.21679997
235.489105 0.537599981
253.156799 0.
257.774292 0.0203000009
272.775604 0.236499995

286.428589 2.70000005
300.035706 0.250699997
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313.162598 0.910700023
377.003204 6.58039999
378.636108 0.
382.462708 9.99999975E-05
384.812195 0.
397.161987 0.618200004
397.187408 3.76480007
442.841187 0.240199998
443.528412 4.08850002
447.436493 2.97110009
470.968994 9.02540016

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Si,0,-2.5543087296,0.0000015394,1.214039261
Si,0,1.3367460073,-2.0684101778,1.3922771696
Si,0,1.3367471345,2.0684117548,1.3922731817
Si,0,-0.0963164156,0.0000023106,2.072327232
Si,0,-0.5814220056,-1.379507265,0.0262871072
Si,0,2.5606315721,0.0000000082,1.0322681666
Si,0,1.6592109953,-1.4574781964,-1.0507404476
Si,0,-0.581421346,1.3795086317,0.0262846722
Si,0,1.6592098829,1.4574750387,-1.0507437641
Si,0,-0.0394956962,-0.0000029191,-2.1254091185
Si,0,3.5640948306,-0.0000017251,-1.173246594

Frequency IR intensities
85.1408997 0.0540999994
85.7796021 0.148000002
106.628601 0.0881000012
120.756500 0.0782999992
128.832108 0.0918999985
129.593094 0.520600021
164.361694 0.500100017
167.691498 0.73360002
167.858200 0.706799984
192.325195 0.379099995
193.693604 0.1061
199.152603 0.225899994
202.117706 0.551999986
211.818100 0.123599999

223.795898 2.54480004
232.871399 2.69720006
240.619202 0.807900012
242.025894 0.195999995
258.010010 1.10039997
266.984009 2.0848
275.797913 7.77099991
284.660309 0.236599997
293.670197 0.981100023
307.457397 0.315699995
310.323792 0.910000026
330.093414 1.36109996
332.445709 0.550499976
344.742096 0.276800007
354.461487 1.79149997
360.489807 0.253300011
377.743195 2.76079988
380.558197 9.95189953
404.171387 10.8743
414.329712 11.2665997
444.786987 0.488799989
454.239807 0.167600006

Si_{15}^{+}
Si,0,-2.2176732289,0.5936330074,-1.4291407195
Si,0,-1.9871498116,2.7016907841,-0.3525523242
Si,0,-2.213572386,0.9420720786,1.2320713065
Si,0,-1.9855427703,-1.6554417301,-2.165869839
Si,0,-2.2153392224,-1.5371298593,0.1992612228
Si,0,-1.9861320707,-1.0479340776,2.5148232594
Si,0,0.1172470236,-0.8932328408,-1.1765922376
Si,0,0.1158261302,1.4640958531,-0.1894150763
Si,0,1.4268067092,0.9609784561,-2.2922029583
Si,0,1.4196314408,1.5057148898,1.9779438173
Si,0,2.6623584544,1.524382419,-0.1911008393
Si,0,2.6654737693,-0.9273054037,-1.2198237921
Si,0,2.659059472,-0.5957720592,1.4219315974
Si,0,0.1155866889,-0.5707819125,1.3587420815
Si,0,1.4234198015,-2.4649696049,0.3119245015

Frequency IR intensities
53.4065018 9.99999975E-05
54.8059998 0.000500000024
61.5648994 9.99999975E-05
118.806999 0.409799993
119.468002 0.417199999

138.024597 0.867900014
140.014801 0.893899977
142.805405 3.17729998
166.664398 0.807600021
168.353897 0.8847
173.714096 1.8779
180.867798 0.725399971
181.057907 1.93079996
181.874207 1.12699997
182.019501 0.0188999996
203.930695 0.00079999998
212.741302 0.228
216.967194 1.54050004
223.816498 0.263900012
224.405502 0.265100002
258.270111 0.223700002
258.984985 0.0225000009
259.840393 0.0167999994
279.436005 4.24490023
279.759399 4.89209986
280.573608 5.94890022
305.045502 0.00109999999
306.961304 0.1171
308.278290 0.120999999
319.064606 0.00329999998
354.492615 10.8271999
354.916290 10.6582003
362.131287 0.187199995
398.783813 4.12270021
399.360107 3.98370004
413.898010 7.84089994
444.411896 0.000199999995
482.291809 12.8469
482.464996 12.8790998

Si_{18}^{+}
Si,0,-2.0478420032,-1.7208725361,-2.0932762645
Si,0,-2.0463935882,-1.7221102111,2.0923277342
Si,0,-3.43477641,-1.7135835466,0.000083274
Si,0,-3.4731021562,0.3495180467,-1.5171909861
Si,0,-3.4725256544,0.3486842183,1.5183522096
Si,0,-0.6855125058,-1.6955230653,-0.0011071718
Si,0,-2.3864694975,1.9491106425,0.0006738938
Si,0,-0.959943407,0.3566061238,-1.4121241769
Si,0,-0.9595039085,0.3557020341,1.411880005
Si,0,0.6300730469,1.9504721308,-2.3007639229

Si,0,0.6300123418,1.9495690916,2.3013327769
Si,0,0.017140696,2.4030874402,0.0003762873
Si,0,1.705797521,-1.4883492621,-0.0001190699
Si,0,3.7985058967,-1.4783379578,-1.3148545719
Si,0,3.7986224216,-1.4787157024,1.3143140215
Si,0,2.2408226713,0.5229395889,1.2153975142
Si,0,2.2406513037,0.5232112952,-1.2152645152
Si,0,4.4044432321,0.5885916696,-0.0000370372

Frequency	IR intensities
32.6324005	1.62720001
67.1183014	0.074000001
81.2703018	0.00870000012
86.2553024	0.0672999993
110.724998	0.00159999996
113.671303	0.00850000046
116.744400	0.746299982
123.736198	0.363999993
129.404297	0.264600009
141.517593	0.765299976
150.183899	0.0864999965
154.144501	0.139599994
165.650406	9.99999975E-05
168.263702	0.633700013
183.603897	0.0789000019
190.863297	8.18050003
199.060699	0.000600000028
202.448898	0.29370001
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216.607697	11.3057003
225.886993	0.221900001
233.543793	1.21159995
240.531296	0.371399999
243.726196	0.799000025
255.623795	2.13569999
256.308990	0.0324999988
276.699799	4.9611001
281.374115	1.39569998
287.485809	5.24130011
290.821106	4.20170021
312.538910	0.760999978
316.684113	4.64519978
327.144409	4.96610022
333.389587	5.84210014
337.928894	0.921500027
340.795593	3.80640006

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431.882294 2.13709998
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439.029114 5.93839979
449.973907 0.0298999995
491.817810 1.01960003