Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information for "Nonlinear effects in infrared action spectroscopy of silicon and vanadium oxide clusters: Experiment and kinetic modeling"

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Contents

1 Quantum chemical data

All quantum chemical calculations were performed using the Gaussian09 software package [1] and the DFT method. All geometries reported below are in Å frequencies and anharmonic couplings in cm^{-1}.

1.1 Silicon clusters

For neutral and cationic silicon clusters the BPW91 functional and the 6-311+G* basis set were used.

— Si_6 —

The optimized neutral geometry of Si_6 in its singlet state (C_{2v} isomer) in Cartesian coordinates and angströms is

```
Si       -1.341597   -1.355247    0.001997
Si        1.616603    1.217421   -0.002172
Si       -1.474571    1.384188    0.000452
Si        1.183128   -1.497230   -0.000130
Si        0.009417    0.126257    1.354535
Si        0.007022    0.124612   -1.354681
```

Its total electronic energy is -1736.53960402 Hartree, and at this geometry the cationic state (doublet spin multiplicity) has an energy of -1736.24079539 Hartree, giving a vertical ionization energy of 8.13 eV. The average rotational constant used to convolute the action spectra is 15.1 cm^{-1}.

Its harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	16.7597	0.202	5	305.684	0.542	9	391.303	0.002
2	51.2309	0.194	6	315.097	0.000	10	435.446	10.435
3	131.7791	0.000	7	371.066	0.006	11	443.578	20.236
4	254.7936	0.022	8	388.494	0.268	12	445.714	5.906

Table S1: Vibrational frequencies and IR intensities of neutral Si_6

The matrix of anharmonic couplings used in the modeling, with the same mode numbering as in table S1, is given as

```
           1             2             3             4             5
 1 -0.533363D+00
 2 -0.680033D+01 -0.574851D+00
 3 -0.392254D+00 -0.293722D+01 -0.576801D+00
 4 -0.283724D+01 -0.225926D+01 -0.260562D+01 -0.568960D+00
 5 -0.179471D+01 -0.363503D+01 -0.192458D+01 -0.677445D+01 -0.948204D+00
 6 -0.957594D+00 -0.873021D-01 -0.733147D+00 -0.145728D+01 -0.202382D+01
 7 -0.306700D+00 -0.925647D+00 -0.675245D+00 -0.534009D+00 -0.132898D+00
 8 -0.135192D+01  0.218614D+00 -0.774723D+00 -0.138324D+01 -0.232669D+01
 9  0.122207D+00 -0.102864D+01 -0.788830D+00  0.861744D+00  0.177348D+01
10 -0.122208D+01 -0.834938D+00 -0.129912D+01  0.367161D+00  0.649008D+00
11 -0.139034D+01  0.248630D+00  0.109423D+01  0.107650D+01 -0.136654D+01
12  0.295010D+01 -0.213975D+01  0.142718D+01  0.480972D+01 -0.185788D+01
           6             7             8             9            10
 6 -0.729742D+00
 7  0.701864D-01 -0.158458D+00
 8 -0.259707D+01  0.102202D+00 -0.729630D+00
 9  0.121868D+01  0.981241D+00  0.112498D+01 -0.204942D+01
10 -0.150678D+01  0.565539D+00 -0.255508D+00 -0.211315D+01  0.652660D-01
11  0.877437D-01  0.191062D+01  0.556090D+00 -0.176597D+01 -0.263424D+00
12  0.657514D+01 -0.292457D+01  0.636410D+01 -0.548452D+01 -0.501622D+00
          11            12
11 -0.560549D+01
12 -0.116542D+02  0.259495D+01
```

— Si_7 —

The optimized neutral geometry of Si_7 in its singlet state is in Cartesian coordinates

```
Si        0.000000   -0.000002    1.277153
Si        0.000000    2.137331   -0.000001
Si        2.032719    0.660473    0.000000
Si        1.256292   -1.729137    0.000000
Si       -1.256292   -1.729137    0.000000
Si       -2.032719    0.660473    0.000000
Si        0.000000   -0.000003   -1.277152
```

Its total electronic energy is -2025.99215898 Hartree, and at this geometry the cationic state (doublet spin multiplicity) has an energy of -2025.68965569 Hartree, giving a vertical ionization energy of 8.23 eV. The average rotational constant used to convolute the action spectra is 13.0 cm^{-1}.

Its harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	168.5375	0.000	6	406.518	12.174	11	329.252	0.000
2	216.5820	0.042	7	168.537	0.000	12	332.630	0.000
3	224.8315	0.591	8	216.582	0.042	13	351.944	0.000
4	284.5745	0.000	9	284.582	0.000	14	406.519	12.174
5	332.6291	0.000	10	329.241	0.000	15	427.079	0.000

Table S2: Vibrational frequencies and IR intensities of neutral Si_7

The matrix of anharmonic couplings used in the modeling is given as

```
           1             2             3             4             5
 1 -0.205785D+00
 2 -0.822184D+00 -0.290603D+00
 3 -0.413201D-01 -0.718743D+00  0.463624D-01
 4 -0.364188D+00 -0.658118D+00 -0.484216D+00 -0.267412D+00
 5 -0.101278D+01 -0.866513D+00 -0.816133D+00 -0.632884D+00 -0.179503D+00
 6 -0.100539D+01 -0.287629D+01 -0.802002D+00 -0.637349D+00  0.239411D+00
 7 -0.751677D+00 -0.108119D+01 -0.304573D+00 -0.477742D+00 -0.551299D+00
 8 -0.209658D+01 -0.108690D+01 -0.576722D+00 -0.103770D+01 -0.484360D+00
 9  0.319416D-01 -0.665955D+00  0.406837D+00 -0.107115D+00 -0.423850D+00
10 -0.818185D+00 -0.202255D+00 -0.718874D+00 -0.562929D+00 -0.287969D+01
11  0.442841D+00  0.362849D+00 -0.422456D-02 -0.135893D-01  0.381256D+00
12 -0.751422D+00 -0.942882D+00 -0.298784D+00 -0.333462D+00 -0.551219D+00
13 -0.212896D+01 -0.648851D+00 -0.722929D+00 -0.194622D+00  0.621904D-01
14 -0.209477D+01 -0.616689D-01 -0.129360D+00 -0.954695D+00 -0.151073D+01
15  0.319276D-01 -0.666373D+00  0.406477D+00 -0.564597D+00 -0.367990D+00
           6             7             8             9            10
 6 -0.175459D+00
 7 -0.550717D+00  0.316035D-01
 8 -0.150868D+01 -0.633384D+00  0.393648D+00
 9 -0.367396D+00 -0.100167D+01  0.256085D+00 -0.136047D+00
10 -0.863011D+00 -0.854554D+00 -0.620627D-01 -0.666152D+00 -0.271917D+00
11  0.397969D+00  0.132544D-01 -0.759732D-01 -0.208096D-01  0.362549D+00
12 -0.550560D+00  0.675668D+00 -0.586957D+00 -0.219269D+00 -0.100578D+01
13  0.848355D-01 -0.647413D+00 -0.194487D+00 -0.582840D-01 -0.652331D+00
14 -0.484058D+00 -0.427541D+00  0.648318D+00  0.255941D+00 -0.644682D+00
15 -0.423276D+00 -0.219109D+00  0.255959D+00 -0.386062D-01 -0.666298D+00
          11            12            13            14            15
11  0.000000D+00
12  0.542636D+00  0.214075D-01
13  0.590275D+00 -0.647424D+00  0.292750D+00
14 -0.865094D-01 -0.500929D+00 -0.194482D+00  0.442340D+00
15  0.299487D-01 -0.114138D+01  0.157210D+00  0.256300D+00 -0.135931D+00
```

