Supplemental Information for "Spectral Characterization for Small Clusters of Silicon and Oxygen: SiO_2, SiO_3, Si_2O_3, & Si_2O_4"

Mason B. Gardner[1], Brent R. Westbrook[1], and Ryan C. Fortenberry[1]

[1]Department of Chemistry & Biochemistry, University of Mississippi, University, MS 38677-1848

Introduction

The explicit CCSD(T)-F12b/cc-pVTZ-F12 force constants for each of the molecules explored. They are given in units of mdyne/(Å^n·rad^m) numbered from the symmetry-internal coordinates given in the text.

Table S1. CCSD(T)-F12b/cc-pVTZ-F12 force constants for SiO_2

4	4	0	0	0.423766259855
3	3	0	0	0.423766211032
2	2	0	0	9.112568406691
1	1	0	0	9.280510189762
4	4	1	0	-0.561596903890
3	3	1	0	-0.561596082870
2	2	1	0	-38.726137784528
1	1	1	0	-39.471154081588
4	4	4	4	0.359773378775
4	4	3	3	0.683611533991
3	3	3	3	0.361891002070
4	4	2	2	-0.804604628590
3	3	2	2	-0.803545817450
2	2	2	2	136.514960010751
4	4	1	1	0.027162155485
3	3	1	1	0.028407813978
2	2	1	1	135.909598842323
1	1	1	1	137.129507870339

Corresponding author: Ryan C. Fortenberry, r410@olemiss.edu

Table S2. CCSD(T)-F12b/cc-pVTZ-F12 force constants for SiO_3

1	1	0	0	9.593251755369	3	2	2	2	-10.841399942476
2	1	0	0	0.020317264205	3	3	1	1	-0.928709892230
2	2	0	0	6.175872995167	3	3	2	1	0.709080890870
3	1	0	0	0.027966975167	3	3	2	2	36.402882897569
3	2	0	0	-1.879514109745	3	3	3	1	0.489792625850
3	3	0	0	6.154725332648	3	3	3	2	-150.627489211387
4	4	0	0	5.400667716233	3	3	3	3	748.599740366254
5	4	0	0	0.060071158680	4	4	1	1	0.044880119037
5	5	0	0	0.338878981838	4	4	2	1	0.216627388092
6	6	0	0	0.500633887434	4	4	2	2	77.105244430278
1	1	1	0	-56.875124864289	4	4	3	1	1.058300987324
2	1	1	0	-0.286271769474	4	4	3	2	12.268129236786
2	2	1	0	-0.061126772121	4	4	3	3	-43.701877754418
2	2	2	0	-24.448452284040	4	4	4	4	78.487904596218
3	1	1	0	-0.249791618390	5	4	1	1	0.000908224868
3	2	1	0	-0.166115607672	5	4	2	1	-0.056241596139
3	2	2	0	6.455600817448	5	4	2	2	-0.168252544859
3	3	1	0	-0.341875325469	5	4	3	1	0.200987409404
3	3	2	0	-21.780762781098	5	4	3	2	-0.043598136539
3	3	3	0	80.965619208057	5	4	3	3	-0.871788790145
4	4	1	0	-0.247019715133	5	4	4	4	0.897134819534
4	4	2	0	-22.141561198732	5	5	1	1	-0.092708702622
4	4	3	0	-2.083042459491	5	5	2	1	0.220987201935
5	4	1	0	-0.115963170075	5	5	2	2	0.008959291030
5	4	2	0	0.010349296600	5	5	3	1	0.166719095925
5	4	3	0	-0.324048573980	5	5	3	2	-0.042676575777
5	5	1	0	-0.344488100188	5	5	3	3	-0.144496289900
5	5	2	0	-0.165531828561	5	5	4	4	-0.281554039784
5	5	3	0	-0.096202691644	5	5	5	4	0.089697331009
6	6	1	0	-0.436942519454	5	5	5	5	0.237161089921
6	6	2	0	-4.626097373435	6	6	1	1	-1.133182657608
6	6	3	0	14.379198844142	6	6	2	1	-0.172767409510
1	1	1	1	279.489567735293	6	6	2	2	14.834754840529
2	1	1	1	-0.003138098573	6	6	3	1	-0.781460413976
2	2	1	1	0.159693594846	6	6	3	2	-57.037475106406
2	2	2	1	-0.269591553292	6	6	3	3	231.184327712308
2	2	2	2	79.322436459600	6	6	4	4	-4.600652854360
3	1	1	1	-0.265877807624	6	6	5	4	-0.421052504480
3	2	1	1	0.336226531556	6	6	5	5	2.021540456128
3	2	2	1	0.094799152526	6	6	6	6	98.159664984538

