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Supplementary Material

The role of aldehydes on sulfur based-new particle formation: a theoretical study

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Table S1. The relative Gibbs free energies (Δ*G*, in kcal/mol) of four isomers in FA-SA-A system.

Method	Isomer-1	Isomer-2	Isomer-3	Isomer-4
MP2/6-311+G (d, p)// B3LYP-D3/6-31G(d)	0.00	0.41	5.36	7.51
MP2/6-311+G (d, p)	0.00	0.18	5.69	6.04
MP2/aug-cc-pvtz// B3LYP-D3/6-31G(d)	0.00	0.24	5.58	8.43
B3LYP-D3/ aug-cc-pvtz	0.00	0.30	6.85	-

Supplementary Figures

Figure S1. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y (X=FA/GL/MG; Y=SA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S2. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y (X=FA/GL/MG; Y=MSA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S3. The energies (in Hartree) and the corresponding geometric information of lowest-energy X-Y clusters from dynamic simulations at 300 K within 100 ps.

Figure S4. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=W) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S5. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=W) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S6. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=A) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S7. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=A) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S8. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=MA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S9. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=MA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

Figure S10. The plots of RDG versus sign(λ_2)ρ function, the visualized bonding isosurfaces for the most stable isomers of X-Y-Z (X=GL; Y=SA/MSA; Z=W/A/MA).

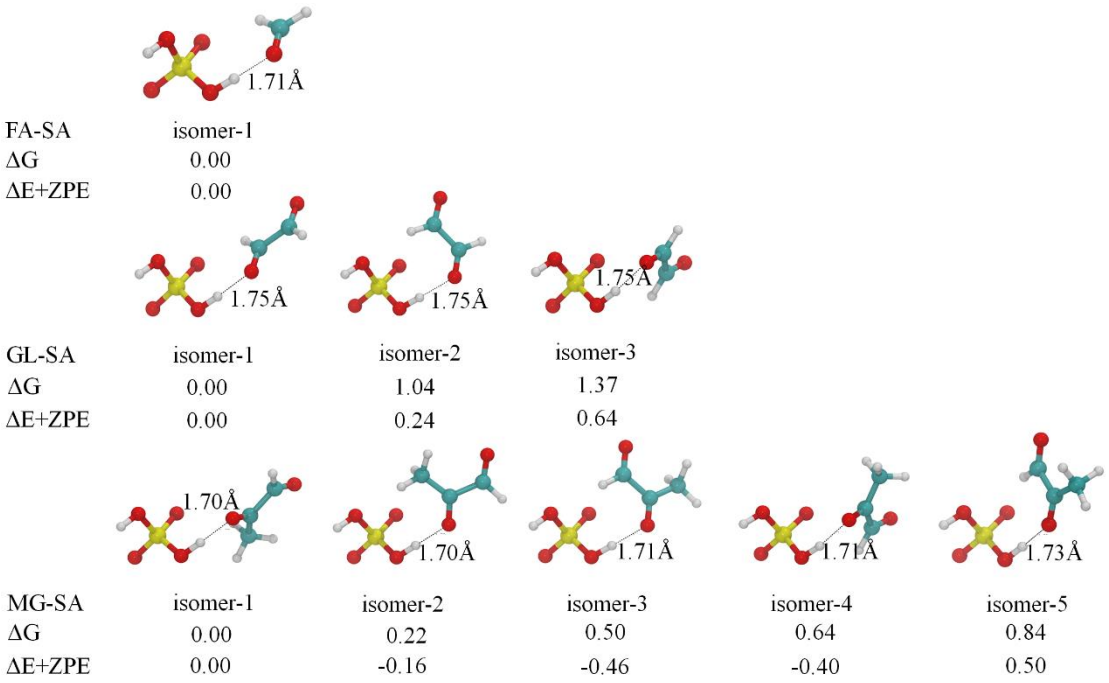
Figure S11. The plots of RDG versus sign(λ_2)ρ function, the visualized bonding isosurfaces for the most stable isomers of X-Y-Z (X=MG; Y=SA/MSA; Z=W/A/MA).

Figure S12. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=W) from dynamic simulations at 300 K within 100 ps.

Figure S13. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=A) from dynamic simulations at 300 K within 100 ps.

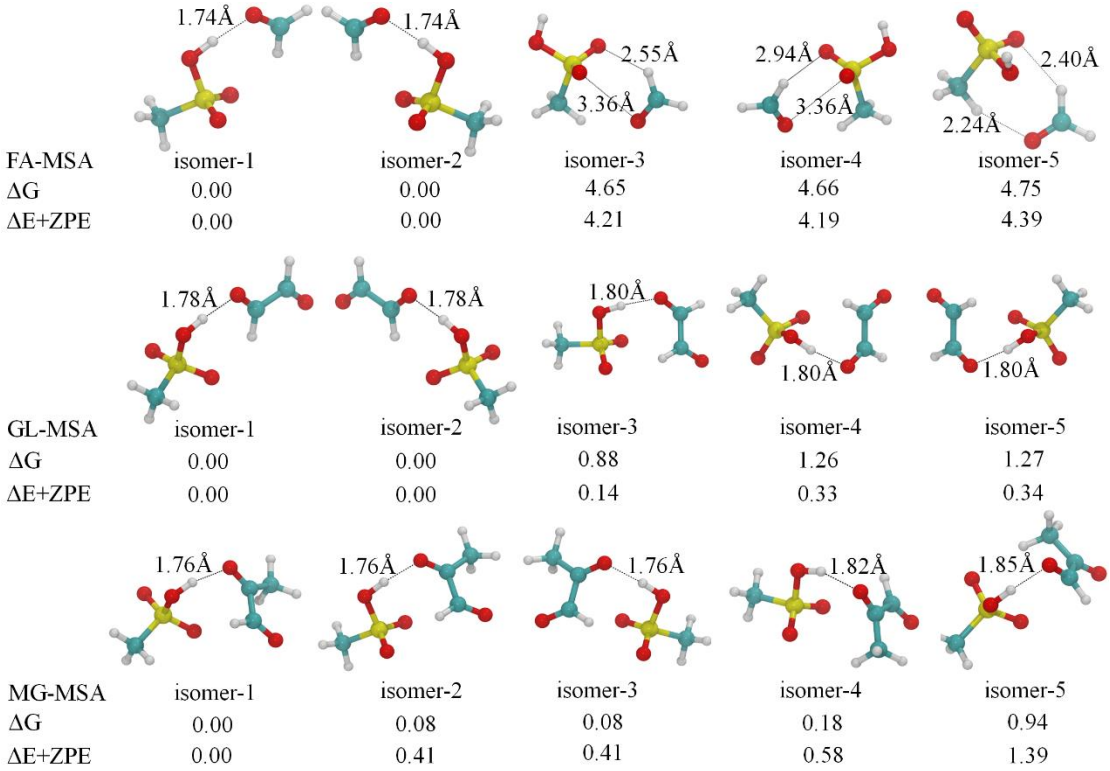
Figure S14. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=MA) from dynamic simulations at 300 K within 100 ps.

Section Frequencies. Details of Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates for all the most stable structures.



FA-SA	isomer-1				
ΔG	0.00				
ΔE+ZPE	0.00				
GL-SA	isomer-1	isomer-2	isomer-3		
ΔG	0.00	1.04	1.37		
ΔE+ZPE	0.00	0.24	0.64		
MG-SA	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	0.22	0.50	0.64	0.84
ΔE+ZPE	0.00	-0.16	-0.46	-0.40	0.50

Figure S1. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y (X=FA/GL/MG; Y=SA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.