— Si_{10} —

The optimized neutral geometry of Si_{10} in its singlet state is in Cartesian coordinates

Si	−0.054941	2.689441	0.000000
Si	2.453375	−0.211794	0.000000
Si	−1.218707	−0.286881	2.120471
Si	−1.218707	−0.286881	−2.120471
Si	0.773507	0.959375	1.373499
Si	−1.604887	0.910780	0.000000
Si	0.773507	0.959375	−1.373499
Si	0.773507	−1.562653	1.284149
Si	−1.450162	−1.608109	0.000000
Si	0.773507	−1.562653	−1.284149

Its total electronic energy is -2894.32023028 Hartree, and at this geometry the cationic state (doublet spin multiplicity) has an energy of -2894.02162120 Hartree, giving a vertical ionization energy of 8.13 eV. The average rotational constant used to convolute the action spectra is 9.4 cm^{-1}.

Its harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	94.9454	0.010	9	299.549	0.387	17	238.187	0.462
2	180.5651	0.007	10	329.844	2.799	18	250.054	0.000
3	208.8242	0.049	11	354.783	0.357	19	276.317	0.021
4	238.1401	0.463	12	369.278	0.203	20	280.469	0.919
5	258.4184	0.231	13	410.047	3.850	21	292.616	0.000
6	276.2947	0.019	14	466.904	0.291	22	294.458	0.325
7	280.4740	0.920	15	95.036	0.010	23	369.276	0.204
8	294.4595	0.327	16	180.587	0.007	24	410.053	3.848

Table S3: Vibrational frequencies and IR intensities of neutral Si_{10}

The matrix of anharmonic couplings used in the modeling is given as

	1	2	3	4	5
1	−0.363702D+00				
2	−0.115881D+01	−0.431316D+00			
3	−0.128694D+01	−0.118001D+01	−0.317855D+00		
4	−0.124988D+01	−0.365192D+00	−0.166748D+01	−0.179349D+00	
5	0.239109D+00	0.362053D+00	0.402792D−02	0.222312D−03	0.000000D+00
6	−0.486616D+00	−0.393885D+00	−0.395052D+00	−0.817749D+00	−0.445287D−03
7	−0.616367D+00	−0.139304D+00	−0.967532D+00	−0.157236D+01	−0.527144D−01
8	−0.323376D+00	−0.226712D+00	−0.287955D+00	−0.149605D+00	0.301671D−05
9	−0.423251D+00	−0.399174D−01	−0.862307D+00	0.147927D+00	0.112113D−01
10	0.568564D+00	−0.941382D−01	0.278198D+00	0.229377D+00	0.120712D−02
11	−0.977852D+00	−0.151128D+01	−0.262211D+00	−0.455541D+00	0.349094D+00
12	−0.375983D+00	−0.729478D+00	−0.230458D+00	−0.125028D+01	−0.235140D−01
13	−0.739287D+00	−0.413678D+00	−0.703247D+00	−0.376371D+00	−0.185254D−02
14	−0.406106D+00	−0.460878D+00	−0.613427D+00	−0.432046D+00	0.391667D−04
15	−0.389297D+00	−0.299249D+00	−0.564810D+00	−0.194884D+00	0.705151D−03
16	−0.398652D+00	−0.577188D+00	−0.353355D+00	−0.509397D+00	−0.100741D−02
17	−0.233169D+00	−0.706256D+00	−0.454013D+00	−0.162867D+01	0.851401D−02
18	−0.481599D+00	−0.106562D+01	−0.116035D+00	−0.539550D+00	0.289403D−02
19	−0.699796D+00	−0.688112D+00	−0.612911D+00	−0.792462D+00	0.303541D−02
20	−0.519208D+00	0.459586D+00	−0.254950D+00	−0.584668D+00	0.166209D−02
21	−0.662758D+00	−0.360447D+00	−0.273622D+00	−0.140575D+00	0.192348D−02
22	−0.650460D+00	−0.517771D+00	−0.800931D−01	−0.658204D+00	0.367770D−02
23	−0.139118D+01	−0.148622D+00	−0.100294D+01	0.165231D+00	0.129020D−01
24	0.923794D+00	0.393604D+00	−0.582481D+00	0.286811D+00	−0.235047D−01

	6	7	8	9	10
6	-0.199306D+00				
7	-0.872729D+00	-0.682333D-01			
8	-0.141969D+00	-0.488951D-01	0.108664D-01		
9	-0.528168D-01	0.744682D+00	0.174905D+00	0.152515D+00	
10	-0.565790D+00	-0.138189D+01	-0.216663D+00	-0.342675D+00	-0.785761D+00
11	-0.721510D+00	-0.314923D+00	-0.559932D+00	0.563058D-01	-0.433287D+00
12	-0.695962D+00	-0.587197D+00	-0.666379D+00	-0.139261D+01	0.918316D+00
13	-0.687548D+00	-0.138932D+00	-0.362558D+00	-0.145285D+00	0.400254D+00
14	-0.640524D+00	-0.480395D+00	-0.203604D+00	-0.129433D+01	-0.829057D-01
15	-0.151207D+00	-0.441425D+00	-0.471773D+00	-0.144338D+01	0.129716D+00
16	-0.306809D+00	-0.281323D+00	-0.142011D+00	0.188990D+00	0.452825D-01
17	-0.568341D+00	-0.964021D+00	-0.273577D+00	-0.100479D+01	-0.533710D+00
18	-0.521297D+00	-0.833579D+00	-0.103040D+00	0.135499D+00	0.525491D+00
19	-0.324713D+00	-0.819529D+00	-0.120415D+00	-0.442580D-02	0.179921D+00
20	-0.245843D+00	-0.535688D+00	-0.217819D+00	0.161516D+00	-0.134921D+01
21	-0.120550D+00	-0.481994D-01	-0.253232D-01	0.934083D-01	0.712281D-01
22	-0.681051D+00	-0.655351D+00	-0.511697D+00	-0.259539D+00	0.142173D+01
23	-0.396915D-02	0.753568D+00	0.878852D-01	-0.307697D+00	-0.520825D+00
24	0.177426D+00	-0.144882D+01	0.105290D+00	-0.521486D+00	-0.450746D+00