Table S3. CCSD(T)-F12b/cc-pVTZ-F12 force constants for Si_2O_3

1	1	0	0	2.393458	7	7	3	0	-0.307534	6	5	2	1	-0.123382	7	7	7	5	0.054256
2	1	0	0	-0.373099	7	7	4	0	-0.149339	6	5	2	2	0.180493	7	7	7	6	0.043820
2	2	0	0	4.352402	8	8	1	0	-0.072243	6	5	3	1	0.124254	7	7	7	7	0.320433
3	1	0	0	-0.019765	8	8	2	0	-0.003489	6	5	3	2	0.154773	8	8	1	1	-0.220340
3	2	0	0	-0.008746	8	8	3	0	-0.074989	6	5	3	3	-0.137814	8	8	2	1	0.118423
3	3	0	0	9.472136	8	8	4	0	-0.012975	6	5	4	1	-0.298211	8	8	2	2	-0.192851
4	1	0	0	0.046657	9	8	5	0	0.007517	6	5	4	2	0.279464	8	8	3	1	0.081792
4	2	0	0	-0.047857	9	8	6	0	-0.068297	6	5	4	3	-0.071500	8	8	3	2	-0.015052
4	3	0	0	0.069924	9	8	7	0	-0.058418	6	5	4	4	0.266195	8	8	3	3	-0.082325
4	4	0	0	0.707882	9	9	1	0	-0.107954	6	5	5	5	1.363429	8	8	4	1	-0.001338
5	5	0	0	2.916534	9	9	2	0	0.004304	6	6	1	1	-0.128485	8	8	4	2	-0.000903
6	5	0	0	0.007948	9	9	3	0	-0.093272	6	6	2	1	0.184040	8	8	4	3	0.055237
6	6	0	0	9.426143	9	9	4	0	-0.017659	6	6	2	2	-0.154850	8	8	4	4	-0.176750
7	5	0	0	0.395335	1	1	1	1	28.956240	6	6	3	1	0.054543	8	8	5	5	-0.237260
7	6	0	0	0.093038	2	1	1	1	1.362428	6	6	3	2	-0.007459	8	8	6	5	0.008520
7	7	0	0	0.469356	2	2	1	1	-2.993502	6	6	3	3	137.841087	8	8	6	6	-0.073964
8	8	0	0	0.132335	2	2	2	1	0.295727	6	6	4	1	-0.049306	8	8	7	5	0.095446
9	9	0	0	0.142333	2	2	2	2	57.510846	6	6	4	2	0.151114	8	8	7	6	0.008743
1	1	1	0	-10.363249	3	1	1	1	0.028078	6	6	4	3	-0.071467	8	8	7	7	-0.130868
2	1	1	0	0.832672	3	2	1	1	0.174634	6	6	4	4	-0.189758	8	8	8	8	-0.026261
2	2	1	0	0.304945	3	2	2	1	-0.263743	6	6	5	5	0.266072	9	8	5	1	-0.010027
2	2	2	0	-16.704375	3	2	2	2	0.148937	6	6	6	5	-0.071918	9	8	5	2	0.025286
3	1	1	0	-0.277536	3	3	1	1	-0.141811	6	6	6	6	137.984264	9	8	5	3	-0.029210
3	2	1	0	0.110273	3	3	2	1	0.217927	7	5	1	1	0.041686	9	8	5	4	0.002615
3	2	2	0	-0.084054	3	3	2	2	-0.129616	7	5	2	1	-0.269436	9	8	6	1	0.129486
3	3	1	0	-0.241230	3	3	3	1	-0.003561	7	5	2	2	0.292064	9	8	6	2	-0.036186
3	3	2	0	-0.036442	3	3	3	2	0.084328	7	5	3	1	-0.143873	9	8	6	3	-0.057985
3	3	3	0	-39.629940	3	3	3	3	137.837264	7	5	3	2	0.113791	9	8	6	4	0.053189
4	1	1	0	0.232653	4	1	1	1	-0.297422	7	5	3	3	-0.070671	9	8	7	1	0.045778
