

Supplementary Information to

“The vibrational overtones of SiH₄ isotopomers: experimental wavenumbers, assignment, *ab initio* dipole moment surfaces, and intensities”

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TABLE I. M_z components of the four-dimensional dipole moment surface of SiH_4 calculated at the CCSD(T)/cc-pVQZ level^a.

r_1 (Å)	r_2 (Å)	r_3 (Å)	r_4 (Å)	M_z (D)
-0.3	-0.3	-0.3	-0.3	0.00000
-0.3	-0.3	-0.3	-0.2	0.06297
-0.3	-0.3	-0.3	-0.1	0.13401
-0.3	-0.3	-0.3	0.0	0.21140
-0.3	-0.3	-0.3	0.1	0.29358
-0.3	-0.3	-0.3	0.2	0.37886
-0.3	-0.3	-0.3	0.3	0.46530
-0.3	-0.3	-0.2	-0.2	0.12453
-0.3	-0.3	-0.2	-0.1	0.19396
-0.3	-0.3	-0.2	0.0	0.26962
-0.3	-0.3	-0.2	0.1	0.35003
-0.3	-0.3	-0.2	0.2	0.43354
-0.3	-0.3	-0.2	0.3	0.51824
-0.3	-0.3	-0.1	-0.1	0.26156
-0.3	-0.3	-0.1	0.0	0.33525
-0.3	-0.3	-0.1	0.1	0.41362
-0.3	-0.3	-0.1	0.2	0.49506
-0.3	-0.3	-0.1	0.3	0.57772
-0.3	-0.3	0.0	0.0	0.40681
-0.3	-0.3	0.0	0.1	0.48294
-0.3	-0.3	0.0	0.2	0.56210
-0.3	-0.3	0.0	0.3	0.64250
-0.3	-0.3	0.1	0.1	0.55670

-0.3	-0.3	0.1	0.2	0.63342
-0.3	-0.3	0.1	0.3	0.71140
-0.3	-0.3	0.2	0.2	0.70764
-0.3	-0.3	0.2	0.3	0.78310
-0.3	-0.3	0.3	0.3	0.85603
-0.3	-0.2	-0.3	-0.2	0.00000
-0.3	-0.2	-0.3	-0.1	0.07115
-0.3	-0.2	-0.3	0.0	0.14877
-0.3	-0.2	-0.3	0.1	0.23129
-0.3	-0.2	-0.3	0.2	0.31699
-0.3	-0.2	-0.3	0.3	0.40392
-0.3	-0.2	-0.2	-0.2	0.06157
-0.3	-0.2	-0.2	-0.1	0.13113
-0.3	-0.2	-0.2	0.0	0.20705
-0.3	-0.2	-0.2	0.1	0.28783
-0.3	-0.2	-0.2	0.2	0.37179
-0.3	-0.2	-0.2	0.3	0.45701
-0.3	-0.2	-0.1	-0.1	0.19889
-0.3	-0.2	-0.1	0.0	0.27287
-0.3	-0.2	-0.1	0.1	0.35164
-0.3	-0.2	-0.1	0.2	0.43356
-0.3	-0.2	-0.1	0.3	0.51678
-0.3	-0.2	0.0	0.0	0.34475
-0.3	-0.2	0.0	0.1	0.42131
-0.3	-0.2	0.0	0.2	0.50099
-0.3	-0.2	0.0	0.3	0.58198
-0.3	-0.2	0.1	0.1	0.49553

-0.3	-0.2	0.1	0.2	0.57282
-0.3	-0.2	0.1	0.3	0.65143
-0.3	-0.2	0.2	0.2	0.64764
-0.3	-0.2	0.2	0.3	0.72377
-0.3	-0.2	0.3	0.3	0.79740
-0.3	-0.1	-0.3	-0.1	0.00000
-0.3	-0.1	-0.3	0.0	0.07773
-0.3	-0.1	-0.3	0.1	0.16048
-0.3	-0.1	-0.3	0.2	0.24652
-0.3	-0.1	-0.3	0.3	0.33383
-0.3	-0.1	-0.2	-0.2	-0.00967
-0.3	-0.1	-0.2	-0.1	0.05990
-0.3	-0.1	-0.2	0.0	0.13597
-0.3	-0.1	-0.2	0.1	0.21700
-0.3	-0.1	-0.2	0.2	0.30132
-0.3	-0.1	-0.2	0.3	0.38697
-0.3	-0.1	-0.1	-0.1	0.12771
-0.3	-0.1	-0.1	0.0	0.20186
-0.3	-0.1	-0.1	0.1	0.28091
-0.3	-0.1	-0.1	0.2	0.36323
-0.3	-0.1	-0.1	0.3	0.44692
-0.3	-0.1	0.0	0.0	0.27394
-0.3	-0.1	0.0	0.1	0.35082
-0.3	-0.1	0.0	0.2	0.43094
-0.3	-0.1	0.0	0.3	0.51244
-0.3	-0.1	0.1	0.1	0.42541
-0.3	-0.1	0.1	0.2	0.50317