	11	12	13	14	15
11	-0.586273D+00				
12	-0.116414D+01	-0.362252D+00			
13	-0.185261D+01	-0.115977D+01	-0.434091D+00		
14	-0.413985D+00	-0.412916D+00	-0.459429D+00	-0.117655D+00	
15	0.267973D-01	-0.391657D+00	-0.303801D+00	-0.390029D+00	-0.434042D+00
16	-0.434281D+00	-0.414324D+00	-0.599649D+00	-0.463475D+00	-0.167315D+00
17	-0.268480D+00	-0.128993D+01	-0.117129D+01	-0.641291D+00	-0.588130D+00
18	-0.301267D+00	-0.692020D+00	-0.128161D+01	-0.548089D+00	-0.164288D+00
19	-0.752111D+00	-0.485688D+00	-0.401738D+00	-0.640602D+00	-0.175829D+00
20	-0.625139D+00	-0.590014D+00	0.426200D+00	-0.440227D+00	-0.656730D-01
21	-0.583455D+00	-0.325944D+00	-0.228092D+00	-0.203093D+00	-0.477816D+00
22	-0.319175D+00	-0.703487D+00	-0.609540D+00	-0.675877D+00	-0.187019D+00
23	0.276856D+00	-0.418740D+00	-0.372672D-01	-0.130153D+01	-0.147157D+01
24	-0.407367D+00	0.564663D+00	-0.121890D+00	-0.829262D-01	0.130067D+00

	16	17	18	19	20
16	-0.807296D-01				
17	-0.379584D+00	-0.304790D+00			
18	-0.386771D+00	-0.617028D+00	-0.150515D+00		
19	-0.352285D+00	-0.392705D+00	-0.471101D+00	-0.200402D+00	
20	-0.262646D+00	-0.272872D+00	-0.229157D+00	-0.249673D+00	-0.365382D-01
21	-0.142133D+00	-0.218725D+00	-0.890046D-01	-0.140994D+00	-0.216606D+00
22	-0.229721D+00	-0.991931D-01	-0.157434D+00	-0.698548D+00	-0.629109D+00
23	0.179744D+00	-0.855866D+00	-0.113081D+00	-0.514872D-01	0.161985D+00
24	0.629496D-02	0.286092D+00	0.832151D+00	-0.574261D+00	-0.134723D+01

	21	22	23	24
21	0.132330D-01			
22	-0.517044D+00	-0.510637D-01		
23	0.172088D+00	-0.259431D+00	0.153277D+00	
24	-0.212075D+00	0.143422D+01	-0.342362D+00	-0.788808D+00

1.2 Vanadium oxide clusters

Bare and xenon-tagged vanadium oxide clusters are modeled using the wB97xD functional, which accounts for the dispersion interaction needed to bind the messenger atom. The QZVP basis was employed in all-electron calculations.

— $V_4O_{10}^+$ —

The optimized geometry of $V_4O_{10}^+$ in its lowest doublet state is in Cartesian coordinates

V	0.095982	1.426827	1.241958
O	0.217419	2.588293	2.240776
O	1.618496	1.042046	0.284479
O	-0.285268	-0.163905	1.988578
O	-1.113087	1.686022	-0.058811
V	-1.374762	0.398538	-1.255220
O	-2.467652	0.715169	-2.288150
O	0.362852	0.145127	-1.915661
O	-1.642582	-1.115428	-0.346715
V	1.649189	-0.240120	-0.873349
V	-0.500265	-1.578048	0.943120
O	3.187241	-0.455689	-1.675147
O	-0.885693	-2.858006	1.701641
O	1.138129	-1.590824	0.012503

Its total electronic energy is -4528.80295158 Hartree and the average rotational constant used to convolute the action spectra is 8.1 cm^{-1}.

Its harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	107.3055	58.558	13	220.983	17.123	25	621.715	122.617
2	146.0725	1.819	14	250.061	2.503	26	631.301	12.830
3	147.0996	0.697	15	251.713	1.403	27	638.957	36.054
4	162.6779	0.536	16	263.175	19.494	28	669.742	1.204
5	170.9174	0.295	17	264.610	10.098	29	671.872	4.979
6	171.5986	6.155	18	268.283	27.553	30	728.026	36.007
7	181.5429	3.038	19	298.416	12.314	31	870.440	362.897
8	181.8329	10.662	20	306.312	4.966	32	875.372	656.612
9	199.5420	4.269	21	370.892	13.624	33	875.497	648.843
10	200.5304	0.156	22	474.705	0.168	34	1130.107	333.549
11	208.8605	1.920	23	492.510	0.001	35	1132.954	355.766
12	209.6816	2.430	24	563.005	22.124	36	1147.383	68.417

Table S4: Vibrational frequencies and IR intensities of $V_4O_{10}^+$

Modeling of the IR-MPD spectra for $V_4O_{10}^+$ required additional calculations for the dissociation products $V_4O_8^+$ and O_2, for which the energies in the optimized configurations were found as -4378.33706667 and -150.397538355 Hartree in their quartet and triplet spin multiplicity states, respectively. This yields a dissociation energy of 1.86 eV.

The unperturbed couplings matrix obtained from the VPT2 calculation was slightly tweaked by decreasing some excessively large aharmonic coefficients involving low-frequency modes. Those coefficients lead to poor convergence of the multicanonical calculation and only affected the thermal population of the associated modes, but did not affect the spectroscopic response in the experimentally relevant range. The matrix of anharmonic couplings used in the modeling is given as

	1	2	3	4	5
1	-0.159892D+01				
2	-0.660914D+01	-0.168931D+01			
3	-0.515519D+01	-0.445874D+01	-0.230853D+01		
4	-0.140146D+00	-0.350888D+00	-0.356391D+00	-0.132353D+01	
5	-0.115208D+00	-0.136090D+00	-0.234316D+00	-0.153750D+01	-0.145493D+01
6	-0.485295D+00	-0.601829D+00	-0.210450D+01	-0.418540D+01	-0.143462D+01
7	-0.382487D+00	-0.366639D+00	-0.820069D+00	-0.688065D+01	0.289598D+00
8	0.558922D+00	-0.142835D+00	-0.153183D+00	-0.446252D+01	-0.236101D+01
9	-0.145537D+00	-0.286749D+00	-0.738373D-01	-0.141807D+01	-0.343921D+01
10	-0.113828D+00	0.255544D+00	-0.674753D-01	-0.205348D+01	-0.420718D+01
11	-0.837487D-01	-0.819881D-01	-0.635174D-01	-0.451993D+01	-0.241705D+01