4	2	1	0	-0.048263	4	2	1	1	0.018656	7	5	4	1	0.293851	9	8	7	2	-0.007847
4	2	2	0	-0.168580	4	2	2	1	-0.170870	7	5	4	2	0.045778	9	8	7	3	0.020055
4	3	1	0	0.110421	4	2	2	2	0.758728	7	5	4	3	0.244149	9	8	7	4	-0.071936
4	3	2	0	-0.105756	4	3	1	1	-0.094170	7	5	4	4	0.169574	9	9	1	1	-0.266283
4	3	3	0	-0.012620	4	3	2	1	-0.038366	7	5	5	5	0.041177	9	9	2	1	0.240934
4	4	1	0	-0.296048	4	3	2	2	0.194763	7	6	1	1	-0.126975	9	9	2	2	-0.295263
4	4	2	0	-0.151536	4	3	3	1	-0.013219	7	6	2	1	0.013951	9	9	3	1	0.136290
4	4	3	0	-0.478874	4	3	3	2	0.112968	7	6	2	2	0.121907	9	9	3	2	-0.025080
4	4	4	0	-0.216592	4	3	3	3	-0.070169	7	6	3	1	-0.057985	9	9	3	3	-0.074787
5	5	1	0	-0.817291	4	4	1	1	-0.466444	7	6	3	2	0.164364	9	9	4	1	-0.008750
5	5	2	0	-16.579513	4	4	2	1	0.381995	7	6	3	3	-0.109951	9	9	4	2	0.034410
5	5	3	0	-0.176111	4	4	2	2	-0.322601	7	6	4	1	0.203603	9	9	4	3	0.045209
5	5	4	0	-0.492544	4	4	3	1	0.133592	7	6	4	2	0.115535	9	9	4	4	-0.140147
6	5	1	0	-0.154152	4	4	3	2	0.201700	7	6	4	3	-0.089376	9	9	5	5	-0.191065
6	5	2	0	0.040981	4	4	3	3	-0.136067	7	6	4	4	0.146073	9	9	6	5	0.008084
6	5	3	0	-0.102121	4	4	4	1	-0.154005	7	6	5	5	-0.104533	9	9	6	6	-0.091616
6	5	4	0	-0.232735	4	4	4	2	0.370248	7	6	6	5	-0.021639	9	9	7	5	0.039641
6	6	1	0	-0.189097	4	4	4	3	0.322628	7	6	6	6	-0.148786	9	9	7	6	0.035338
6	6	2	0	-0.039021	4	4	4	4	0.043179	7	7	1	1	-0.270117	9	9	7	7	-0.078860
6	6	3	0	-39.432886	5	5	1	1	0.130113	7	7	2	1	0.210683	9	9	8	8	-0.006235
6	6	4	0	-0.060308	5	5	2	1	0.690360	7	7	2	2	-0.204245	9	9	9	9	0.126351
7	5	1	0	0.457745	5	5	2	2	61.435452	7	7	3	1	0.261198					
7	5	2	0	-0.392158	5	5	3	1	-0.429202	7	7	3	2	0.130117					
7	5	3	0	-0.151860	5	5	3	2	0.659301	7	7	3	3	0.040517					
7	5	4	0	-0.278160	5	5	3	3	0.048027	7	7	4	1	-0.094842					
7	6	1	0	0.119511	5	5	4	1	-0.696981	7	7	4	2	0.335970					
7	6	2	0	-0.124389	5	5	4	2	0.292178	7	7	4	3	0.115132					
7	6	3	0	-0.119890	5	5	4	3	0.205913	7	7	4	4	0.286891					
7	6	4	0	-0.310597	5	5	4	4	-0.495095	7	7	5	5	0.069345					
7	7	1	0	-0.382576	5	5	5	5	57.935564	7	7	6	5	0.306510					
7	7	2	0	-0.100966	6	5	1	1	0.260963	7	7	6	6	0.065356					