FA-MSA	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	0.00	4.65	4.66	4.75
ΔE+ZPE	0.00	0.00	4.21	4.19	4.39
GL-MSA	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	0.00	0.88	1.26	1.27
ΔE+ZPE	0.00	0.00	0.14	0.33	0.34
MG-MSA	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	0.08	0.08	0.18	0.94
ΔE+ZPE	0.00	0.41	0.41	0.58	1.39

Figure S2. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y (X=FA/GL/MG; Y=MSA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

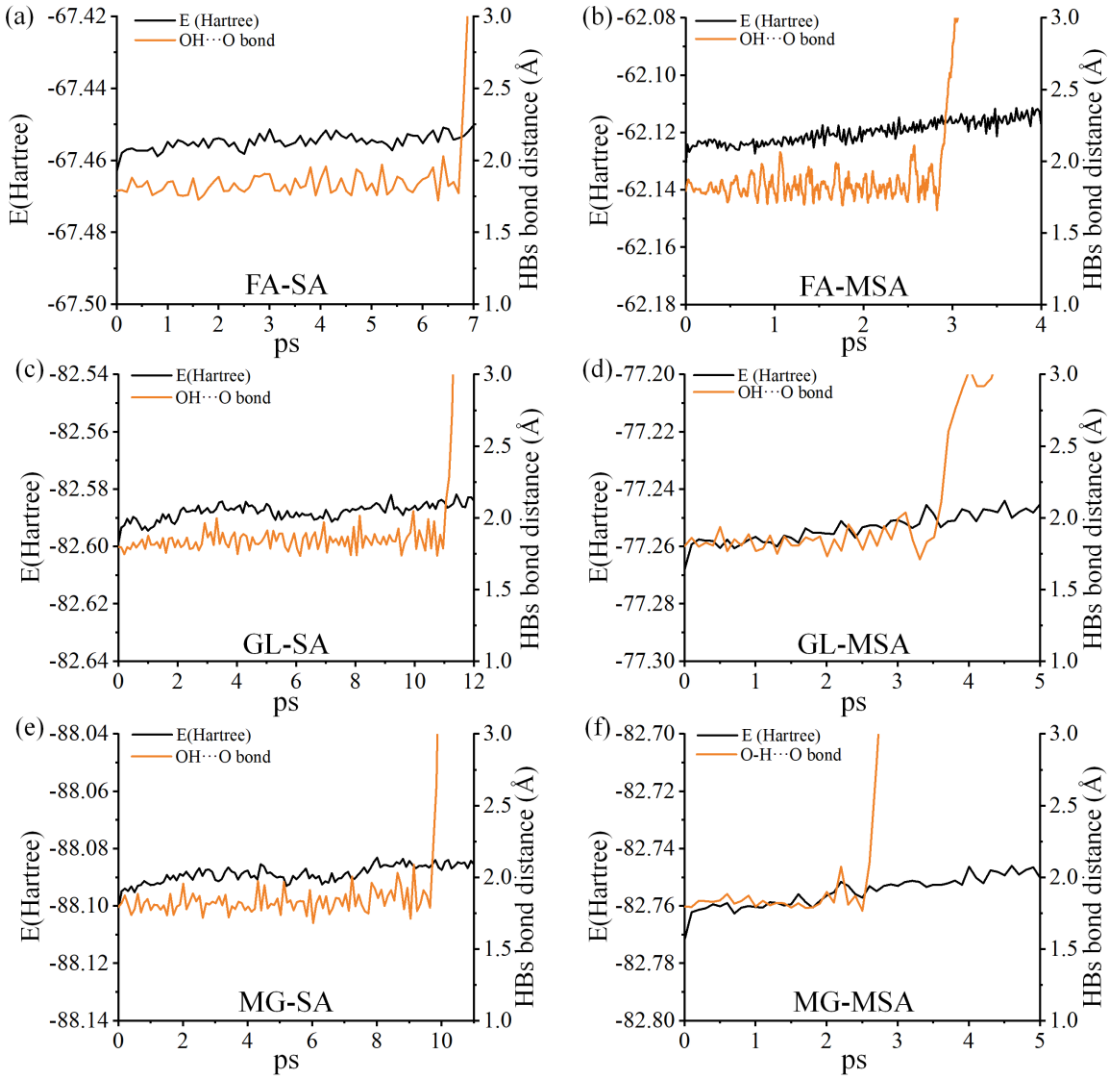
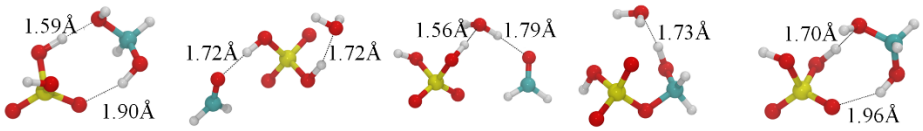
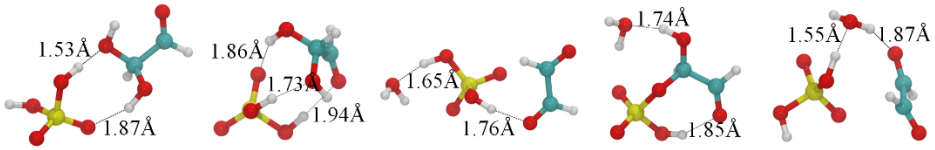


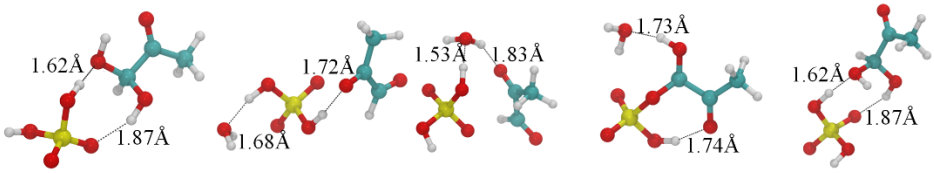
Figure S3. The energies (in Hartree) and the corresponding geometric information of lowest-energy X-Y clusters from dynamic simulations at 300 K within 100 ps.



FA-SA-W	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	1.53	2.70	2.95	4.36
ΔE+ZPE	0.00	2.27	3.73	2.62	4.26



GL-SA-W	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	2.73	3.06	3.35	3.56
ΔE+ZPE	0.11	2.03	4.98	2.73	5.16



MG-SA-W	isomer-1	isomer-2	isomer-3	isomer-4	isomer-5
ΔG	0.00	0.87	2.52	2.56	3.33
ΔE+ZPE	0.00	2.69	4.07	1.92	3.86

Figure S4. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=W) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

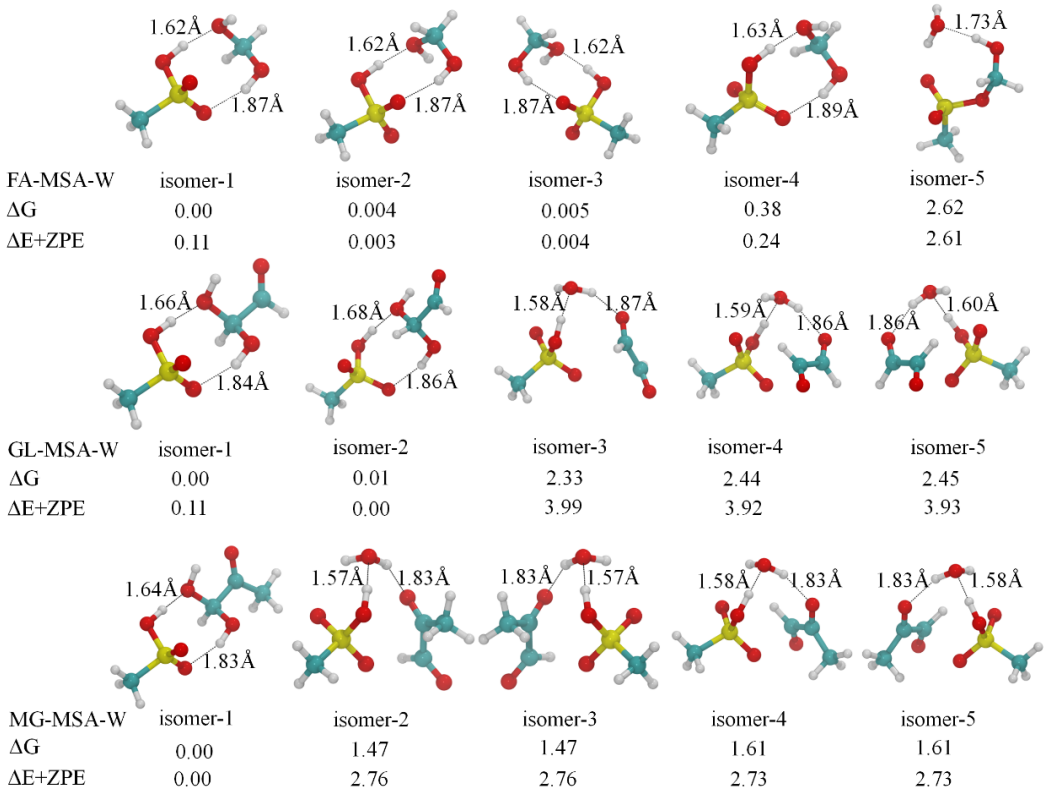


Figure S5. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=W) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