-0.3	-0.1	0.1	0.3	0.58232
-0.3	-0.1	0.2	0.2	0.57850
-0.3	-0.1	0.2	0.3	0.65522
-0.3	-0.1	0.3	0.3	0.72948
-0.3	0.0	-0.3	0.0	0.00000
-0.3	0.0	-0.3	0.1	0.08286
-0.3	0.0	-0.3	0.2	0.16911
-0.3	0.0	-0.3	0.3	0.25672
-0.3	0.0	-0.2	-0.2	-0.08751
-0.3	0.0	-0.2	-0.1	-0.01802
-0.3	0.0	-0.2	0.0	0.05806
-0.3	0.0	-0.2	0.1	0.13923
-0.3	0.0	-0.2	0.2	0.22380
-0.3	0.0	-0.2	0.3	0.30978
-0.3	0.0	-0.1	-0.1	0.04970
-0.3	0.0	-0.1	0.0	0.12390
-0.3	0.0	-0.1	0.1	0.20313
-0.3	0.0	-0.1	0.2	0.28573
-0.3	0.0	-0.1	0.3	0.36978
-0.3	0.0	0.0	0.0	0.19606
-0.3	0.0	0.0	0.1	0.27315
-0.3	0.0	0.0	0.2	0.35358
-0.3	0.0	0.0	0.3	0.43549
-0.3	0.0	0.1	0.1	0.34798
-0.3	0.0	0.1	0.2	0.42610
-0.3	0.0	0.1	0.3	0.50571
-0.3	0.0	0.2	0.2	0.50183

-0.3	0.0	0.2	0.3	0.57904
-0.3	0.0	0.3	0.3	0.65384
-0.3	0.1	-0.3	0.1	0.00000
-0.3	0.1	-0.3	0.2	0.08635
-0.3	0.1	-0.3	0.3	0.17415
-0.3	0.1	-0.2	-0.2	-0.17035
-0.3	0.1	-0.2	-0.1	-0.10108
-0.3	0.1	-0.2	0.0	-0.02509
-0.3	0.1	-0.2	0.1	0.05611
-0.3	0.1	-0.2	0.2	0.14080
-0.3	0.1	-0.2	0.3	0.22701
-0.3	0.1	-0.1	-0.1	-0.03355
-0.3	0.1	-0.1	0.0	0.04058
-0.3	0.1	-0.1	0.1	0.11986
-0.3	0.1	-0.1	0.2	0.20263
-0.3	0.1	-0.1	0.3	0.28695
-0.3	0.1	0.0	0.0	0.11270
-0.3	0.1	0.0	0.1	0.18988
-0.3	0.1	0.0	0.2	0.27051
-0.3	0.1	0.0	0.3	0.35272
-0.3	0.1	0.1	0.1	0.26484
-0.3	0.1	0.1	0.2	0.34319
-0.3	0.1	0.1	0.3	0.42314
-0.3	0.1	0.2	0.2	0.41920
-0.3	0.1	0.2	0.3	0.49680
-0.3	0.1	0.3	0.3	0.57204
-0.3	0.2	-0.3	0.2	0.00000

-0.3	0.2	-0.3	0.3	0.08789
-0.3	0.2	-0.2	-0.2	-0.25647
-0.3	0.2	-0.2	-0.1	-0.18751
-0.3	0.2	-0.2	0.0	-0.11171
-0.3	0.2	-0.2	0.1	-0.03059
-0.3	0.2	-0.2	0.2	0.05413
-0.3	0.2	-0.2	0.3	0.14045
-0.3	0.2	-0.1	-0.1	-0.12027
-0.3	0.2	-0.1	0.0	-0.04630
-0.3	0.2	-0.1	0.1	0.03291
-0.3	0.2	-0.1	0.2	0.11574
-0.3	0.2	-0.1	0.3	0.20022
-0.3	0.2	0.0	0.0	0.02566
-0.3	0.2	0.0	0.1	0.10281
-0.3	0.2	0.0	0.2	0.18354
-0.3	0.2	0.0	0.3	0.26595
-0.3	0.2	0.1	0.1	0.17778
-0.3	0.2	0.1	0.2	0.25627
-0.3	0.2	0.1	0.3	0.33645
-0.3	0.2	0.2	0.2	0.33245
-0.3	0.2	0.2	0.3	0.41033
-0.3	0.2	0.3	0.3	0.48588
-0.3	0.3	-0.3	0.3	0.00000
-0.3	0.3	-0.2	-0.2	-0.34387
-0.3	0.3	-0.2	-0.1	-0.27530
-0.3	0.3	-0.2	0.0	-0.19978
-0.3	0.3	-0.2	0.1	-0.11883