12	-0.126125D+00	0.562053D-01	-0.437006D-01	-0.465630D+01	-0.116767D+01
13	0.201730D+00	-0.360781D-01	0.105528D-01	-0.879526D+00	-0.587645D+00
14	-0.297321D+00	0.142669D+00	-0.216669D+00	-0.394939D+01	-0.326207D+01
15	0.554355D+00	-0.112358D+00	-0.162569D+00	-0.803771D+00	-0.306394D+01
16	-0.192460D+00	-0.748548D+00	0.650574D+00	-0.397888D+01	-0.616202D+00
17	-0.465450D-01	-0.439554D-01	-0.506503D-01	-0.473854D+00	-0.500401D+00
18	-0.551153D-02	-0.153800D-01	0.447437D-02	-0.918759D+00	-0.269843D+00
19	-0.177244D+00	-0.562179D+00	-0.247363D+00	-0.485068D+01	-0.292016D+01
20	-0.316635D+00	-0.658465D+00	-0.428364D+00	-0.292206D+01	-0.185056D+01
21	-0.241395D-01	-0.183881D+00	-0.106506D+00	-0.709936D+00	-0.681469D+00
22	-0.125809D+00	-0.124604D+00	-0.119662D+00	-0.448671D+00	0.251190D-01
23	-0.902227D-01	-0.102161D+00	-0.120279D+00	0.528385D+00	-0.384328D+00
24	-0.102415D-01	-0.166396D-02	-0.207231D-01	-0.640494D+00	-0.567537D+00
25	-0.752630D-01	-0.101359D+00	-0.836506D-02	-0.441101D+00	-0.452492D+00
26	-0.142612D+00	-0.107816D+00	-0.193961D+00	-0.365810D+00	-0.339469D+00
27	-0.188334D+00	-0.174279D+00	-0.165422D+00	-0.834646D-01	0.182546D+00
28	-0.244023D+00	-0.231914D+00	-0.283286D+00	0.159930D+01	0.139344D+01
29	0.212392D+00	0.143802D+00	-0.829785D-01	0.373132D+00	0.671712D+00
30	-0.263430D+00	-0.254678D+00	-0.230824D+00	-0.521797D-01	0.100023D+00
31	-0.170500D+00	-0.194797D+00	-0.212061D+00	0.399872D+00	0.410290D+00
32	0.216346D-01	-0.157662D-01	0.107111D+00	0.569890D-01	-0.325198D+00
33	0.215173D+00	0.216251D+00	-0.215953D-01	-0.376657D+00	-0.338834D+00
34	-0.226281D-01	-0.707624D-01	0.651692D-01	0.484190D+00	0.573512D-02
35	-0.329374D+00	-0.289105D+00	-0.232281D+00	-0.122204D+00	0.376743D+00
36	-0.129921D+00	-0.172079D+01	0.266078D+01	0.337922D+01	-0.184314D+01

	6	7	8	9	10
6	-0.274116D+01				
7	-0.611818D+01	-0.508255D+01			
8	-0.195285D+01	-0.484004D+00	-0.712120D+00		
9	-0.233923D+01	-0.162213D+01	-0.995026D+01	-0.963276D+00	
10	-0.548526D+01	-0.225151D+01	-0.208604D+02	-0.357347D+01	-0.157746D+01
11	-0.224160D+01	-0.207629D+00	-0.249636D+01	-0.148217D+02	-0.228293D+02
12	-0.162237D+01	-0.179800D+00	-0.112316D+01	-0.209078D+01	-0.210480D+01
13	-0.930671D+00	-0.331277D+00	-0.909933D+00	-0.345223D+01	-0.770170D+01
14	0.159213D+00	-0.717880D-01	-0.877005D+00	-0.129531D+01	-0.140488D+01
15	-0.391215D+01	0.153509D+00	0.487366D+00	-0.444058D+02	-0.700739D+02
16	-0.766986D+01	-0.868973D+01	-0.285648D+02	0.272249D+00	-0.662789D+01
17	-0.103352D+01	-0.756504D+00	0.618437D-01	-0.315942D+00	-0.211156D+01
18	-0.139876D+01	-0.517710D+00	-0.206756D+00	-0.303692D+00	-0.279671D+01
19	-0.108916D+01	0.102884D+01	-0.148614D+01	-0.358910D+01	-0.505200D+01
20	-0.863337D+00	0.472174D+00	-0.118491D+01	-0.244547D+01	0.160668D+01
21	-0.606989D+00	-0.601941D+00	-0.254503D+00	0.190158D+00	-0.572171D-01
22	-0.128534D+01	0.160741D+00	-0.322708D-01	-0.327265D+00	0.110107D+00
23	-0.114032D+01	-0.264172D+00	-0.167862D+00	0.960952D-01	0.105295D+01
24	-0.329762D+00	-0.219803D+00	-0.107228D-01	0.103387D+00	0.744611D+00
25	-0.183925D+00	0.446077D-01	-0.156797D+00	-0.254129D+00	-0.628448D+00
26	0.119780D+00	0.997582D-01	-0.119685D+00	-0.311540D+00	-0.127926D+00
27	-0.342033D+00	-0.172605D+00	-0.165636D+00	-0.262397D+01	-0.882310D-01
28	0.123036D+00	-0.340843D+00	-0.159871D+01	-0.237815D+01	-0.181189D+00
29	0.185902D+00	-0.273544D+00	-0.193448D+01	-0.842584D+00	0.378256D+00
30	0.150899D+00	-0.378048D+00	-0.262891D+00	-0.100749D+01	-0.375220D+00
31	0.171169D+00	-0.222384D+00	-0.203484D+00	0.958718D-02	0.455346D+00
32	0.578538D+00	0.158300D+00	0.919124D-01	0.686764D+00	0.172774D+00
33	-0.407292D+00	-0.546392D-01	-0.236277D+00	0.419146D+00	-0.209054D-01
34	0.303116D+00	-0.100953D+01	0.434521D-01	0.326978D+01	0.214119D+01
35	0.403050D+00	-0.110482D+01	-0.112096D+00	-0.547332D+00	-0.786628D-01
36	0.159677D+01	-0.637054D+01	-0.340988D+02	0.631142D+01	0.188383D+02

