

Supplementary data

Lifetimes and decay mechanisms of isotopically substituted
ozone above the dissociation threshold: Matching quantum and
classical dynamics

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Below are given energies of bound vibrational states of the $^{16}\text{O}^{16}\text{O}^{18}\text{O}$ isotopologue of ozone as well as energies and widths of resonant vibrational states of the molecule. The states of A and B symmetries are separated (the B states are in the lower part of the table). The energies and widths are given in units of cm^{-1} . The origin of energies is at the ground vibrational level of the molecule.

Bound A states

<i>Energy</i>	<i>Energy</i>	<i>Energy</i>	<i>Energy</i>
0.00000	5202.96592	6791.80362	7851.32522
14.22262	5233.13850	6799.51764	7856.77965
693.14433	5254.56987	6810.68940	7856.89985
698.55938	5256.15990	6813.10630	7867.77492
1041.85187	5271.94702	6854.91690	7869.27879
1074.18671	5273.67929	6855.13114	7888.32461
1104.57567	5289.85663	6857.28144	7892.58977
1380.40062	5298.42343	6860.72007	7904.76005
1383.78053	5353.96155	6877.42308	7906.78590
1710.31813	5354.82705	6896.59533	7910.10546
1759.86608	5380.53059	6904.38756	7928.05931
1781.22720	5398.87949	6923.19254	7946.18223
1992.06515	5416.39388	6925.51502	7949.33569
2042.11318	5443.28795	6929.18570	7956.91046
2059.72714	5472.72278	6937.45578	7958.18161
2071.88420	5482.63195	6948.32673	7974.83379
2104.26759	5494.77709	6974.43231	7980.00100
2143.01832	5495.64523	6985.85483	7984.74870
2186.62029	5527.18157	6986.39518	7988.07056
2375.79623	5540.13714	7003.90843	7992.17343
2442.85263	5572.60106	7012.56885	7996.94513
2455.26383	5574.29029	7026.08628	8020.58705
2654.74942	5606.86231	7030.12784	8021.19595
2695.10092	5607.75998	7051.86819	8038.26534
2736.47474	5627.12962	7062.82238	8042.36303
2757.41790	5634.66943	7067.22191	8045.84143
2762.47996	5653.92777	7071.69224	8045.90947
2821.00924	5660.05583	7094.07614	8051.62442
2855.71422	5695.38289	7094.64781	8068.05677
2992.70039	5718.52572	7108.65971	8076.90792
3012.31200	5741.94496	7115.98161	8081.06430

Supplementary data

3038.21422	5763.21501	7120.57778	8085.33323
3074.24288	5777.59477	7151.82463	8088.82615
3123.02343	5787.26870	7153.96749	8090.16493
3126.54774	5797.54565	7155.73380	8104.76020
3161.95991	5809.09382	7164.24135	8131.51741
3203.31851	5816.84402	7169.53918	8132.88853
3260.16382	5856.50910	7174.99570	8139.19316
3314.27233	5864.39456	7202.68196	8140.25360
3344.60076	5881.60781	7211.79986	8146.75191
3410.57329	5883.08892	7213.30702	8155.30352
3417.20821	5907.44409	7227.84710	8158.32559
3440.33327	5915.85513	7230.99241	8173.72398
3495.98918	5921.07873	7237.29493	8182.52690
3521.87865	5932.91863	7256.45895	8191.72270
3643.86739	5951.66819	7267.63598	8192.60490
3650.06343	5966.65360	7275.77034	8196.06467
3697.41176	5988.59256	7285.59071	8200.20526
3713.90939	6012.71230	7315.49021	8203.64010
3794.86913	6015.24895	7327.44681	8220.12456
3800.18446	6025.73285	7336.79596	8238.58595
3810.30508	6030.13684	7339.40138	8241.67459
3872.76969	6040.92892	7345.93077	8242.56627
3881.36804	6079.07147	7346.73068	8257.75173
3921.43172	6098.71722	7347.94594	8268.57724
3947.04738	6132.02545	7358.12953	8274.27690
3970.58873	6135.05974	7359.00116	8274.93395
3990.56959	6142.28920	7373.80104	8283.91122
4016.17333	6144.47049	7394.28334	8288.38217
4019.35218	6145.78287	7403.47939	8288.82925
4067.91879	6165.93808	7406.06821	8289.87025
4082.04427	6190.75800	7421.15504	8296.09501
4105.73811	6213.07903	7453.34896	8296.19214
4120.57153	6225.74516	7464.23615	8306.03883
4167.50059	6226.87079	7470.79044	8313.06197
4184.70278	6230.74213	7477.24457	8313.93158
4212.63887	6267.83927	7478.48708	8329.77760
4255.22782	6284.18274	7484.69299	8331.53812
4283.80528	6289.91978	7485.57619	8332.04604
4290.83253	6290.12685	7498.13180	8332.77491
4324.84126	6297.85052	7500.59870	8345.26812
4349.14149	6332.63436	7507.35845	8347.51971
4353.50971	6332.67743	7510.65239	8354.14961
4453.74047	6340.15316	7515.47745	8355.34186
4459.91406	6379.86680	7558.86584	8356.68235
4474.02063	6382.36655	7559.96550	8360.33026
4512.12615	6388.74340	7569.23896	8361.40520
4541.02955	6405.06731	7573.32196	8366.76619
4567.76057	6426.98845	7579.99462	8366.97635
4580.35413	6427.44604	7589.04438	8372.84093