Table S4. CCSD(T)-F12b/cc-pVTZ-F12 force constants for Si_2O_4

12	12	0	0	1.5052177	6	6	1	0	-10.8955301
11	11	0	0	3.4380046	5	5	1	0	-0.1769573
11	10	0	0	1.6085544	5	4	1	0	-0.1344538
10	10	0	0	1.4861017	4	4	1	0	-13.2745196
9	9	0	0	4.7880909	3	3	1	0	-0.2114673
9	8	0	0	0.2305831	3	2	1	0	0.0426781
8	8	0	0	9.5984462	2	2	1	0	-2.4634107
7	7	0	0	0.4874767	3	1	1	0	-0.1104480
7	6	0	0	-0.0153111	2	1	1	0	0.3392645
6	6	0	0	4.4563956	1	1	1	0	-13.5017494
5	5	0	0	0.3862562	12	12	12	12	-60.5367835
5	4	0	0	0.3156321	12	12	11	11	-5.2442897
4	4	0	0	3.1459507	11	11	11	11	16.9170223
3	3	0	0	9.6515276	12	12	11	10	-12.0536259
3	2	0	0	-0.0367923	11	11	11	10	-4.3405671
2	2	0	0	2.5458314	12	12	10	10	-26.9068233
3	1	0	0	0.0198368	11	11	10	10	-3.0261947
2	1	0	0	-0.2676806	11	10	10	10	-6.7489281
1	1	0	0	4.9711604	10	10	10	10	-13.8197903
12	11	9	0	-1.0666611	12	12	9	9	-0.4256177
12	10	9	0	-0.3821905	11	11	9	9	-17.3925953
12	11	8	0	-1.8473227	11	10	9	9	0.6057806
12	10	8	0	-1.9713577	10	10	9	9	-0.5366798
12	12	3	0	-1.8895568	9	9	9	9	12.4008141
11	11	3	0	-1.7806184	12	12	9	8	0.4400029
11	10	3	0	-1.7734222	11	11	9	8	1.2760603
10	10	3	0	-1.7677520	11	10	9	8	0.9857538
9	9	3	0	-0.5732631	10	10	9	8	0.3291087
9	8	3	0	-0.3637721	9	9	9	8	0.7429297
8	8	3	0	-40.2930191	12	12	8	8	1.2515269
7	7	3	0	-0.3695357	11	11	8	8	-0.2294819
7	6	3	0	-0.0931883	11	10	8	8	0.9048638
6	6	3	0	-0.0080361	10	10	8	8	1.4965264
5	5	3	0	-0.2740490	9	9	8	8	0.1401472
5	4	3	0	-0.2180328	9	8	8	8	-0.1735030
4	4	3	0	-0.2760485	8	8	8	8	140.1888729
3	3	3	0	-40.3875189	12	11	9	7	-0.0366224
12	12	2	0	-0.5724076	12	10	9	7	0.0021799
11	11	2	0	0.1741417	12	11	8	7	0.0209271
11	10	2	0	0.2190144	12	10	8	7	0.0344425
10	10	2	0	-0.5099257	12	12	7	7	0.5598222
9	9	2	0	1.7294489	11	11	7	7	1.4604507
9	8	2	0	0.1170418	11	10	7	7	1.9644730
8	8	2	0	0.0312180	10	10	7	7	1.7362410
7	7	2	0	0.1757038	9	9	7	7	0.2997647
7	6	2	0	0.0986588	9	8	7	7	0.2535532
6	6	2	0	-0.4822610	8	8	7	7	-0.1066505
5	5	2	0	0.1242985	7	7	7	7	0.2006736
5	4	2	0	0.1166824	12	11	9	6	-0.0379303
4	4	2	0	0.7144730	12	10	9	6	-0.0021799
3	3	2	0	0.0705488	12	11	8	6	-0.0034878
3	2	2	0	-0.0955508	12	10	8	6	0.0170032
2	2	2	0	0.1699830	12	12	7	6	-0.9139685
12	12	1	0	0.0622657	11	11	7	6	-1.1572764
11	11	1	0	5.5537311	11	10	7	6	-0.2733603
11	10	1	0	-0.3252612	10	10	7	6	-0.0699389
10	10	1	0	-0.0309021	9	9	7	6	0.3680479
9	9	1	0	-11.7737133	9	8	7	6	0.1953196
9	8	1	0	-0.2848449	8	8	7	6	0.1212824
8	8	1	0	-0.1776558	7	7	7	6	0.1756657
7	7	1	0	-0.1778230	12	12	6	6	-1.3918542
7	6	1	0	-0.0917942	11	11	6	6	-20.7202227

Table S5. CCSD(T)-F12b/cc-pVTZ-F12 force constants for Si_2O_4 contd.