	11	12	13	14	15

```
11 -0.808622D+00
12 -0.101669D+01 -0.555806D+00
13 -0.478072D+00 -0.105720D+01 -0.515245D+00
14  0.128329D+01 -0.357377D+01 -0.226169D+01  0.152481D+01
15 -0.804767D+00 -0.180181D+01 -0.342798D+01  0.208200D+01  0.154319D+01
16 -0.450721D+02 -0.793306D+00 -0.235207D+02  0.241031D+01 -0.247182D+03
17  0.678594D-01  0.537945D+00  0.100005D+00 -0.102935D+01 -0.522272D+00
18  0.113740D+00  0.953716D+00 -0.262370D+00 -0.119599D+01 -0.145588D+00
19  0.481775D+01  0.238003D+01 -0.452379D+01  0.164252D+01 -0.100102D+03
20  0.106050D+01  0.582586D+00 -0.204732D+01  0.137871D+01 -0.634939D+02
21  0.203970D+00  0.489015D+00  0.104229D+01 -0.140186D+01  0.851687D+00
22  0.129505D+01 -0.412548D+00  0.517392D+00  0.380267D+00 -0.963046D+00
23  0.702673D+00 -0.941046D+00  0.779518D-01  0.182008D+00 -0.553346D+00
24 -0.392402D-01  0.630978D+00  0.379744D+00 -0.139725D+00  0.618722D-01
25  0.347938D+00 -0.532277D-01 -0.228600D+00 -0.250045D+00  0.102378D-01
26 -0.341640D+00 -0.225377D+00  0.240963D-01 -0.272444D+00  0.507893D+00
27 -0.429283D-01 -0.267155D-01 -0.544662D+00 -0.155831D+01  0.389660D+01
28 -0.323626D+00 -0.210413D+00 -0.231608D+00  0.906886D-01  0.239728D+00
29 -0.138681D+00  0.486265D+00 -0.258416D-01  0.262222D+01 -0.152112D+02
30 -0.186705D+00 -0.368768D+00  0.729688D-01  0.120859D+01  0.108321D+00
31 -0.366420D+00 -0.272195D+00  0.905448D-01  0.793858D-01 -0.410330D+00
32  0.147450D+01 -0.304826D+00  0.188568D+01 -0.101453D+01 -0.109537D+02
33 -0.383538D+00 -0.747340D+00  0.728045D-01 -0.397446D+00  0.182269D+01
34  0.969093D+00  0.130711D+00  0.974798D+00 -0.549074D+00 -0.260668D+01
35  0.211058D+00 -0.205168D+00 -0.445485D+00  0.191742D-01 -0.445984D+00
36 -0.531492D+01  0.408501D+01 -0.858792D+01 -0.249798D+01 -0.264956D+03
          16            17            18            19            20
16  0.207337D+02
17 -0.234204D+02  0.799553D-01
18 -0.561831D+02  0.229554D+00  0.476841D+00
19 -0.368984D+01 -0.188922D+02 -0.265866D+02 -0.467232D+01
20  0.104063D+02 -0.112676D+02 -0.160738D+02 -0.397790D+01  0.239133D+01
21 -0.270675D+01 -0.161128D+00  0.244287D+00 -0.253726D+00 -0.212997D+00
22 -0.183827D+01 -0.155615D+00  0.195451D+00  0.802930D-01 -0.416930D+00
23 -0.126040D+01 -0.171721D+00 -0.358032D+00  0.104237D+01  0.502053D+00
24 -0.117327D+01 -0.229829D+00  0.257896D+00 -0.164411D+01 -0.742225D+00
25 -0.550745D+00 -0.139338D+01 -0.700698D+00 -0.194973D+00 -0.413514D-01
26 -0.208228D+01 -0.350438D-01 -0.246103D-01 -0.159988D+01 -0.916920D+00
27  0.102923D+01 -0.105065D-01 -0.432039D+00 -0.181667D+01 -0.101392D+01
28 -0.326151D+02  0.104250D+00  0.371007D-01 -0.196895D+02 -0.835874D+01
29  0.555812D+01 -0.182426D+01 -0.377762D+01  0.361587D+00 -0.581472D+00
30 -0.144353D+01  0.179248D+00 -0.126427D+00 -0.293940D+01 -0.596855D+01
31 -0.159288D+01 -0.431380D-01 -0.538607D+00 -0.866589D+00 -0.280251D+01
32  0.510242D+01 -0.422942D+01 -0.375393D+01 -0.128412D+01 -0.441583D+01
33 -0.262295D+01 -0.665393D+00 -0.435091D+00 -0.348803D+00 -0.902507D+00
34  0.596580D+01  0.250168D+01 -0.601447D+01 -0.394156D+01 -0.227856D+01
35 -0.989937D+01 -0.207541D+00 -0.319404D+00 -0.422540D+01 -0.191207D+01
36  0.820948D+02 -0.561830D+02 -0.105959D+03 -0.398021D+02 -0.151931D+02
          21            22            23            24            25
21  0.393979D+00
22  0.209427D+00  0.327695D-01
23 -0.951965D-02 -0.254856D+00  0.889372D-02
24  0.187922D+01  0.465566D+00  0.246500D+00  0.416274D+00
25  0.480794D+00 -0.264264D+00  0.588109D-01  0.380490D+00 -0.509498D-01
26 -0.375570D+00  0.215427D+00 -0.613131D+00  0.385644D+00 -0.488691D+00
27 -0.248418D+00 -0.338835D+00 -0.298776D+00 -0.354754D+00 -0.142955D+00
28 -0.269938D+00  0.213099D+00 -0.299785D+00 -0.150723D+00 -0.441135D+00
29 -0.242297D+00 -0.504887D+00  0.189673D+00 -0.215407D+00 -0.225547D+00
```

```
30 -0.502574D+00  0.272401D+00 -0.110129D+00 -0.422121D+00 -0.433920D+00
31 -0.510187D+00  0.295479D+00 -0.833161D-01 -0.256544D+00 -0.576102D+00
32 -0.213829D+00 -0.305912D+00 -0.159348D+00 -0.773618D+00 -0.381843D+00
33 -0.158544D+00 -0.144489D+00 -0.205370D+00 -0.143772D+00 -0.133117D+00
34  0.984365D+00 -0.204733D+00 -0.869772D+00 -0.257650D+01 -0.552042D+00
35 -0.406483D+00 -0.611353D-01 -0.779875D+00 -0.158194D+00 -0.403005D+00
36 -0.297087D+01 -0.268721D+01  0.256289D+01 -0.724581D+01 -0.747511D-01
          26            27            28            29            30
26 -0.559080D-01
27 -0.178947D+00 -0.736628D-01
28 -0.551584D+00 -0.504228D+00 -0.190008D-01
29 -0.293816D+00 -0.755498D+00 -0.410258D+01  0.141450D+00
30  0.114594D+00 -0.544729D+00  0.412909D+00 -0.162034D+01  0.634630D-01
31 -0.474638D+00 -0.465613D+00  0.238203D+00 -0.319865D+00  0.594853D+00
32 -0.153102D-01 -0.185729D+00 -0.255686D+01 -0.897474D-03 -0.117009D+01
33 -0.349801D+00 -0.131240D+00 -0.231760D+00 -0.785712D+00 -0.178106D+00
34 -0.119728D+00 -0.210856D+00 -0.440193D+01  0.103840D+01 -0.649190D+00
35 -0.277008D+00 -0.664943D+00 -0.712185D+00 -0.253335D+01  0.560798D-02
36 -0.437072D+01 -0.109783D+01 -0.873956D+02 -0.707169D+01 -0.105452D+02
          31            32            33            34            35
31  0.157133D+00
32 -0.554157D+00 -0.368434D+00
33 -0.211159D+00 -0.548244D-01 -0.605671D-01
34 -0.103218D+01  0.153551D+01 -0.465110D+00 -0.423187D+00
35  0.713458D+00 -0.149076D+01 -0.348553D+00 -0.349578D+01 -0.518776D-01
36  0.424290D+00 -0.645259D+01 -0.986931D+01  0.855075D+01 -0.377356D+02
          36
36 -0.481150D+02
```