-0.3	0.3	-0.2	0.2	-0.03417
-0.3	0.3	-0.2	0.3	0.05218
-0.3	0.3	-0.1	-0.1	-0.20842
-0.3	0.3	-0.1	0.0	-0.13472
-0.3	0.3	-0.1	0.1	-0.05564
-0.3	0.3	-0.1	0.2	0.02714
-0.3	0.3	-0.1	0.3	0.11168
-0.3	0.3	0.0	0.0	-0.06298
-0.3	0.3	0.0	0.1	0.01405
-0.3	0.3	0.0	0.2	0.09477
-0.3	0.3	0.0	0.3	0.17727
-0.3	0.3	0.1	0.1	0.08893
-0.3	0.3	0.1	0.2	0.16745
-0.3	0.3	0.1	0.3	0.24777
-0.3	0.3	0.2	0.2	0.24370
-0.3	0.3	0.2	0.3	0.32175
-0.3	0.3	0.3	0.3	0.39753
-0.2	-0.2	-0.2	-0.2	0.00000
-0.2	-0.2	-0.2	-0.1	0.06968
-0.2	-0.2	-0.2	0.0	0.14584
-0.2	-0.2	-0.2	0.1	0.22697
-0.2	-0.2	-0.2	0.2	0.31138
-0.2	-0.2	-0.2	0.3	0.39711
-0.2	-0.2	-0.1	-0.1	0.13758
-0.2	-0.2	-0.1	0.0	0.21183
-0.2	-0.2	-0.1	0.1	0.29098
-0.2	-0.2	-0.1	0.2	0.37339

-0.2	-0.2	-0.1	0.3	0.45716
-0.2	-0.2	0.0	0.0	0.28401
-0.2	-0.2	0.0	0.1	0.36099
-0.2	-0.2	0.0	0.2	0.44119
-0.2	-0.2	0.0	0.3	0.52277
-0.2	-0.2	0.1	0.1	0.43567
-0.2	-0.2	0.1	0.2	0.51352
-0.2	-0.2	0.1	0.3	0.59275
-0.2	-0.2	0.2	0.2	0.58893
-0.2	-0.2	0.2	0.3	0.66573
-0.2	-0.2	0.3	0.3	0.74007
-0.2	-0.1	-0.2	-0.1	0.00000
-0.2	-0.1	-0.2	0.0	0.07628
-0.2	-0.1	-0.2	0.1	0.15765
-0.2	-0.1	-0.2	0.2	0.24240
-0.2	-0.1	-0.2	0.3	0.32855
-0.2	-0.1	-0.1	-0.1	0.06793
-0.2	-0.1	-0.1	0.0	0.14233
-0.2	-0.1	-0.1	0.1	0.22176
-0.2	-0.1	-0.1	0.2	0.30454
-0.2	-0.1	-0.1	0.3	0.38877
-0.2	-0.1	0.0	0.0	0.21470
-0.2	-0.1	0.0	0.1	0.29199
-0.2	-0.1	0.0	0.2	0.37261
-0.2	-0.1	0.0	0.3	0.45469
-0.2	-0.1	0.1	0.1	0.36702
-0.2	-0.1	0.1	0.2	0.44532