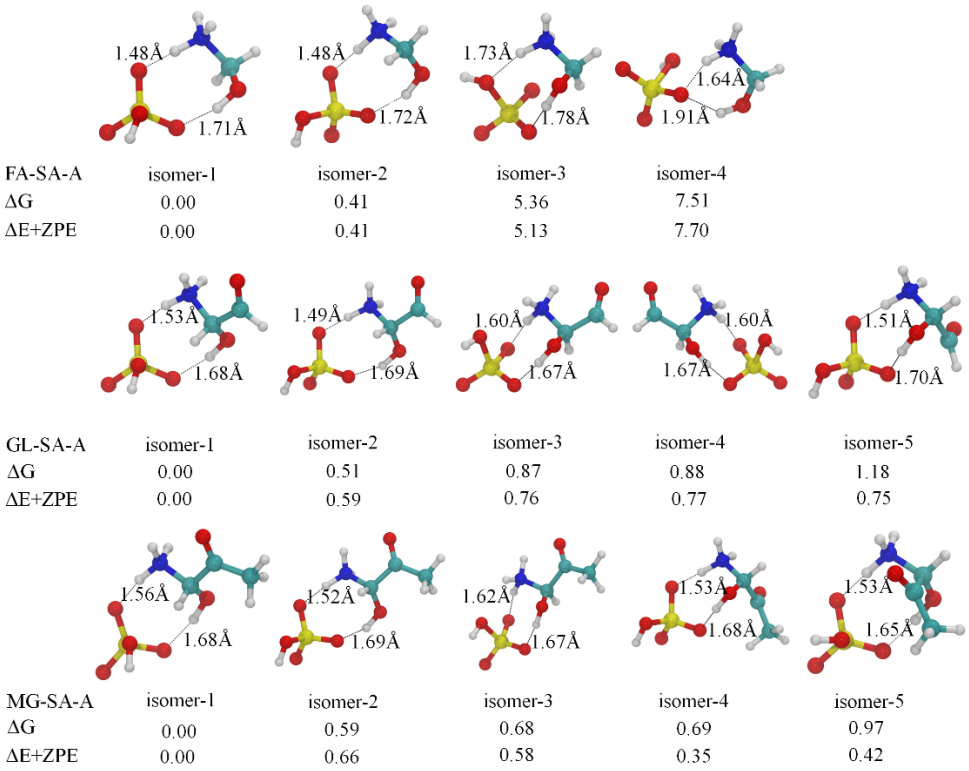


Figure S6. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=A) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

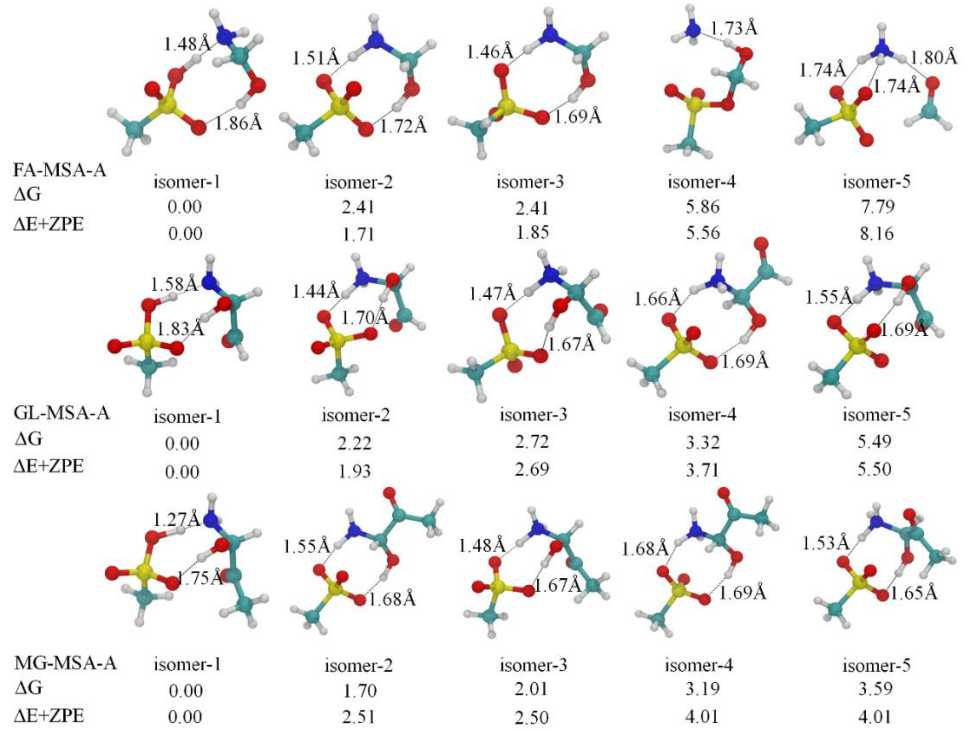


Figure S7. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=A) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

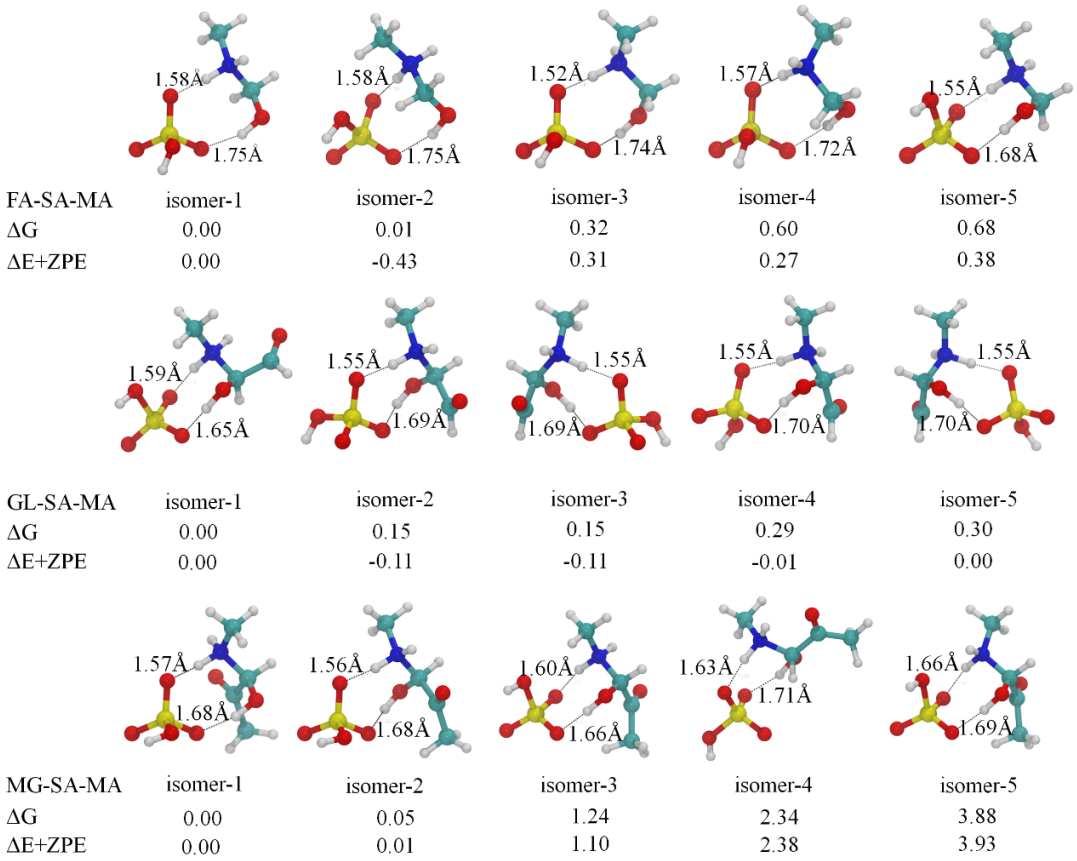


Figure S8. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=SA; Z=MA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