— $V_3O_7^+$ —

For the $V_3O_7^+$ cluster two closeby structures exist, whose relative stability is affected by the presence of the tagging Xe atom. Calculations of IRMPD spectra were carried out with data corresponding to the most stable isomer of $V_3O_7^+$Xe, in which the cluster forms a ring of alternating vanadium and oxygen ions.

The optimized neutral geometry of the most stable isomer of $V_3O_7^+$Xe in its singlet state is in Cartesian coordinates

```
V       -0.048938   -0.911761    1.263101
V       -0.048938   -0.911761   -1.263101
V        0.079655    1.930422    0.000000
O       -0.162019   -1.822877    2.496519
O       -0.162019   -1.822877   -2.496519
O        1.134438   -1.348362    0.000000
O       -1.290754   -1.135334    0.000000
O        0.054842    0.934232   -1.412120
O        0.054842    0.934232    1.412120
O        1.348525    2.794883    0.000000
Xe      -2.049739    3.673361    0.000000
```

Its total electronic energy is -3688.23965701 Hartree and the average rotational constant is 10.6 cm^{-1}.

Its harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	1191.1400	105.660	10	509.040	11.370	19	225.570	0.650
2	1164.2100	477.650	11	441.230	1.510	20	183.100	2.720
3	1163.8600	269.470	12	403.130	0.220	21	180.640	9.870
4	868.4800	839.540	13	374.840	8.350	22	178.660	0.160
5	817.3100	477.680	14	351.440	58.430	23	160.680	3.700
6	811.9000	12.430	15	328.270	0.160	24	130.780	1.380
7	791.2100	103.070	16	275.190	8.160	25	101.310	3.410
8	652.9700	6.760	17	253.380	1.460	26	45.770	0.210
9	628.2200	60.760	18	233.280	1.140	27	20.840	0.510

Table S5: Vibrational frequencies and IR intensities of $V_3O_7^+Xe$ in the ring isomer of $V_3O_7^+$

Likewise the optimized geometry of the bare cluster in the same ring isomer reads

```
V       -0.093098   -0.845242    1.263234
V       -0.093098   -0.845242   -1.263234
V       -0.022082    2.023889    0.000000
O       -0.161015   -1.773830    2.482899
O       -0.161015   -1.773830   -2.482899
O        1.108319   -1.222064    0.000000
O       -1.319275   -1.125052    0.000000
O       -0.066605    1.025724   -1.392599
O       -0.066605    1.025724    1.392599
O        1.284365    2.824081    0.000000
```

Its total electronic energy is -3358.75510778 Hartree, which together with the energy of the xenon atom alone (-329.447081410 Hartree) yields a dissociation energy of 1.02 eV.

For this cluster the harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	1197.2100	73.370	9	339.930	51.780	17	650.440	8.360
2	1169.6700	289.760	10	260.180	9.010	18	485.290	8.430
3	881.4300	633.490	11	218.520	3.210	19	402.450	0.270
4	815.8300	13.870	12	178.390	1.670	20	337.410	0.350
5	794.8400	104.960	13	173.400	14.540	21	246.410	0.640
6	606.7700	89.890	14	53.630	5.600	22	230.360	1.280
7	440.4200	0.620	15	1170.190	461.800	23	165.530	0.020
8	368.8700	1.130	16	825.390	535.790	24	148.810	5.530

Table S6: Vibrational frequencies and IR intensities of bare $V_3O_7^+$ in the ring isomer

In the case of the bare cluster $V_3O_7^+$, another isomer forming a cage structure with a triply coordinated oxygen turns out to be slightly more stable. We only provide below its structural and harmonic IR spectra features.

```
V        0.631656   -1.342568    0.465052
V        0.631656    1.342568    0.465052
V       -1.008804   -0.000000   -1.183381
O        0.631656   -2.530428    1.432813
O        0.631656    2.530428    1.432813
O       -0.702561    0.000000    0.699677
O        1.800820    0.000000    0.701979
O       -0.072759    1.524762   -1.170256
O       -0.072759   -1.524762   -1.170256
O       -2.460558   -0.000000   -1.673489
```

Its total electronic energy is -3358.76536833 Hartree.

For this cluster the harmonic frequencies (cm^{-1}) and associated IR intensities (km/mol) are given in the table below.

#	ω	I	#	ω	I	#	ω	I
1	1205.453	72.373	9	669.771	68.835	17	243.538	0.034
2	1175.609	403.083	10	464.178	0.499	18	243.535	0.049
3	1175.520	402.776	11	462.710	2.624	19	208.328	0.000
4	803.375	252.970	12	461.784	2.134	20	172.848	10.421
5	801.962	251.835	13	383.125	0.068	21	172.419	10.635
6	726.974	233.683	14	346.583	9.959	22	147.853	0.690
7	726.819	235.289	15	344.797	9.980	23	147.587	0.758
8	724.290	47.280	16	298.838	29.876	24	120.097	23.249

Table S7: Vibrational frequencies and IR intensities of bare $V_3O_7^+$ in the cage isomer

In the harmonic limit, the IR spectra of the bare and xenon-tagged $V_3O_7^+$ clusters are relatively similar, as shown in Fig. S2 below.