-0.2	-0.1	0.1	0.3	0.52510
-0.2	-0.1	0.2	0.2	0.52124
-0.2	-0.1	0.2	0.3	0.59861
-0.2	-0.1	0.3	0.3	0.67357
-0.2	0.0	-0.2	0.0	0.00000
-0.2	0.0	-0.2	0.1	0.08149
-0.2	0.0	-0.2	0.2	0.16647
-0.2	0.0	-0.2	0.3	0.25293
-0.2	0.0	-0.1	-0.1	-0.00845
-0.2	0.0	-0.1	0.0	0.06597
-0.2	0.0	-0.1	0.1	0.14555
-0.2	0.0	-0.1	0.2	0.22860
-0.2	0.0	-0.1	0.3	0.31318
-0.2	0.0	0.0	0.0	0.13840
-0.2	0.0	0.0	0.1	0.21587
-0.2	0.0	0.0	0.2	0.29679
-0.2	0.0	0.0	0.3	0.37926
-0.2	0.0	0.1	0.1	0.29113
-0.2	0.0	0.1	0.2	0.36978
-0.2	0.0	0.1	0.3	0.44998
-0.2	0.0	0.2	0.2	0.44607
-0.2	0.0	0.2	0.3	0.52392
-0.2	0.0	0.3	0.3	0.59941
-0.2	0.1	-0.2	0.1	0.00000
-0.2	0.1	-0.2	0.2	0.08508
-0.2	0.1	-0.2	0.3	0.17175
-0.2	0.1	-0.1	-0.1	-0.09005

-0.2	0.1	-0.1	0.0	-0.01571
-0.2	0.1	-0.1	0.1	0.06389
-0.2	0.1	-0.1	0.2	0.14708
-0.2	0.1	-0.1	0.3	0.23190
-0.2	0.1	0.0	0.0	0.05664
-0.2	0.1	0.0	0.1	0.13418
-0.2	0.1	0.0	0.2	0.21528
-0.2	0.1	0.0	0.3	0.29803
-0.2	0.1	0.1	0.1	0.20953
-0.2	0.1	0.1	0.2	0.28840
-0.2	0.1	0.1	0.3	0.36893
-0.2	0.1	0.2	0.2	0.36496
-0.2	0.1	0.2	0.3	0.44317
-0.2	0.1	0.3	0.3	0.51907
-0.2	0.2	-0.2	0.2	0.00000
-0.2	0.2	-0.2	0.3	0.08676
-0.2	0.2	-0.1	-0.1	-0.17512
-0.2	0.2	-0.1	0.0	-0.10099
-0.2	0.2	-0.1	0.1	-0.02147
-0.2	0.2	-0.1	0.2	0.06175
-0.2	0.2	-0.1	0.3	0.14670
-0.2	0.2	0.0	0.0	-0.02881
-0.2	0.2	0.0	0.1	0.04866
-0.2	0.2	0.0	0.2	0.12983
-0.2	0.2	0.0	0.3	0.21275
-0.2	0.2	0.1	0.1	0.12400
-0.2	0.2	0.1	0.2	0.20297

-0.2	0.2	0.1	0.3	0.28371
-0.2	0.2	0.2	0.2	0.27967
-0.2	0.2	0.2	0.3	0.35814
-0.2	0.2	0.3	0.3	0.43433
-0.2	0.3	-0.2	0.3	0.00000
-0.2	0.3	-0.1	-0.1	-0.26168
-0.2	0.3	-0.1	0.0	-0.18784
-0.2	0.3	-0.1	0.1	-0.10850
-0.2	0.3	-0.1	0.2	-0.02534
-0.2	0.3	-0.1	0.3	0.05963
-0.2	0.3	0.0	0.0	-0.11594
-0.2	0.3	0.0	0.1	-0.03860
-0.2	0.3	0.0	0.2	0.04252
-0.2	0.3	0.0	0.3	0.12551
-0.2	0.3	0.1	0.1	0.03660
-0.2	0.3	0.1	0.2	0.11557
-0.2	0.3	0.1	0.3	0.19642
-0.2	0.3	0.2	0.2	0.19231
-0.2	0.3	0.2	0.3	0.27093
-0.2	0.3	0.3	0.3	0.34731
-0.1	-0.1	-0.1	-0.1	0.00000
-0.1	-0.1	-0.1	0.0	0.07453
-0.1	-0.1	-0.1	0.1	0.15421
-0.1	-0.1	-0.1	0.2	0.23736
-0.1	-0.1	-0.1	0.3	0.32203
-0.1	-0.1	0.0	0.0	0.14707
-0.1	-0.1	0.0	0.1	0.22465