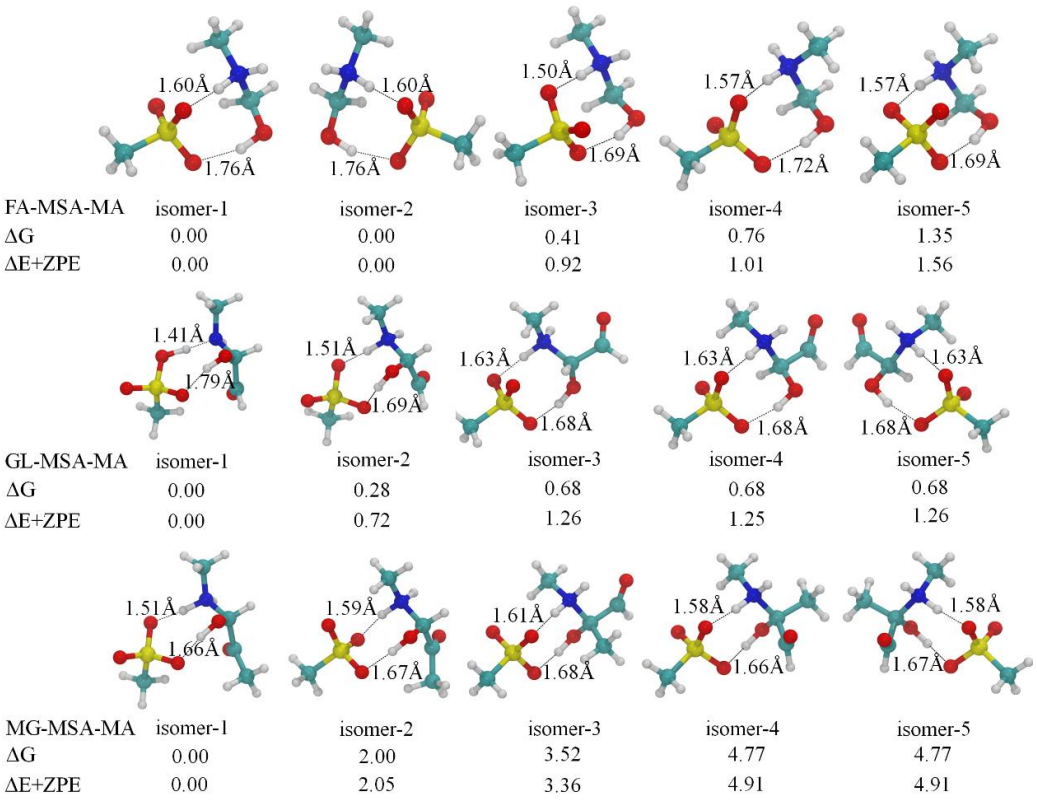


Figure S9. Structures, relative energies with zero-point energy correction (ΔE, kcal/mol) and relative Gibbs free energy (ΔG, kcal/mol) of the X-Y-Z (X=FA/GL/MG; Y=MSA; Z=MA) system at the MP2/6-311+G(d,p)//B3LYP-D3/6-31G(d) level.

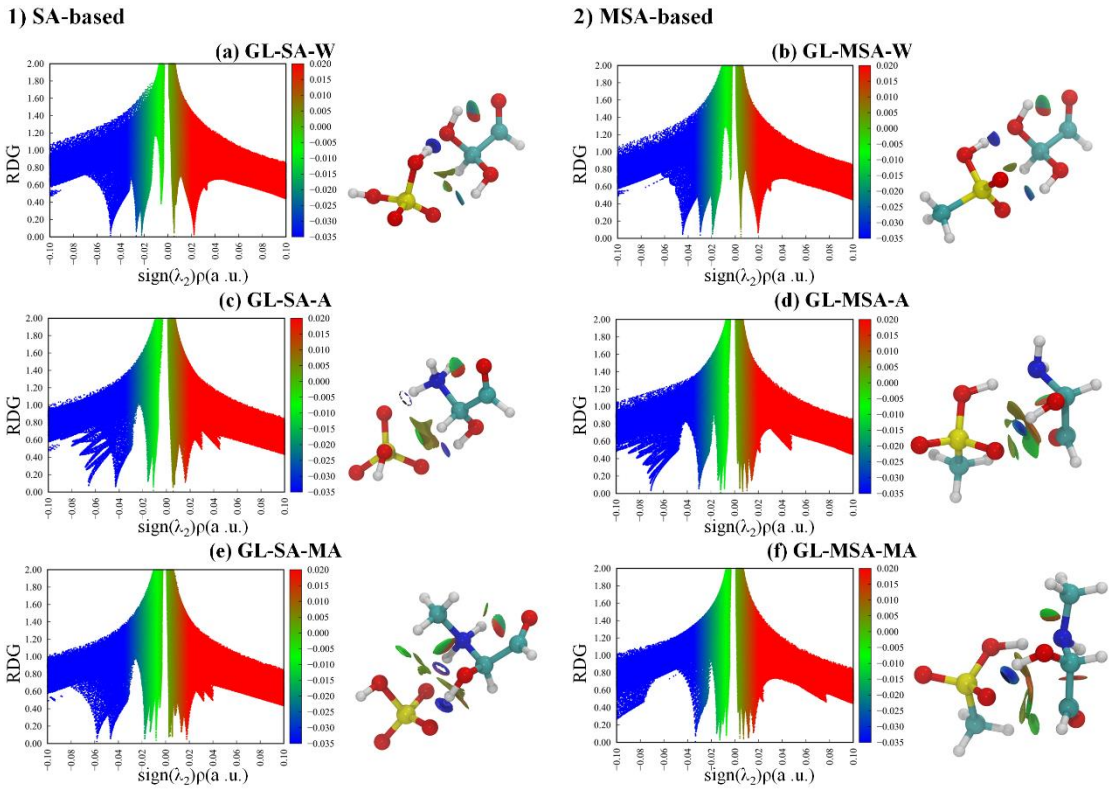


Figure S10. The plots of RDG versus sign(λ_2)ρ function, the visualized bonding isosurfaces for the most stable isomers of X-Y-Z (X=GL; Y=SA/MSA; Z=W/A/MA).

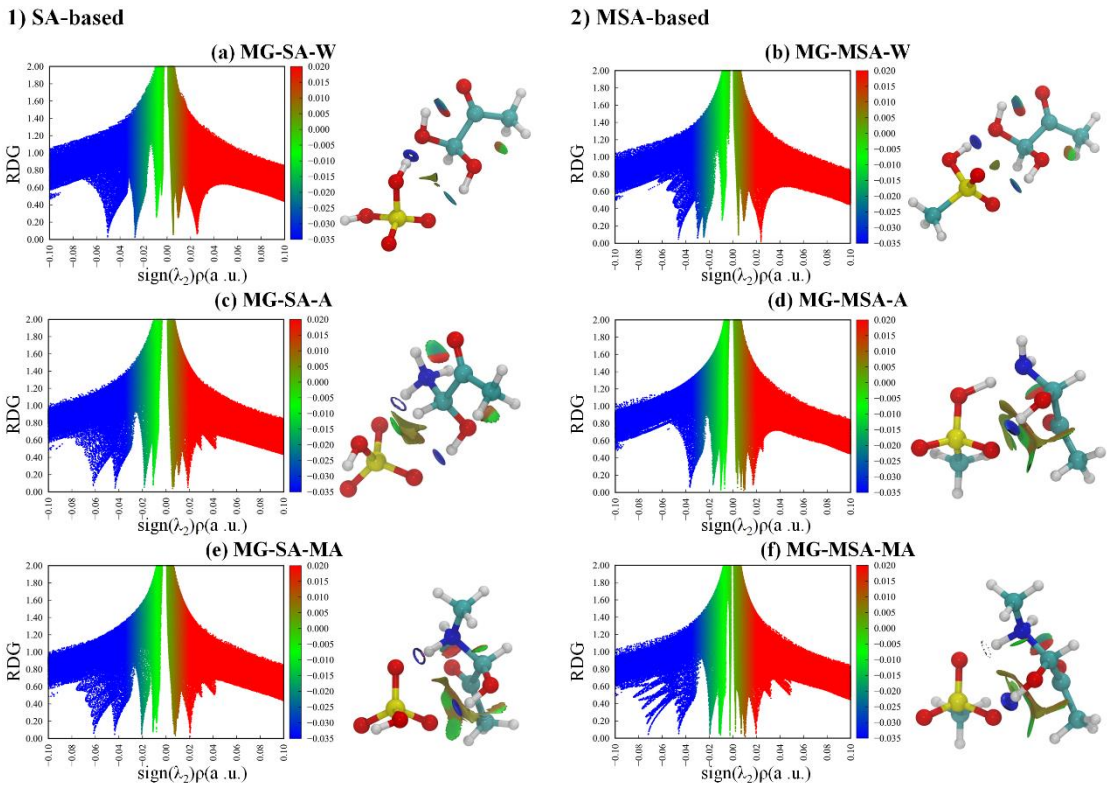


Figure S11. The plots of RDG versus sign(λ_2)ρ function, the visualized bonding isosurfaces for the most stable isomers of X-Y-Z (X=MG; Y=SA/MSA; Z=W/A/MA).