Supplementary data

4623.69045	6445.98236	7593.62795	8375.68760
4632.80115	6467.45754	7601.36530	8377.96534
4637.86254	6472.03418	7632.17620	8384.01129
4657.71695	6482.58205	7634.87953	8384.63331
4714.10202	6489.65367	7644.02756	8388.42468
4733.27829	6500.29143	7646.61557	8390.13089
4750.66682	6515.90387	7649.82732	8392.45263
4781.67608	6539.09894	7675.09871	8400.77309
4798.06274	6540.13712	7678.47456	8403.97785
4834.56656	6542.03924	7686.10759	8406.55860
4839.16586	6566.53412	7691.07033	8411.03338
4843.34116	6572.16881	7694.68557	8411.44823
4852.91048	6582.60356	7698.54177	8419.08705
4913.60494	6593.52793	7706.37224	8420.94865
4917.32346	6613.56086	7720.85587	8423.53037
4923.07983	6624.39196	7728.36625	8424.10264
4933.61701	6628.12658	7741.44044	8425.29084
4977.90054	6634.01110	7749.26113	8425.93756
4980.73686	6643.84879	7750.23096	8428.25929
5005.60418	6663.84662	7755.31954	8437.10253
5024.46731	6694.25812	7776.65614	8439.79918
5028.43336	6730.83352	7781.49538	8441.37992
5090.74223	6738.47664	7785.25810	8443.83206
5121.14002	6740.78000	7789.96621	8443.87474
5127.76266	6745.44514	7816.55278	8447.56183
5140.15988	6752.30506	7831.70004	8448.58152
5143.98973	6767.15163	7832.40090	8451.53386
5185.12522	6769.55515	7845.40612	8451.76914

Resonant A states

<i>Energy</i>	<i>Width</i>
8467.47835	0.000456
8468.42629	0.000793
8471.93998	0.000234
8473.44404	0.000198
8475.04710	0.000190
8478.06443	0.001612
8479.13222	0.018497
8481.91254	0.027720
8482.73791	0.003206
8485.17370	0.000900
8486.85962	0.005581
8489.76889	0.021105
8490.35010	0.070373
8491.54107	0.132007
8492.07228	0.016103
8493.17605	0.002331
8493.93951	0.037295
8497.03900	0.052986
8497.69282	0.064438

Supplementary data

8500.61619	0.229075
8502.23402	0.209003
8502.55690	0.145353
8504.58270	0.132675
8505.03892	1.744144
8505.99363	1.083996
8505.99638	0.286592
8509.80628	0.577768
8511.25163	0.532148
8515.18267	0.216428
8515.76411	0.327919
8515.98730	1.356077
8516.45193	0.253850
8518.40886	3.182789
8518.99747	0.870216
8521.22541	2.124773
8522.22662	0.650844
8523.30867	1.755257
8524.11177	1.458643
8526.09831	0.829442
8527.56839	2.001107
8528.11473	2.199522
8530.37251	0.881446
8532.52907	2.777031
8533.15651	0.822757
8535.93719	2.130706
8536.22990	3.431121
8539.23518	1.917428
8540.58499	1.538340
8542.82518	2.061560
8545.88257	1.986959
8548.87503	3.288872
8550.10543	2.047023
8551.98747	2.586079
8557.16062	2.650119
8558.14276	3.067719
8570.26761	3.055805
8579.88399	3.019214
8581.23309	2.794017
8594.61885	3.777553
8595.58990	1.575304
8599.12421	1.589654
8604.02026	3.274300
8624.37690	1.708304
8625.92196	2.348709
8662.30187	2.575091
8666.06043	1.153984
8671.35059	1.601354
8671.82093	0.403627