-0.1	-0.1	0.0	0.2	0.30567
-0.1	-0.1	0.0	0.3	0.38823
-0.1	-0.1	0.1	0.1	0.30001
-0.1	-0.1	0.1	0.2	0.37876
-0.1	-0.1	0.1	0.3	0.45906
-0.1	-0.1	0.2	0.2	0.45515
-0.1	-0.1	0.2	0.3	0.53310
-0.1	-0.1	0.3	0.3	0.60867
-0.1	0.0	-0.1	0.0	0.00000
-0.1	0.0	-0.1	0.1	0.07980
-0.1	0.0	-0.1	0.2	0.16320
-0.1	0.0	-0.1	0.3	0.24820
-0.1	0.0	0.0	0.0	0.07256
-0.1	0.0	0.0	0.1	0.15030
-0.1	0.0	0.0	0.2	0.23161
-0.1	0.0	0.0	0.3	0.31454
-0.1	0.0	0.1	0.1	0.22587
-0.1	0.0	0.1	0.2	0.30494
-0.1	0.0	0.1	0.3	0.38565
-0.1	0.0	0.2	0.2	0.38170
-0.1	0.0	0.2	0.3	0.46010
-0.1	0.0	0.3	0.3	0.53616
-0.1	0.1	-0.1	0.1	0.00000
-0.1	0.1	-0.1	0.2	0.08351
-0.1	0.1	-0.1	0.3	0.16873
-0.1	0.1	0.0	0.0	-0.00734
-0.1	0.1	0.0	0.1	0.07043

-0.1	0.1	0.0	0.2	0.15189
-0.1	0.1	0.0	0.3	0.23508
-0.1	0.1	0.1	0.1	0.14607
-0.1	0.1	0.1	0.2	0.22533
-0.1	0.1	0.1	0.3	0.30634
-0.1	0.1	0.2	0.2	0.30232
-0.1	0.1	0.2	0.3	0.38106
-0.1	0.1	0.3	0.3	0.45751
-0.1	0.2	-0.1	0.2	0.00000
-0.1	0.2	-0.1	0.3	0.08532
-0.1	0.2	0.0	0.0	-0.09095
-0.1	0.2	0.0	0.1	-0.01326
-0.1	0.2	0.0	0.2	0.06822
-0.1	0.2	0.0	0.3	0.15156
-0.1	0.2	0.1	0.1	0.06232
-0.1	0.2	0.1	0.2	0.14165
-0.1	0.2	0.1	0.3	0.22284
-0.1	0.2	0.2	0.2	0.21875
-0.1	0.2	0.2	0.3	0.29771
-0.1	0.2	0.3	0.3	0.37443
-0.1	0.3	-0.1	0.3	0.00000
-0.1	0.3	0.0	0.0	-0.17626
-0.1	0.3	0.0	0.1	-0.09876
-0.1	0.3	0.0	0.2	-0.01734
-0.1	0.3	0.0	0.3	0.06602
-0.1	0.3	0.1	0.1	-0.02333
-0.1	0.3	0.1	0.2	0.05596

-0.1	0.3	0.1	0.3	0.13722
-0.1	0.3	0.2	0.2	0.13307
-0.1	0.3	0.2	0.3	0.21214
-0.1	0.3	0.3	0.3	0.28901
0.0	0.0	0.0	0.0	0.00000
0.0	0.0	0.0	0.1	0.07788
0.0	0.0	0.0	0.2	0.15943
0.0	0.0	0.0	0.3	0.24272
0.0	0.0	0.1	0.1	0.15361
0.0	0.0	0.1	0.2	0.23298
0.0	0.0	0.1	0.3	0.31408
0.0	0.0	0.2	0.2	0.31007
0.0	0.0	0.2	0.3	0.38890
0.0	0.0	0.3	0.3	0.46544
0.0	0.1	0.0	0.1	0.00000
0.0	0.1	0.0	0.2	0.08167
0.0	0.1	0.0	0.3	0.16519
0.0	0.1	0.1	0.1	0.07577
0.0	0.1	0.1	0.2	0.15530
0.0	0.1	0.1	0.3	0.23667
0.0	0.1	0.2	0.2	0.23259
0.0	0.1	0.2	0.3	0.31173
0.0	0.1	0.3	0.3	0.38862
0.0	0.2	0.0	0.2	0.00000
0.0	0.2	0.0	0.3	0.08362
0.0	0.2	0.1	0.1	-0.00599
0.0	0.2	0.1	0.2	0.07356

0.0	0.2	0.1	0.3	0.15508
0.0	0.2	0.2	0.2	0.15094
0.0	0.2	0.2	0.3	0.23026
0.0	0.2	0.3	0.3	0.30738
0.0	0.3	0.0	0.3	0.00000
0.0	0.3	0.1	0.1	-0.08970
0.0	0.3	0.1	0.2	-0.01021
0.0	0.3	0.1	0.3	0.07134
0.0	0.3	0.2	0.2	0.06713
0.0	0.3	0.2	0.3	0.14653
0.0	0.3	0.3	0.3	0.22377
0.1	0.1	0.1	0.1	0.00000
0.1	0.1	0.1	0.2	0.07965
0.1	0.1	0.1	0.3	0.16125
0.1	0.1	0.2	0.2	0.15711
0.1	0.1	0.2	0.3	0.23653
0.1	0.1	0.3	0.3	0.31372
0.1	0.2	0.1	0.2	0.00000
0.1	0.2	0.1	0.3	0.08171
0.1	0.2	0.2	0.2	0.07750
0.1	0.2	0.2	0.3	0.15706
0.1	0.2	0.3	0.3	0.23444
0.1	0.3	0.1	0.3	0.00000
0.1	0.3	0.2	0.2	-0.00428
0.1	0.3	0.2	0.3	0.07531
0.1	0.3	0.3	0.3	0.15278
0.2	0.2	0.2	0.2	0.00000