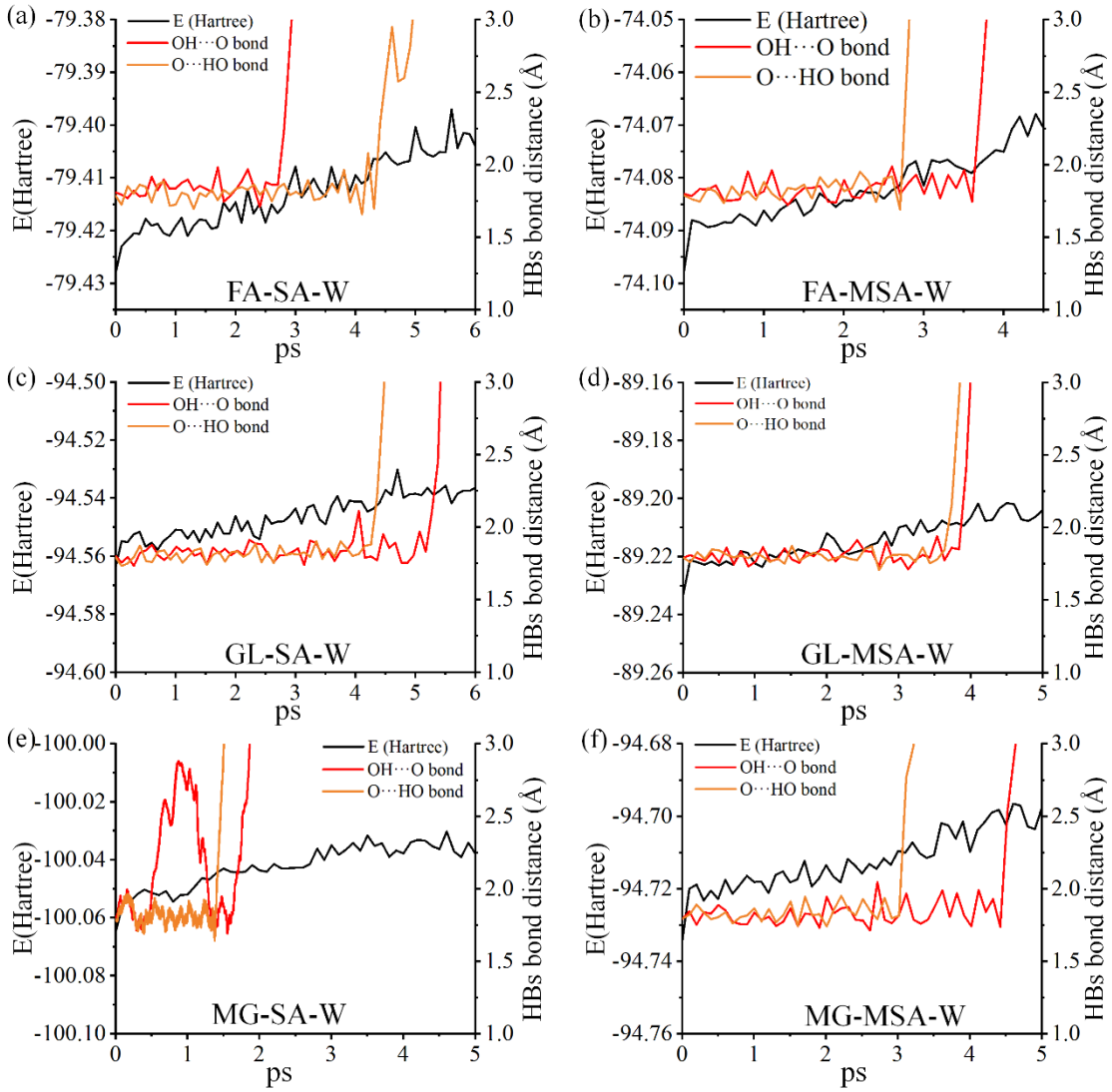


Figure S12. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=W) from dynamic simulations at 300 K within 100 ps.

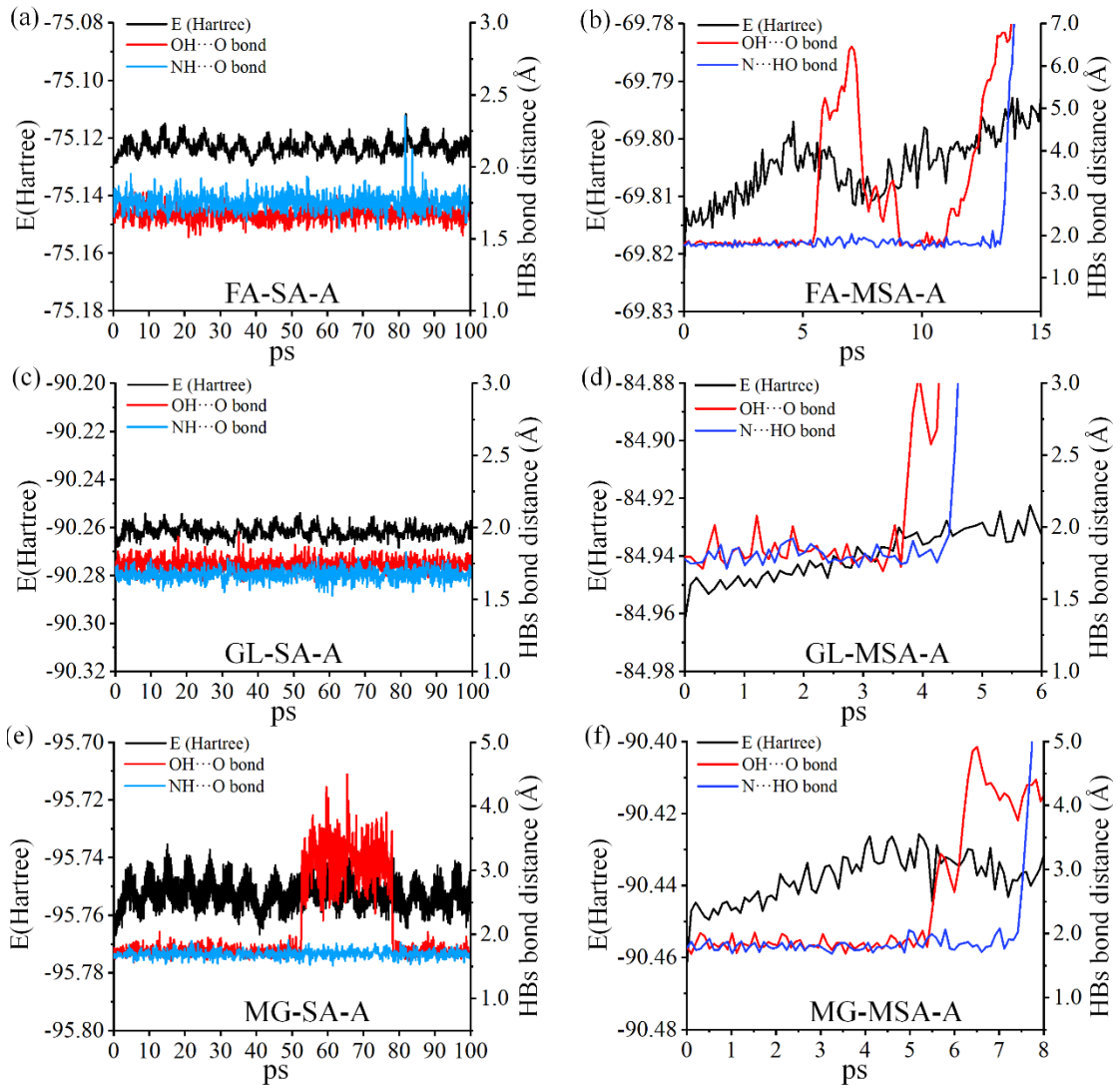


Figure S13. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=A) from dynamic simulations at 300 K within 100 ps.