Supplementary data

8673.02546	0.930929
8682.81265	3.672626
8688.44317	2.294264
8691.00948	0.775550
8701.43925	1.598574
8706.41772	0.785422
8718.84105	3.928412
8733.02541	1.527350
8734.23850	0.912018
8739.03464	2.876286
8751.90064	2.823397
8769.09972	3.283326
8792.51230	2.873665
8797.58614	0.118066
8804.50563	1.708944
8815.30871	0.161556
8817.11418	2.848933
8827.38597	2.613102
8838.18178	3.982467
8867.68667	3.349780
8886.20383	3.096298
8895.42076	0.334626
8904.21964	2.472557
8905.30524	3.068536
8927.04986	3.022009
8954.82033	1.582650
8964.09156	2.196595
8971.29434	1.669465
8985.86124	0.710752
8988.17688	2.916550
9003.88564	2.591090
9021.87379	0.046272
9100.68393	1.217616
9152.91170	0.247451
9236.78781	3.008582
9240.22206	2.251220
9303.31060	3.884798
9316.72945	2.890996
9340.23410	1.195212
9344.68949	3.014485
9385.37365	0.074074
9426.92087	0.687664
9448.13080	2.274063
9498.99908	3.545497
9518.59839	1.872189
9543.61897	2.908449
9545.84241	2.284941
9557.75531	1.789467
9572.81674	1.220024

Supplementary data

9592.48122	3.943575
9653.92687	0.361720
9667.14188	3.718393
9726.86935	3.886111
9743.33053	1.106926
9803.94065	2.418267
9813.23731	3.740549
9816.58746	2.943846
9818.47793	2.565634
9821.49031	3.874265
9873.37402	2.295377
9890.30889	3.939851
9902.31010	3.319357
9903.57358	3.268308
9905.82056	2.306429
9912.08837	3.842958
9918.54639	3.282917
9922.59149	2.715711
9926.48894	2.981270
9931.45549	0.474069
9941.44482	1.617467
9943.24873	1.979845
9953.73680	0.799410
9955.05915	0.049745
9958.20992	2.487335
9959.20808	1.074767
9961.81653	1.722129
9962.46152	0.995007
9975.43375	0.571571
9977.19027	3.753666
9980.78202	2.418639
9985.27443	3.608592
9985.73301	2.011859
9988.08670	2.300471
9992.07448	3.411712
9994.10026	3.202364
9994.19847	0.454262

Bound B states

<i>Energy</i>	<i>Energy</i>	<i>Energy</i>	<i>Energy</i>
14.22259	5353.96147	6877.41951	7892.58348
698.55935	5354.82700	6880.55470	7894.99661
1007.95478	5379.21647	6896.59474	7906.34709
1041.85185	5380.53057	6904.38584	7906.77854
1104.57564	5416.39386	6919.56957	7910.10161
1380.40060	5426.86819	6925.51407	7928.05575
1685.77959	5443.28785	6929.18484	7949.32867
1710.31811	5482.63188	6937.45567	7956.90181
1781.22717	5495.64519	6958.50415	7959.85139