0.2	0.2	0.2	0.3	0.07966
0.2	0.2	0.3	0.3	0.15719
0.2	0.3	0.2	0.3	0.00000
0.2	0.3	0.3	0.3	0.07756
0.3	0.3	0.3	0.3	0.00000

^a Only the M_z components were calculated. The M_x , M_y components can be derived by symmetry considerations. See text for details.

TABLE II. Comparison of the calculated and observed band intensities for SiH₄^a.

Sym	$\tilde{\nu}_{\text{cal}}$	$(n_1 n_2 n_3 n_4)$	$I_{\text{obs}}^b / \text{m}^{-2} \text{atm}^{-1}$	$I_{\text{cal}}^b / \text{m}^{-2} \text{atm}^{-1}$
F_{2z}	2188.757	(1 0 0 0)	0.113E+4	0.121E+4
F_{2z}	4308.965	(2 0 0 0)	0.722E+1	0.627E+1
F_{2z}	4377.616	(1 1 0 0)	0.670E-0	0.546E-0
F_{2z}	6362.149	(3 0 0 0)	0.224E-2	0.100E-1
F_{2z}	6498.565	(2 1 0 0)	0.362E-1	0.109E-1
F_{2z}	6500.368	(2 1 0 0)	0.406E-3	0.969E-3
F_{2z}	6569.735	(0 1 1 1)	...	0.309E-3
F_{2z}	8348.314	(4 0 0 0)	0.679E-2	0.154E-1
F_{2z}	8553.576	(3 1 0 0)	0.322E-3	0.385E-3
F_{2z}	8556.061	(3 1 0 0)	0.222E-4	0.944E-4
F_{2z}	8624.235	(2 2 0 0)	0.400E-4	0.138E-4
F_{2z}	10267.207	(5 0 0 0)	0.155E-2	0.286E-2
F_{2z}	10541.528	(4 1 0 0)	...	0.262E-4
F_{2z}	10544.112	(4 1 0 0)	...	0.210E-5
F_{2z}	12118.820	(6 0 0 0)	0.556E-4	0.425E-3
F_{2z}	13903.148	(7 0 0 0)	0.116E-4	0.633E-4
F_{2z}	15620.193	(8 0 0 0)	0.133E-5	0.100E-4
F_{2z}	17269.989	(9 0 0 0)	0.366E-6	0.171E-5

^a Experimental data from Refs. 13 and 23.

^b 1 atm=10⁵ Pa.

TABLE III. Comparison of the calculated and observed band intensities for SiH₃D.

Sym	$\tilde{\nu}_{\text{cal}}$	$(n_1 n_2 n_3)(m_1)^a$	$I_{\text{obs}}^b/\text{m}^{-2}\text{atm}^{-1}$	$I_{\text{cal}}^b/\text{m}^{-2}\text{atm}^{-1}$
A_1	1587.610	(0 0 0) (1)	...	0.155E+3
A_1	2186.219	(1 0 0) (0)	0.115E+3	0.105E+3
E	2188.525	(1 0 0) (0)	0.460E+3	0.813E+3
A_1	3140.445	(0 0 0) (2)	...	0.586E-0
A_1	3774.928	(1 0 0) (1)	0.30E+1	0.573E-1
E	3777.333	(1 0 0) (1)	...	0.135E-0
A_1	4307.650	(2 0 0) (0)	0.101E+1	0.532E-0
E	4308.521	(2 0 0) (0)	0.401E+1	0.416E+1
A_1	4375.606	(0 1 1) (0)	0.33E-0	0.938E-1
E	4377.965	(0 1 1) (0)	0.33E-0	0.180E-0
A_1	5897.629	(2 0 0) (1)	0.24E-1	0.416E-4
E	5898.502	(2 0 0) (1)	...	0.186E-2
A_1	6361.413	(3 0 0) (0)	0.34E-3	0.813E-3
E	6361.460	(3 0 0) (0)	0.14E-2	0.669E-2
A_1	6498.194	(2 1 0) (0)	0.12E-1	0.102E-2
E	6498.692	(2 1 0) (0)	...	0.432E-2
E	6500.044	(2 1 0) (0)	...	0.489E-3
A_1	7952.647	(3 0 0) (1)	...	0.126E-4
E	7952.694	(3 0 0) (1)	...	0.477E-4
A_1	8347.366	(4 0 0) (0)	0.92E-3	0.128E-2
E	8347.373	(4 0 0) (0)	0.37E-2	0.103E-1
A_1	8552.672	(3 1 0) (0)	...	0.171E-4
E	8553.533	(3 1 0) (0)	...	0.141E-3
E	8555.160	(3 1 0) (0)	...	0.772E-4
A_1	10266.007	(5 0 0) (0)	...	0.238E-3