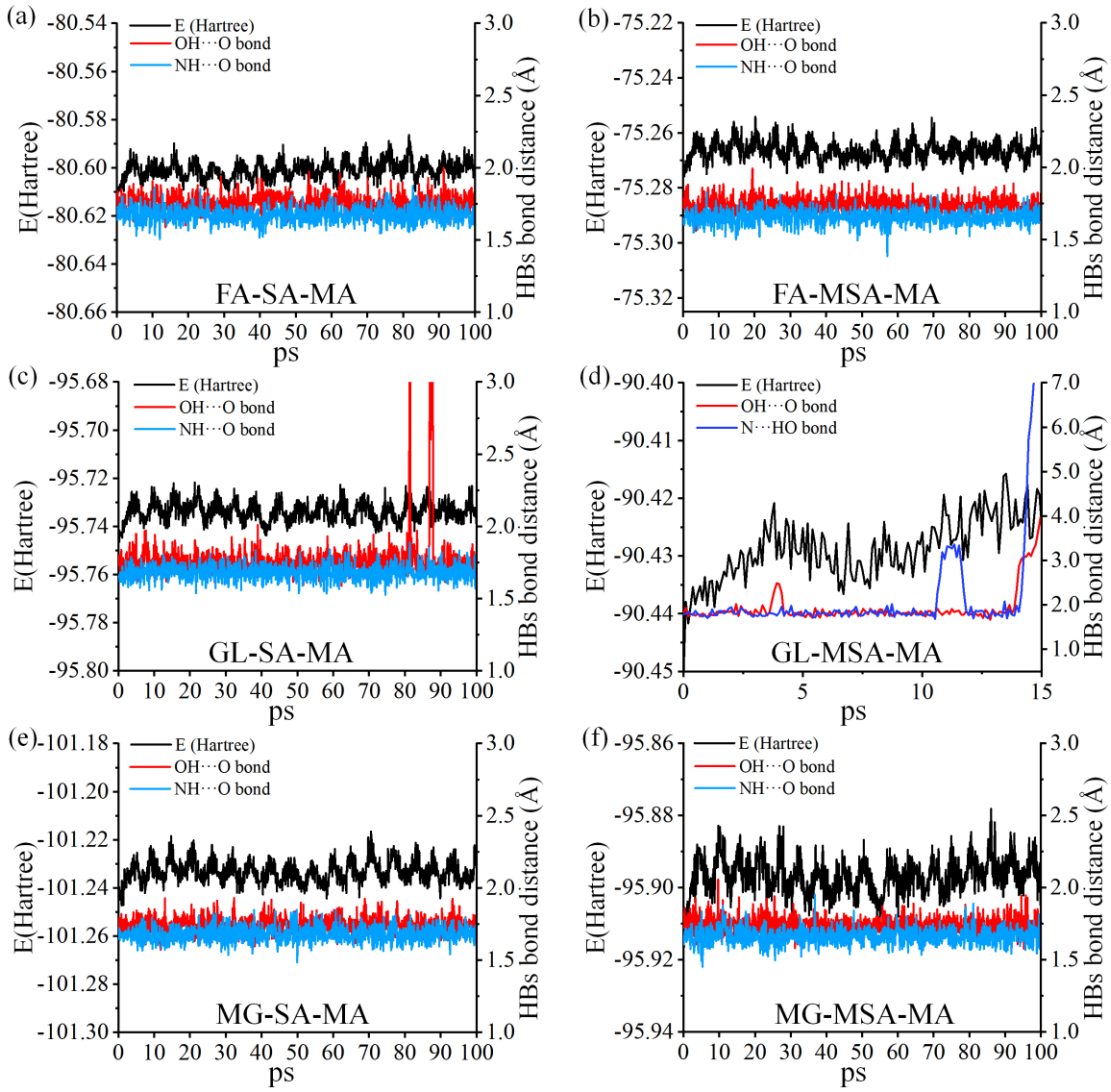


Figure S14. The energies (in Hartree) and the corresponding geometric information of lowest-energy structures in X-Y-Z (X=MG; Y=SA/MSA; Z=MA) from dynamic simulations at 300 K within 100 ps.

Section Frequencies. Details of Harmonic frequencies (cm**-1), IR intensities (KM/Mole), Raman scattering activities (A**4/AMU), depolarization ratios for plane and unpolarized incident light, reduced masses (AMU), force constants (mDyne/A), and normal coordinates for all the most stable structures.

FA-SA:

	1	2	3
	A	A	A
Frequencies --	39.8609	86.5150	135.1494
Red. masses --	3.7653	8.5140	11.6604
Frc consts --	0.0035	0.0375	0.1255
IR Inten --	14.6135	1.0732	1.6754
	4	5	6
	A	A	A
Frequencies --	168.1929	220.2504	281.4278
Red. masses --	5.1387	3.8205	1.0736
Frc consts --	0.0856	0.1092	0.0501
IR Inten --	0.6801	66.0985	1.9028
	7	8	9
	A	A	A
Frequencies --	340.9616	388.3201	472.6869
Red. masses --	2.8973	7.8996	1.6061
Frc consts --	0.1985	0.7018	0.2114
IR Inten --	18.0535	5.8976	50.3134
	10	11	12
	A	A	A
Frequencies --	509.3705	535.5155	539.7011
Red. masses --	5.2228	12.5900	10.0062
Frc consts --	0.7984	2.1273	1.7172
IR Inten --	17.3266	12.4399	72.1348
	13	14	15
	A	A	A
Frequencies --	765.2677	851.7863	882.8081
Red. masses --	12.9573	8.2960	1.1562
Frc consts --	4.4709	3.5463	0.5309
IR Inten --	135.8146	229.2068	181.5746
	16	17	18
	A	A	A
Frequencies --	1153.7031	1172.5533	1243.5657
Red. masses --	7.8179	1.3219	1.3429
Frc consts --	6.1310	1.0708	1.2236
IR Inten --	230.2615	62.6203	7.5591
	19	20	21
	A	A	A
Frequencies --	1300.6404	1326.3090	1418.1239

Red. masses -- 1.3161 1.6382 2.4331
Frc consts -- 1.3117 1.6979 2.8829
IR Inten -- 2.5908 122.5681 277.4894

	22	23	24
	A	A	A
Frequencies --	1561.8847	1760.3163	2999.5551
Red. masses --	1.1436	6.0132	1.0520
Frc consts --	1.6437	10.9783	5.5769
IR Inten --	14.2100	81.1457	136.4499

	25	26	27
	A	A	A
Frequencies --	3115.5219	3191.0421	3716.0248
Red. masses --	1.1182	1.0725	1.0660
Frc consts --	6.3948	6.4342	8.6732
IR Inten --	10.9031	1343.1424	125.9338

FA-MSA:

	1	2	3
	A	A	A
Frequencies --	40.6579	81.4621	122.8675
Red. masses --	3.7064	7.4478	7.3674
Frc consts --	0.0036	0.0291	0.0655
IR Inten --	16.1654	2.4243	3.7668

	4	5	6
	A	A	A
Frequencies --	161.2876	213.4170	232.0150
Red. masses --	4.8321	2.9371	1.0974
Frc consts --	0.0741	0.0788	0.0348
IR Inten --	1.7660	56.7814	5.1612

	7	8	9
	A	A	A
Frequencies --	292.5796	316.9620	331.4922
Red. masses --	1.0663	3.8298	3.9447
Frc consts --	0.0538	0.2267	0.2554
IR Inten --	1.5779	0.5439	16.0226