Supplementary data

2042.11315	5521.73039	6986.39422	7974.81616
2049.14204	5527.18141	6993.08855	7983.16036
2059.72712	5540.13706	7003.90782	7988.06809
2104.26757	5543.54138	7012.56537	7992.16258
2186.62027	5606.86223	7026.34048	7995.02087
2360.73184	5622.13685	7030.12502	7996.93162
2375.79621	5627.12958	7039.19011	8020.57862
2455.26381	5634.66907	7062.82210	8038.26189
2695.10089	5653.92773	7067.22170	8045.82625
2717.59474	5688.02319	7071.69116	8045.90846
2736.47472	5690.67032	7094.64436	8051.61325
2762.47994	5695.38269	7108.65584	8057.24728
2855.71420	5718.52563	7120.57643	8063.79060
2951.19704	5741.94480	7130.51809	8076.89217
3012.31198	5777.59474	7149.28316	8081.04188
3032.72594	5787.26845	7153.96619	8082.00124
3038.21420	5795.11169	7155.73163	8085.33051
3074.24286	5795.58513	7159.76801	8088.82348
3095.10474	5797.54553	7169.53889	8104.75134
3126.54771	5864.39442	7174.99448	8131.51213
3161.95989	5881.60770	7193.21196	8134.82714
3260.16380	5883.08879	7213.30463	8139.18569
3344.60073	5890.96336	7227.84654	8142.18735
3382.45119	5907.44400	7230.98874	8155.29800
3410.57326	5932.91784	7251.82603	8158.30151
3417.20818	5966.65331	7256.45413	8162.13449
3521.87863	5984.22237	7275.76895	8173.70836
3598.94437	5988.59249	7279.20729	8191.72104
3650.06340	5994.16556	7285.58916	8192.59158
3697.41174	6015.24858	7300.88141	8195.69446
3701.64718	6025.73279	7313.90367	8203.62145
3713.90937	6040.92863	7315.48979	8206.73156
3753.32552	6062.40429	7336.79065	8220.11166
3794.86910	6079.07144	7339.39752	8237.85725
3810.30505	6098.71704	7345.92899	8238.57181
3904.42642	6132.02516	7347.94483	8242.55082
3921.43170	6135.05963	7358.99869	8257.73977
3947.04735	6145.78255	7394.28327	8266.88174
3990.56957	6150.25931	7398.37649	8274.24848
4016.17330	6155.95396	7403.46571	8274.82060
4043.30538	6165.93790	7406.06723	8283.89747
4067.91876	6181.21236	7408.45186	8284.92776
4082.04424	6226.17061	7421.15109	8288.37505
4105.73809	6226.87010	7427.58975	8289.86250
4131.07391	6230.74195	7464.23599	8296.09272
4184.70276	6267.83906	7470.57945	8306.00864
4212.63885	6284.18231	7470.78528	8307.36676
4243.27318	6290.12673	7477.24349	8313.95081
4283.80525	6297.85045	7484.69014	8329.77391

Supplementary data

4324.84124	6313.86132	7500.58937	8331.53564
4349.14146	6332.63418	7502.86790	8332.07290
4353.50969	6340.15253	7507.35628	8332.18238
4367.34832	6342.98211	7514.35064	8342.93969
4406.58540	6382.36604	7515.47482	8347.47826
4453.74044	6398.41983	7545.86495	8354.11895
4459.91404	6405.06694	7559.95939	8354.99162
4538.53687	6419.06047	7569.23875	8356.69522
4567.76054	6422.56169	7579.99277	8361.41404
4580.35410	6426.98841	7589.02918	8366.79203
4632.80112	6427.44598	7601.36005	8366.85003
4637.86250	6472.03370	7604.56882	8368.13785
4699.55448	6482.58067	7632.16332	8377.26623
4714.10200	6500.29076	7636.74633	8381.71394
4733.27825	6513.22956	7638.14406	8384.64531
4750.66679	6515.90343	7644.01389	8388.01295
4765.24957	6539.09687	7649.82512	8389.69560
4784.81695	6540.13692	7674.90353	8390.95681
4839.16582	6572.16840	7678.46976	8401.52432
4843.34113	6578.41465	7686.10271	8404.14679
4852.91045	6582.60236	7691.06939	8406.37460
4884.19268	6613.56071	7694.68250	8408.06533
4913.60490	6628.12543	7706.35311	8411.90848
4923.07977	6629.07908	7716.79655	8419.13496
4925.60194	6634.01020	7728.35517	8420.30531
4977.90052	6663.84628	7749.25546	8420.95431
4980.73682	6682.49739	7755.30786	8423.54282
5005.60415	6688.01434	7755.36174	8425.27421
5028.43327	6694.25764	7776.64918	8425.41359
5029.63650	6738.47661	7781.49122	8428.28386
5053.24300	6740.77888	7783.71893	8437.11963
5090.74219	6741.36482	7789.96526	8439.72164
5121.13999	6745.44310	7816.54736	8441.25452
5127.76262	6752.30484	7829.79103	8442.13613
5160.55921	6786.07167	7832.40010	8447.31044
5168.55667	6791.80319	7844.91201	8447.86296
5185.12515	6799.51619	7845.40147	8448.93006
5233.13847	6801.86460	7851.31461	8450.97793
5254.56981	6810.68591	7855.66761	8451.22147
5256.15985	6830.89510	7855.77248	
5271.94697	6854.91652	7867.74324	
5350.29232	6860.71835	7869.26344	