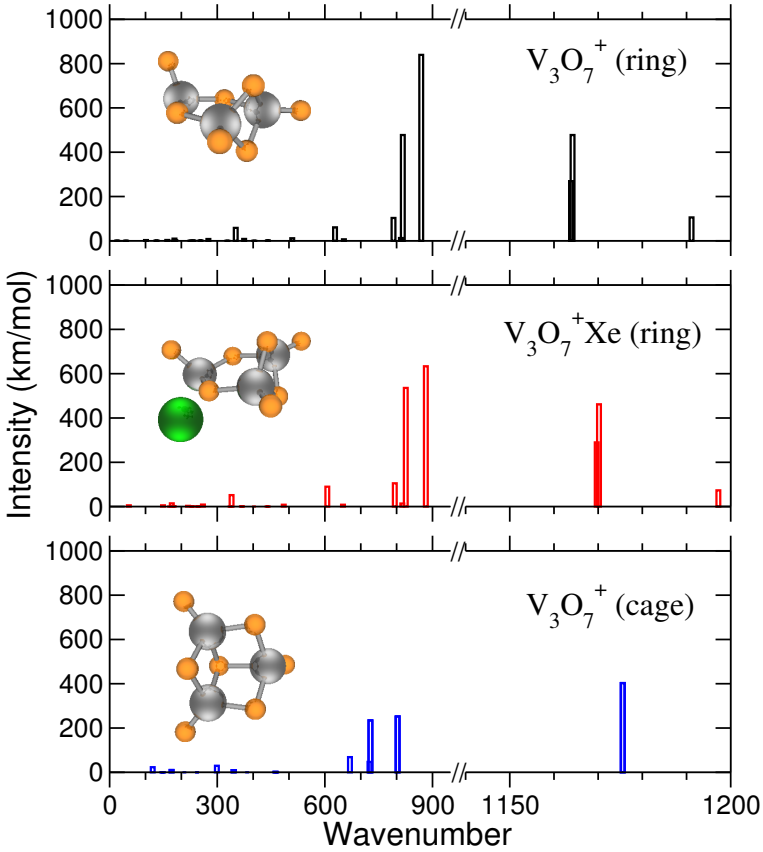

Fig. S1: Harmonic spectra of bare and xenon-tagged $V_3O_7^+$ clusters

The presence of the messenger atom slightly shifts the vibrational lines to the red, but does not by itself splits the intense lines near 1100 cm^{-1}. The harmonic IR spectrum of the cage isomer shows essentially one peak in this spectral range, blue shifted relative to the ring structure. This spectral difference further supports the hypothesis that the splitting seen in experiment could originate from multiple isomers that differ either in the $V_3O_7^+$ cluster itself, or in the position of the xenon atom on the vanadium oxide cluster.

The VPT2 anharmonic calculation for $V_3O_7^+Xe$ was not conclusive due to divergences in the perturbation expansion and strong Fermi resonances. We suspect that the xenon-tagged $V_3O_7^+$ cluster is excessively anharmonic to be properly described by perturbation theory. In order to carry some modeling despite those limitations, we have employed the anharmonic coefficients obtained for the bare cluster and give in the following matrix, with the same mode ordering as in Table S6:

```
              1             2             3             4             5
1 -0.173039D+01
2 -0.152313D+01 -0.337482D+01
3 -0.681514D-01  0.109398D+01 -0.226526D+01
```

```
 4 -0.152412D+00  0.257818D+00 -0.184426D+00 -0.981404D+00
 5 -0.655804D-01  0.317321D+00 -0.255091D+00 -0.381595D+01 -0.148759D+01
 6 -0.103823D+00  0.382390D+00 -0.103371D+01 -0.441877D+00  0.179736D+01
 7  0.312295D+00  0.751232D+00  0.629695D+00  0.209050D+01 -0.581753D+00
 8  0.229969D+00  0.124540D+01 -0.114193D+00  0.235215D+01 -0.925396D+00
 9  0.248628D+00  0.635406D+00 -0.113892D+01 -0.265511D+00 -0.197854D+00
10  0.284095D+00  0.190855D+01 -0.100193D+01 -0.970663D+00 -0.137940D+01
11  0.647686D+00  0.189161D+01 -0.141159D+01 -0.516009D+00 -0.718826D+00
12  0.553144D+00  0.222069D+01 -0.252886D+00 -0.281733D+00  0.815305D+00
13  0.758783D+00  0.162530D+01 -0.605963D+00 -0.742790D+00  0.647387D+00
14  0.163298D+01  0.548811D+01 -0.257227D+01 -0.327870D+01 -0.383115D+01
15 -0.740612D+01 -0.911096D-01 -0.148433D+00  0.140275D+00 -0.130207D+00
16 -0.655651D-01 -0.936575D+00 -0.560749D+01 -0.201166D+01 -0.412565D+01
17 -0.944838D-02  0.325027D+00 -0.178381D+01 -0.135036D+01 -0.567367D+01
18 -0.168011D+00 -0.557753D-01 -0.488718D+01 -0.108851D+01 -0.341129D+01
19 -0.320093D+00  0.697038D+00  0.165118D+00 -0.816494D+00 -0.717401D+01
20  0.281136D+00 -0.113685D+01 -0.660428D+00 -0.491479D+00 -0.121499D+00
21  0.142032D+00  0.114468D+01 -0.449275D-01  0.339791D+00 -0.778279D+00
22  0.254403D+00  0.127564D+01  0.226449D+01 -0.721617D+00 -0.416560D+00
23  0.735757D+00  0.203611D+01  0.177712D-01 -0.230925D+00 -0.887474D+00
24  0.786343D+00  0.217344D+01 -0.157257D+00  0.226436D-02 -0.877845D+00
          6             7             8             9            10
 6 -0.782776D+00
 7 -0.135576D+01 -0.574182D+00
 8 -0.809312D-01 -0.307474D+01  0.471765D-01
 9 -0.237626D+00 -0.570389D+00 -0.114029D+00 -0.602560D+00
10  0.118832D+00 -0.205190D+00 -0.255280D+00 -0.166523D+01 -0.678417D+00
11  0.168971D+00  0.530448D-01 -0.953110D-01 -0.849191D+00 -0.691567D+00
12 -0.150756D+01  0.891035D+00  0.103348D+01  0.976238D+00  0.203545D-01
13 -0.262834D+01  0.274034D+00  0.884375D+00 -0.824747D+00 -0.874613D+00
14 -0.225505D+01 -0.262677D+01 -0.415967D+01 -0.750741D+01 -0.701889D+01
15  0.422646D+00  0.264338D+00  0.201307D+00  0.196124D+00  0.112831D+00
16 -0.424689D+01 -0.129081D+01 -0.818453D+00 -0.524315D+00 -0.265446D+00
17 -0.171080D+01 -0.137403D+01 -0.836718D+00  0.379181D+00 -0.902529D+00
18 -0.731388D+01 -0.195914D+01 -0.341575D+01 -0.172939D+01 -0.329684D+00
19 -0.174075D+01 -0.358743D+01 -0.234202D+01 -0.105820D+01 -0.251888D+01
20 -0.435953D+00  0.801975D-01 -0.788229D-01 -0.119494D+01 -0.410182D+00
21 -0.506345D+00 -0.916102D+00 -0.512158D+00 -0.157081D+00 -0.265870D+01
22  0.202621D+01 -0.147805D+01  0.388465D-01  0.231094D+00 -0.507959D+00
23 -0.977604D+00 -0.126060D+00 -0.103455D+00 -0.461480D+00 -0.363820D+00
24 -0.130833D+01 -0.450472D-01  0.123927D+01 -0.110951D+01 -0.501382D+00
          11            12            13            14            15
11 -0.359696D+00
12 -0.113240D+00 -0.319589D+00
13 -0.378519D+00  0.563286D+00  0.550276D+00
14 -0.627977D+01 -0.176496D+01 -0.237355D+01 -0.750272D+01
15  0.484367D+00  0.264273D+00  0.542282D+00  0.889908D+00 -0.196475D+01
16 -0.116029D+01 -0.106816D+00 -0.715234D+00 -0.312901D+01 -0.145432D+00
17  0.205813D+00 -0.359618D+00 -0.948994D+00 -0.333832D+01 -0.114806D+00
18 -0.131832D+01 -0.127716D+01 -0.414437D+01 -0.875103D+01  0.983973D-03
19 -0.127264D+01 -0.214515D-01 -0.256753D+01 -0.812736D+01 -0.406281D+00
20  0.449069D-01 -0.550146D+00 -0.567281D+00 -0.283689D+01  0.413924D+00
21 -0.192721D+00 -0.522680D-02  0.328021D+00 -0.523361D+01  0.172915D+00
22 -0.317823D+00 -0.527489D+00 -0.345883D+00 -0.550531D+01  0.161108D+00
23 -0.706179D-02  0.396366D+00 -0.572836D+00 -0.846258D+01  0.554745D+00
24 -0.831862D-01 -0.568165D-01 -0.934491D+00 -0.991893D+01  0.522498D+00
          16            17            18            19            20
16 -0.101199D+01
```

```
17 -0.323374D+01 -0.984060D+00
18 -0.951440D+00 -0.125277D+00 -0.108600D+00
19 -0.167848D+01 -0.449952D+00  0.175952D+01 -0.550477D+00
20  0.738082D+00 -0.163701D+00 -0.156635D+01 -0.110009D+01 -0.576941D+00
21 -0.573518D+00  0.279467D-01 -0.341853D+00 -0.134886D+01 -0.623778D+00
22 -0.293852D+01 -0.254577D+01 -0.234948D+01 -0.103136D+01 -0.423176D+00
23 -0.437459D+00 -0.277084D+00 -0.174389D+01 -0.221128D+01 -0.470123D+00
24 -0.552651D+00 -0.940968D+00 -0.316545D+01 -0.191184D+01 -0.603207D+00
          21            22            23            24
21  0.243303D+00
22  0.978679D-01  0.489240D-01
23 -0.797177D+00  0.436817D-01 -0.389205D+00
24 -0.112480D+01 -0.870880D+00 -0.143727D+01 -0.551467D+00
```