	10	11	12
	A	A	A
Frequencies --	456.5367	491.5209	513.4835
Red. masses --	7.0248	8.0764	7.2235
Frc consts --	0.8627	1.1496	1.1221
IR Inten --	6.7155	24.8706	30.2569

	13	14	15
	A	A	A
Frequencies --	726.7718	811.5144	827.7446
Red. masses --	6.6812	1.2468	3.8863

Frc consts --	2.0792	0.4838	1.5688
IR Inten --	29.5165	116.7226	188.5008
	16	17	18
	A	A	A
Frequencies --	1001.0239	1014.4209	1128.2431
Red. masses --	1.3529	1.4262	8.9651
Frc consts --	0.7987	0.8647	6.7238
IR Inten --	2.4789	21.4608	132.7398
	19	20	21
	A	A	A
Frequencies --	1246.8458	1296.6415	1308.4514
Red. masses --	1.3421	3.2994	1.5583
Frc consts --	1.2293	3.2683	1.5719
IR Inten --	4.5741	247.7973	66.4645
	22	23	24
	A	A	A
Frequencies --	1337.9015	1391.4209	1468.7689
Red. masses --	1.2914	1.2268	1.0473
Frc consts --	1.3620	1.3994	1.3311
IR Inten --	124.2812	18.7665	3.5512
	25	26	27
	A	A	A
Frequencies --	1476.1040	1564.4115	1758.8607
Red. masses --	1.0435	1.1446	5.9247
Frc consts --	1.3396	1.6505	10.7988
IR Inten --	6.4829	17.3462	71.4541
	28	29	30
	A	A	A
Frequencies --	2991.3283	3099.3967	3105.7592
Red. masses --	1.0517	1.0298	1.1189
Frc consts --	5.5447	5.8287	6.3588
IR Inten --	124.4150	0.0294	15.9757
	31	32	33
	A	A	A
Frequencies --	3214.1033	3221.1029	3237.9608
Red. masses --	1.1062	1.1076	1.0705
Frc consts --	6.7332	6.7708	6.6126
IR Inten --	3.1640	0.0827	1251.3683

GL-SA:

	1	2	3
	A	A	A
Frequencies --	29.0234	68.8615	84.3348
Red. masses --	4.7423	8.0964	4.9883
Frc consts --	0.0024	0.0226	0.0209

IR Inten --	3.2053	0.5946	0.6473
	4	5	6
	A	A	A
Frequencies --	96.2441	118.1096	128.2405
Red. masses --	3.5651	5.3563	11.6218
Frc consts --	0.0195	0.0440	0.1126
IR Inten --	3.1679	21.6522	1.6653
	7	8	9
	A	A	A
Frequencies --	158.4940	338.5215	362.9082
Red. masses --	9.2103	3.2154	4.4791
Frc consts --	0.1363	0.2171	0.3476
IR Inten --	12.3782	12.7563	96.7313
	10	11	12
	A	A	A
Frequencies --	385.4316	470.0924	506.7335
Red. masses --	7.9205	1.5940	4.7397
Frc consts --	0.6933	0.2075	0.7171
IR Inten --	6.3757	46.4436	21.6499
	13	14	15
	A	A	A
Frequencies --	534.8002	537.3475	574.7070
Red. masses --	12.0936	10.9539	9.8984
Frc consts --	2.0379	1.8635	1.9262
IR Inten --	13.2605	66.6374	5.0177
	16	17	18
	A	A	A
Frequencies --	762.0340	799.4551	848.1520
Red. masses --	4.8908	1.3168	10.4862
Frc consts --	1.6733	0.4958	4.4444
IR Inten --	60.7485	164.8613	316.4901
	19	20	21
	A	A	A
Frequencies --	867.1127	1094.8813	1100.1181
Red. masses --	1.2357	1.8038	4.4619
Frc consts --	0.5474	1.2740	3.1816
IR Inten --	13.0421	0.0857	2.6224
	22	23	24
	A	A	A
Frequencies --	1154.7108	1170.9949	1300.9170
Red. masses --	7.1053	1.3423	1.3926
Frc consts --	5.5819	1.0845	1.3886
IR Inten --	220.0026	59.1172	85.1456
	25	26	27

	A	A	A
Frequencies --	1366.7792	1403.8723	1415.3928
Red. masses --	1.1894	1.4150	2.4922
Frc consts --	1.3091	1.6431	2.9416
IR Inten --	6.1221	96.2109	229.7863
	28	29	30
	A	A	A
Frequencies --	1741.4730	1771.0599	2996.6264
Red. masses --	10.2059	9.2679	1.0897
Frc consts --	18.2362	17.1276	5.7654
IR Inten --	115.8014	41.0698	60.2292
	31	32	33
	A	A	A
Frequencies --	3088.8415	3294.1044	3714.7322
Red. masses --	1.0922	1.0704	1.0661
Frc consts --	6.1399	6.8435	8.6675
IR Inten --	9.1507	1322.3820	131.0964

GL-MSA:

	1	2	3
	A	A	A
Frequencies --	35.3378	66.4879	82.1729
Red. masses --	5.3300	8.5336	5.0797
Frc consts --	0.0039	0.0222	0.0202
IR Inten --	5.0259	0.8858	3.9803
	4	5	6
	A	A	A
Frequencies --	101.3415	118.7711	119.6181
Red. masses --	3.3407	5.4465	4.8813
Frc consts --	0.0202	0.0453	0.0412
IR Inten --	0.6368	8.2415	16.9241
	7	8	9
	A	A	A
Frequencies --	147.8222	229.3938	313.6322
Red. masses --	5.8858	1.0548	4.2451
Frc consts --	0.0758	0.0327	0.2460
IR Inten --	9.9286	0.1982	0.8453
	10	11	12
	A	A	A
Frequencies --	327.8492	362.6240	452.5123
Red. masses --	3.8285	4.5731	6.5027
Frc consts --	0.2425	0.3543	0.7845
IR Inten --	5.9219	98.1014	4.6159
	13	14	15
	A	A	A

Frequencies --	489.1052	511.8891	573.7975
Red. masses --	7.8261	7.3300	9.9167
Frc consts --	1.1031	1.1316	1.9237
IR Inten --	27.6393	29.8796	3.4266

	16	17	18
	A	A	A
Frequencies --	720.4146	734.9451	817.9718
Red. masses --	3.4238	1.2908	7.5850
Frc consts --	1.0469	0.4108	2.9901
IR Inten --	35.6097	98.0020	209.6815

	19	20	21
	A	A	A
Frequencies --	866.8136	1001.6082	1013.8782
Red. masses --	1.2298	1.3517	1.4239
Frc consts --	0.5444	0.7990	0.8624
IR Inten --	0.6449	2.5866	20.4700

	22	23	24
	A	A	A
Frequencies --	1098.4823	1101.0450	1128.0081
Red. masses --	2.5560	2.5606	7.9783
Frc consts --	1.8172	1.8289	5.9811
IR Inten --	2.4630	4.2192	115.6574

	25	26	27
	A	A	A
Frequencies --	1289.9046	1319.0769	1369.6839
Red. masses --	1.8947	2.4392	1.1881
Frc consts --	1.8574	2.5006	1.3133
IR Inten --	196.5469	247.0047	6.0469

	28	29	30
	A	A	A
Frequencies --	1390.9454	1411.9560	1468.6664
Red. masses --	1.2272	1.2326	1.0474
Frc consts --	1.3989	1.4479	1.3311
IR Inten --	14.6518	1.9799	3.5360

	31	32	33
	A	A	A
Frequencies --	1475.5296	1739.1388	1771.3513
Red. masses --	1.0434	10.1144	9.3076
Frc consts --	1.3384	18.0242	17.2066
IR Inten --	6.8416	102.0256	46.3996

	34	35	36
	A	A	A
Frequencies --	2992.7528	3079.5044	3099.2691
Red. masses --	1.0895	1.0930	1.0298

Frc consts --	5.7493	6.1069	5.8281
IR Inten --	63.8398	7.5935	0.0253

	37	38	39
	A	A	A
Frequencies --	3213.9580	3221.6153	3337.8545
Red. masses --	1.1062	1.1077	1.0687
Frc consts --	6.7322	6.7735	7.0154
IR Inten --	0.2923	0.2180	1183.6248