11	10	6	6	-1.0847806	7	7	3	3	-0.0495594	10	10	2	1	0.1199264
10	10	6	6	-0.7618291	7	6	3	3	0.1069137	9	9	2	1	-1.1132032
9	9	6	6	22.8318894	6	6	3	3	-0.0445515	9	8	2	1	-0.1822402
9	8	6	6	-0.1671688	5	5	3	3	0.0117510	8	8	2	1	0.1123403
8	8	6	6	-0.0105761	5	4	3	3	0.0489730	7	7	2	1	-0.1596248
7	7	6	6	-0.1256472	4	4	3	3	0.0624784	7	6	2	1	0.0422901
7	6	6	6	-0.0035225	3	3	3	3	139.9007595	6	6	2	1	-0.6736468
6	6	6	6	8.4062955	12	11	9	2	-0.2737962	5	5	2	1	-0.1547418
12	11	9	5	-0.0095915	12	10	9	2	0.4346734	5	4	2	1	-0.5768033
12	10	9	5	0.0130794	12	11	8	2	-0.1630570	4	4	2	1	-0.8850106
12	11	8	5	-0.0265948	12	10	8	2	0.6975701	3	3	2	1	0.0429104
12	10	8	5	-0.0217990	12	12	3	2	0.7942119	3	2	2	1	-0.0489036
12	12	5	5	1.1787742	11	11	3	2	-0.7329291	2	2	2	1	-1.5685296
11	11	5	5	1.3014890	11	10	3	2	-0.1704687	12	12	1	1	-0.4674084
11	10	5	5	1.7212389	10	10	3	2	0.7097331	11	11	1	1	-14.8873326
10	10	5	5	1.7070058	9	9	3	2	-0.3591187	11	10	1	1	-0.1126219
9	9	5	5	0.1282888	9	8	3	2	-0.1286145	10	10	1	1	-0.3973593
9	8	5	5	0.2611828	8	8	3	2	0.2124528	9	9	1	1	26.4259966
8	8	5	5	0.0371393	7	7	3	2	-0.0707606	9	8	1	1	0.1957724
7	7	5	5	0.2099587	7	6	3	2	-0.1177149	8	8	1	1	0.0225191
7	6	5	5	0.2263975	6	6	3	2	0.1049398	7	7	1	1	0.0108889
6	6	5	5	-0.0715429	5	5	3	2	-0.2044325	7	6	1	1	0.0867209
5	5	5	5	0.2269462	5	4	3	2	-0.8846061	6	6	1	1	25.0526085
12	11	9	4	0.0187471	4	4	3	2	-0.0984891	5	5	1	1	0.1028190
12	10	9	4	0.0148233	3	3	3	2	0.1909926	5	4	1	1	0.5953724
12	11	8	4	0.0418542	12	12	2	2	-0.1244722	4	4	1	1	35.9583554
12	10	8	4	-0.0122074	11	11	2	2	-1.6415210	3	3	1	1	0.0621003
12	12	5	4	1.5234718	11	10	2	2	-0.7655843	3	2	1	1	0.0698978
11	11	5	4	0.4546069	10	10	2	2	-0.2286635	2	2	1	1	2.5511729
11	10	5	4	0.7215491	9	9	2	2	-2.5925774	3	1	1	1	-0.0718655
10	10	5	4	1.1744121	9	8	2	2	0.1984342	2	1	1	1	-0.0444305
9	9	5	4	0.3825392	8	8	2	2	-0.1801460	1	1	1	1	30.6720701
9	8	5	4	0.2097070	7	7	2	2	0.0566748					
8	8	5	4	0.0878158	7	6	2	2	0.2737798					
7	7	5	4	0.2131604	6	6	2	2	-4.2422336					
7	6	5	4	0.0222350	5	5	2	2	0.0153139					
6	6	5	4	-0.0305531	5	4	2	2	0.1479179					
5	5	5	4	0.2803003	4	4	2	2	-5.5748232					
12	12	4	4	-0.1449868	3	3	2	2	-0.1857288					
11	11	4	4	-21.2976080	3	2	2	2	0.0399136					
11	10	4	4	0.8828468	2	2	2	2	6.2780710					
10	10	4	4	0.3297905	12	11	9	1	0.2057832					
9	9	4	4	31.6385350	12	10	9	1	-0.0326986					
9	8	4	4	0.3666903	12	11	8	1	0.3016991					
8	8	4	4	0.1059420	12	10	8	1	0.0034878					
7	7	4	4	-0.0075751	12	12	3	1	-0.0565573					
7	6	4	4	0.1832354	11	11	3	1	0.2790852					
6	6	4	4	30.5400374	11	10	3	1	0.3147785					
5	5	4	4	0.0852797	10	10	3	1	-0.0618522					
5	4	4	4	0.3448255	9	9	3	1	0.4928468					
4	4	4	4	54.9654774	9	8	3	1	0.2663846					
12	11	9	3	0.8113613	8	8	3	1	-0.0176873					
12	10	9	3	0.0928640	7	7	3	1	0.1346881					
12	11	8	3	0.5327692	7	6	3	1	0.1312303					
12	10	8	3	1.0223763	6	6	3	1	-0.1373641					
12	12	3	3	0.5912478	5	5	3	1	0.2713247					
11	11	3	3	-0.2043077	5	4	3	1	0.8671669					
11	10	3	3	0.5730161	4	4	3	1	0.2756845					
10	10	3	3	0.7799912	3	3	3	1	-0.0098185					
9	9	3	3	0.0537292	12	12	2	1	-0.0301654					
9	8	3	3	-0.2179968	11	11	2	1	0.3182979					
8	8	3	3	139.9578700	11	10	2	1	-0.0174392					