<i>E</i>	10266.007	(5 0 0) (0)	...	0.190 <i>E</i> -2
<i>A</i> ₁	12117.354	(6 0 0) (0)	...	0.354 <i>E</i> -4
<i>E</i>	12117.354	(6 0 0) (0)	...	0.283 <i>E</i> -3
<i>A</i> ₁	13901.412	(7 0 0) (0)	...	0.527 <i>E</i> -5
<i>E</i>	13901.412	(7 0 0) (0)	...	0.422 <i>E</i> -4
<i>A</i> ₁	15618.192	(8 0 0) (0)	...	0.834 <i>E</i> -6
<i>E</i>	15618.192	(8 0 0) (0)	...	0.667 <i>E</i> -5
<i>A</i> ₁	17267.804	(9 0 0) (0)	...	0.143 <i>E</i> -6
<i>E</i>	17267.804	(9 0 0) (0)	...	0.114 <i>E</i> -5

^a m_i and n_i denote the Si-D and Si-H bonds excitation, respectively.

^b 1 atm=10⁵ Pa.

TABLE IV. Comparison of the calculated and observed band intensities for SiH₂D₂.

Sym	$\tilde{\nu}_{\text{cal}}$	$(n_1 n_2)(m_1 m_2)^a$	$I_{\text{obs}}^b/\text{m}^{-2}\text{atm}^{-1}$	$I_{\text{cal}}^b/\text{m}^{-2}\text{atm}^{-1}$
A_1	1578.019	(0 0) (1 0)	0.114E+3	0.100E+3
B_2	1596.849	(0 0) (1 0)	0.231E+3	0.212E+3
A_1	2186.781	(1 0) (0 0)	0.621E+3	0.208E+3
B_1	2188.293	(1 0) (0 0)		0.407E+3
A_1	3132.177	(0 0) (2 0)	0.152E+1	0.433E-0
B_2	3140.408	(0 0) (2 0)		0.767E-0
A_1	3765.915	(1 0) (1 0)	0.38E-0	0.292E-3
B_1	3767.490	(1 0) (1 0)		0.133E-0
B_2	3784.784	(1 0) (1 0)	0.40E-0	0.124E-0
A_1	4307.496	(2 0) (0 0)	0.253E+1	0.105E+1
B_1	4308.076	(2 0) (0 0)		0.207E+1
A_1	4376.741	(1 1) (0 0)	0.51E-0	0.919E-1
A_1	5887.847	(2 0) (1 0)	0.58E-2	0.601E-3
B_1	5888.428	(2 0) (1 0)		0.181E-2
B_2	5906.759	(2 0) (1 0)	0.24E-2	0.713E-4
B_2	5975.959	(1 1) (1 0)	0.96E-2	0.723E-4
A_1	6138.147	(0 0) (4 0)	0.96E-2	0.518E-3
A_1	6360.738	(3 0) (0 0)	0.70E-3	0.164E-2
B_1	6360.769	(3 0) (0 0)		0.335E-2
A_1	6498.674	(2 1) (0 0)	0.48E-2	0.987E-3
B_1	6498.733	(2 1) (0 0)		0.926E-3
A_1	7942.322	(3 0) (1 0)	...	0.312E-4
B_1	7942.354	(3 0) (1 0)	...	0.467E-4
A_1	8346.425	(4 0) (0 0)	0.33E-2	0.257E-2
B_1	8346.430	(4 0) (0 0)		0.515E-2

A_1	10264.804	(5 0) (0 0)	...	$0.477E-3$
B_1	10264.804	(5 0) (0 0)	...	$0.954E-3$
A_1	12115.884	(6 0) (0 0)	...	$0.709E-4$
B_1	12115.884	(6 0) (0 0)	...	$0.141E-3$
A_1	13899.669	(7 0) (0 0)	...	$0.105E-4$
B_1	13899.669	(7 0) (0 0)	...	$0.211E-4$
A_1	15616.178	(8 0) (0 0)	...	$0.166E-5$
B_1	15616.178	(8 0) (0 0)	...	$0.333E-5$
A_1	17265.554	(9 0) (0 0)	...	$0.285E-6$
B_1	17265.554	(9 0) (0 0)	...	$0.570E-6$

^a m_i and n_i denote the Si-D and Si-H bonds excitation, respectively.