Resonant B states

<i>Energy</i>	<i>Width</i>
8454.79023	0.00015
8459.37725	0.00000
8462.50061	0.00000
8464.96998	0.00000
8466.94451	0.00045

Supplementary data

8468.57495	0.00067
8469.30074	0.00000
8470.72490	0.00017
8472.94601	0.00017
8474.39141	0.00018
8477.39811	0.00045
8478.24502	0.00366
8478.60837	0.00399
8479.64441	0.01547
8482.36217	0.02942
8483.05189	0.00310
8488.82484	0.00094
8490.64245	0.10743
8491.51130	0.12425
8492.42784	0.01606
8493.99314	0.01940
8494.38848	0.01682
8497.42884	0.08144
8498.11329	0.02265
8500.99507	0.17024
8501.53434	0.34608
8502.96235	0.11010
8504.29386	0.18264
8505.06421	1.70323
8506.05401	1.22567
8508.63294	0.38064
8509.59983	0.04026
8510.00031	0.52008
8513.76211	0.20902
8514.43139	0.78753
8516.44231	0.81350
8518.40954	3.43703
8520.21976	1.42221
8521.12413	1.86278
8522.34589	1.69153
8523.11718	1.86977
8524.70803	0.48394
8524.94403	1.48732
8527.69043	0.67212
8529.07051	1.52191
8530.37177	0.66096
8536.09121	3.97227
8539.68724	3.55601
8542.28503	1.31661
8542.43252	2.28976
8545.44390	0.42159
8546.80455	2.63137
8547.30503	1.60420
8550.11975	0.92618

Supplementary data

8550.84256	1.36055
8552.26872	2.25721
8556.89628	3.06274
8557.43194	2.11642
8558.55559	1.82091
8564.23775	2.11721
8575.97789	1.49002
8580.39045	2.68581
8595.60053	1.52150
8597.51585	3.90635
8599.13336	1.72561
8636.20825	2.43577
8662.19523	3.02619
8671.31596	1.30767
8673.12555	1.51584
8682.65745	3.14474
8688.09354	2.93089
8690.95990	0.61126
8693.00511	1.51804
8701.70954	1.98451
8706.28075	0.78211
8713.18486	3.46343
8719.60580	1.86149
8733.24546	1.68829
8738.95370	2.80962
8759.54952	1.80915
8769.14993	3.22616
8792.55300	3.00897
8815.24739	0.16621
8816.51024	0.40123
8817.09382	2.73125
8838.19490	3.85978
8840.48602	0.37173
8853.85198	2.35138
8867.69580	3.31177
8875.91938	2.27524
8886.16617	3.11055
8895.27076	0.35005
8905.21340	3.06744
8954.72463	1.57539
8960.71728	3.76339
8985.79221	0.72192
8988.09725	2.91133
9032.91401	2.16828
9072.46015	2.37729
9100.62411	1.20547
9152.84884	0.24624
9190.44507	0.24497
9236.68392	3.00815

Supplementary data

9303.20847	3.92311
9340.21458	1.18739
9426.55343	0.75442
9461.57493	2.37423
9475.28090	0.42541
9518.45250	1.71559
9524.83015	3.43315
9543.22973	2.94033
9557.48245	1.80951
9572.58155	1.22479
9653.48156	0.36084
9726.86964	3.88802
9742.95705	1.08202
9763.42586	3.76760
9803.63247	2.47571
9812.54550	3.81641
9813.23782	3.74215
9815.11188	0.79661
9816.39194	2.90165
9820.50990	0.22621
9890.21442	3.91125
9902.31011	3.31984
9904.80516	1.96541
9911.97504	3.94058
9919.47577	3.28817
9922.87188	2.52031
9941.33567	1.32424
9951.53833	3.98514
9955.09993	0.14051
9957.70477	3.59468
9958.13330	2.59967
9961.72038	1.56027
9962.45545	0.94666
9975.31282	1.03904
9978.05633	2.48511
9979.44091	2.28337
9984.73572	2.24608
9987.57324	2.06906
9988.80529	1.83708
9992.10598	2.60429
9994.10037	3.20211
9994.28809	0.48477
9997.47926	3.05390