2 Additional results obtained for Si_{10}

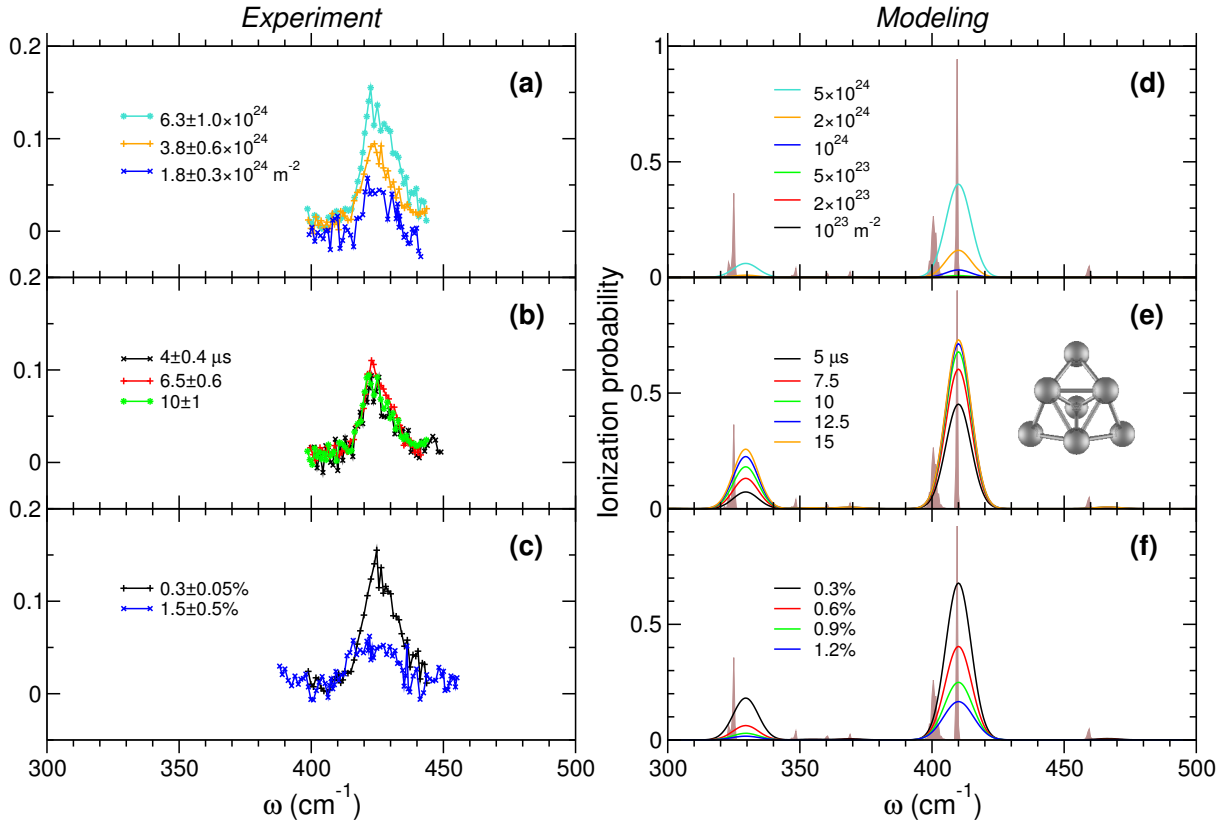

Fig. S2: IR-UV two-photon ionization probability of Si_{10} as a function of laser wavelength, measured experimentally (left panel) and obtained from modeling (right panels) for different IR laser conditions. In (a) and (d) the laser fluence is varied for a macropulse length of 10 μs; In (b) and (e) the macropulse length is varied at fixed photon exposure of 5×10^{24} m^{-2}; In (c) and (f) the IR laser bandwidth is varied while the photon exposure is constant at 5×10^{24} m^{-2} and for a macropulse length of 10 μs. The theoretical linear absorption spectrum at equilibrium is superimposed on the calculated action spectra as brown histograms.

3 Complete reference for Gaussian09

[1] Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; 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.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.