^b 1 atm= 10^5 Pa.

TABLE V. Comparison of the calculated and observed band intensities for SiHD₃.

Sym	$\tilde{\nu}_{\text{cal}}$	$(m_1 m_2 m_3)(n_1)^a$	$I_{\text{obs}}^b/\text{m}^{-2}\text{atm}^{-1}$	$I_{\text{cal}}^b/\text{m}^{-2}\text{atm}^{-1}$
A_1	1568.407	(1 0 0) (0)	0.97E+2	0.492E+2
E	1596.683	(1 0 0) (0)	0.225E+3	0.425E+3
A_1	2187.317	(0 0 0) (1)	0.255E+3	0.309E+3
A_1	3120.613	(2 0 0) (0)	...	0.229E-0
E	3136.610	(2 0 0) (0)	0.18E+1	0.161E+1
A_1	3756.852	(1 0 0) (1)	0.25E-0	0.704E-1
E	3785.188	(1 0 0) (1)	0.30E-0	0.123E-0
A_1	4307.339	(0 0 0) (2)	0.102E+1	0.155E+1
A_1	4646.643	(3 0 0) (0)	...	0.480E-4
E	4651.298	(3 0 0) (0)	...	0.141E-2
A_1	4698.303	(2 1 0) (0)	0.60E-3	0.575E-3
E	4717.368	(2 1 0) (0)	0.25E-2	0.164E-2
E	4745.985	(2 1 0) (0)	...	0.121E-2
A_1	5310.217	(2 0 0) (1)	...	0.185E-4
E	5326.279	(2 0 0) (1)	0.30E-2	0.146E-2
A_1	5878.042	(1 0 0) (2)	0.33E-2	0.174E-2
A_1	6133.810	(4 0 0) (0)	0.25E-3	0.235E-3
E	6134.465	(4 0 0) (0)		0.194E-2
A_1	6360.061	(0 0 0) (3)	0.84E-3	0.249E-2
A_1	7583.182	(5 0 0) (0)	0.20E-4	0.334E-4
E	7583.251	(5 0 0) (0)		0.265E-3
A_1	7931.977	(1 0 0) (3)	0.25E-4	0.570E-4
A_1	8345.482	(0 0 0) (4)	0.15E-2	0.386E-2
A_1	10263.599	(0 0 0) (5)	...	0.715E-3
A_1	12114.410	(0 0 0) (6)	...	0.106E-3

A_1	13897.920	(0 0 0) (7)	$0.34E-4$	$0.158E-4$
A_1	15614.152	(0 0 0) (8)	$0.13E-5$	$0.250E-5$

^a m_i and n_i denote the Si-D and Si-H bonds excitation, respectively.

^b 1 atm= 10^5 Pa.

TABLE VI. Calculated band intensities for SiD₄.

Sym	$\tilde{\nu}_{\text{cal}}$	$(m_1 m_2 m_3 m_4)^a$	$I^b/\text{m}^{-2}\text{atm}^{-1}$
F_{2z}	1596.517	(1 0 0 0)	0.639E+3
F_{2z}	3131.966	(2 0 0 0)	0.251E+1
F_{2z}	3182.697	(1 1 0 0)	0.180E-1
F_{2z}	4645.938	(3 0 0 0)	0.104E-2
F_{2z}	4704.982	(2 1 0 0)	0.468E-2
F_{2z}	4742.465	(2 1 0 0)	0.209E-2
F_{2z}	6129.791	(4 0 0 0)	0.262E-2
F_{2z}	7579.125	(5 0 0 0)	0.379E-3
F_{2z}	8993.256	(6 0 0 0)	0.414E-4
F_{2z}	10372.292	(7 0 0 0)	0.443E-5
F_{2z}	11716.345	(8 0 0 0)	0.499E-6
F_{2z}	13025.515	(9 0 0 0)	0.604E-7

^a m_i denotes the Si-D bond excitation.

^b 1 atm=10⁵ Pa.