MG-SA:

	1	2	3
	A	A	A
Frequencies --	35.3378	66.4879	82.1729
Red. masses --	5.3300	8.5336	5.0797
Frc consts --	0.0039	0.0222	0.0202
IR Inten --	5.0259	0.8858	3.9803

	4	5	6
	A	A	A
Frequencies --	101.3415	118.7711	119.6181
Red. masses --	3.3407	5.4465	4.8813
Frc consts --	0.0202	0.0453	0.0412
IR Inten --	0.6368	8.2415	16.9241

	7	8	9
	A	A	A
Frequencies --	147.8222	229.3938	313.6322
Red. masses --	5.8858	1.0548	4.2451
Frc consts --	0.0758	0.0327	0.2460
IR Inten --	9.9286	0.1982	0.8453

	10	11	12
	A	A	A
Frequencies --	327.8492	362.6240	452.5123
Red. masses --	3.8285	4.5731	6.5027
Frc consts --	0.2425	0.3543	0.7845
IR Inten --	5.9219	98.1014	4.6159

	13	14	15
	A	A	A
Frequencies --	489.1052	511.8891	573.7975
Red. masses --	7.8261	7.3300	9.9167
Frc consts --	1.1031	1.1316	1.9237
IR Inten --	27.6393	29.8796	3.4266

	16	17	18
	A	A	A
Frequencies --	720.4146	734.9451	817.9718
Red. masses --	3.4238	1.2908	7.5850
Frc consts --	1.0469	0.4108	2.9901

IR Inten --	35.6097	98.0020	209.6815
	19	20	21
	A	A	A
Frequencies --	866.8136	1001.6082	1013.8782
Red. masses --	1.2298	1.3517	1.4239
Frc consts --	0.5444	0.7990	0.8624
IR Inten --	0.6449	2.5866	20.4700
	22	23	24
	A	A	A
Frequencies --	1098.4823	1101.0450	1128.0081
Red. masses --	2.5560	2.5606	7.9783
Frc consts --	1.8172	1.8289	5.9811
IR Inten --	2.4630	4.2192	115.6574
	25	26	27
	A	A	A
Frequencies --	1289.9046	1319.0769	1369.6839
Red. masses --	1.8947	2.4392	1.1881
Frc consts --	1.8574	2.5006	1.3133
IR Inten --	196.5469	247.0047	6.0469
	28	29	30
	A	A	A
Frequencies --	1390.9454	1411.9560	1468.6664
Red. masses --	1.2272	1.2326	1.0474
Frc consts --	1.3989	1.4479	1.3311
IR Inten --	14.6518	1.9799	3.5360
	31	32	33
	A	A	A
Frequencies --	1475.5296	1739.1388	1771.3513
Red. masses --	1.0434	10.1144	9.3076
Frc consts --	1.3384	18.0242	17.2066
IR Inten --	6.8416	102.0256	46.3996
	34	35	36
	A	A	A
Frequencies --	2992.7528	3079.5044	3099.2691
Red. masses --	1.0895	1.0930	1.0298
Frc consts --	5.7493	6.1069	5.8281
IR Inten --	63.8398	7.5935	0.0253
	37	38	39
	A	A	A
Frequencies --	3213.9580	3221.6153	3337.8545
Red. masses --	1.1062	1.1077	1.0687
Frc consts --	6.7322	6.7735	7.0154
IR Inten --	0.2923	0.2180	1183.6248

MG-MSA:

	1	2	3
	A	A	A
Frequencies --	51.1372	59.5296	84.0610
Red. masses --	3.8589	9.3443	6.4677
Frc consts --	0.0059	0.0195	0.0269
IR Inten --	8.7490	0.5929	3.7364
	4	5	6
	A	A	A
Frequencies --	95.1469	142.4086	155.1603
Red. masses --	9.2396	5.2985	4.0838
Frc consts --	0.0493	0.0633	0.0579
IR Inten --	0.5301	0.6363	0.9718
	7	8	9
	A	A	A
Frequencies --	168.7463	204.2107	228.6825
Red. masses --	1.1698	3.7396	1.0794
Frc consts --	0.0196	0.0919	0.0333
IR Inten --	2.5371	45.0067	1.7084
	10	11	12
	A	A	A
Frequencies --	263.6092	311.5653	331.8986
Red. masses --	3.6664	4.2294	3.8726
Frc consts --	0.1501	0.2419	0.2513
IR Inten --	14.5120	0.1751	11.6194
	13	14	15
	A	A	A
Frequencies --	450.8275	471.2187	485.7349
Red. masses --	6.3856	2.8463	7.3073
Frc consts --	0.7647	0.3724	1.0158
IR Inten --	4.1367	5.9785	28.6835
	16	17	18
	A	A	A
Frequencies --	502.5339	511.2297	581.1774
Red. masses --	3.4333	7.5787	4.4827
Frc consts --	0.5109	1.1670	0.8921
IR Inten --	37.3571	20.0032	8.1071
	19	20	21
	A	A	A
Frequencies --	717.1183	760.5385	807.7907
Red. masses --	6.7981	1.0988	3.7777
Frc consts --	2.0598	0.3745	1.4524
IR Inten --	33.3892	146.5271	13.5954
	22	23	24
	A	A	A

Frequencies --	812.5397	924.1987	1000.5633
Red. masses --	7.6864	1.3549	1.3547
Frc consts --	2.9899	0.6819	0.7990
IR Inten --	194.4171	0.8615	2.2717

	25	26	27
	A	A	A
Frequencies --	1012.4106	1031.0711	1073.9351
Red. masses --	1.4216	1.7295	1.9082
Frc consts --	0.8585	1.0833	1.2967
IR Inten --	16.9703	1.8800	4.4885

	28	29	30
	A	A	A
Frequencies --	1122.7460	1279.5654	1297.5408
Red. masses --	8.1145	2.8717	2.1140
Frc consts --	6.0267	2.7702	2.0970
IR Inten --	120.2119	32.9070	183.6711

	31	32	33
	A	A	A
Frequencies --	1313.6692	1390.5189	1397.8464
Red. masses --	2.2310	1.2263	1.2258
Frc consts --	2.2684	1.3970	1.4111
IR Inten --	281.3126	18.3964	3.3842

	34	35	36
	A	A	A
Frequencies --	1411.2546	1467.2093	1475.8963
Red. masses --	1.3784	1.0472	1.0433
Frc consts --	1.6174	1.3282	1.3389
IR Inten --	36.6671	3.5644	6.5751

	37	38	39
	A	A	A
Frequencies --	1480.0414	1482.6575	1753.8300
Red. masses --	1.0554	1.0655	10.3115
Frc consts --	1.3621	1.3800	18.6873
IR Inten --	18.0176	9.7058	153.3996

	40	41	42
	A	A	A
Frequencies --	1775.0574	3010.9109	3065.6403
Red. masses --	10.1541	1.0897	1.0396
Frc consts --	18.8502	5.8203	5.7566
IR Inten --	42.6812	55.0652	0.8417

	43	44	45
	A	A	A
Frequencies --	3098.9616	3151.5271	3204.3011
Red. masses --	1.0298	1.0926	1.1059

Frc consts --	5.8266	6.3935	6.6903
IR Inten --	0.0991	2.9310	1.5009

	46	47	48
	A	A	A
Frequencies --	3214.1412	3220.9960	3295.5425
Red. masses --	1.1062	1.1077	1.0692
Frc consts --	6.7332	6.7707	6.8414
IR Inten --	0.4932	0.2074	954.8466

FA-SA-W:

	1	2	3
	A	A	A
Frequencies --	86.1684	94.8110	133.8215
Red. masses --	8.3908	6.4162	6.6757
Frc consts --	0.0367	0.0340	0.0704
IR Inten --	0.7799	1.3093	3.3178

	4	5	6
	A	A	A
Frequencies --	151.8019	205.7684	250.2443
Red. masses --	5.1105	3.6968	4.1077
Frc consts --	0.0694	0.0922	0.1516
IR Inten --	0.0567	8.8662	40.5903

	7	8	9
	A	A	A
Frequencies --	342.6515	393.0671	464.3927
Red. masses --	2.8340	8.1189	1.5746
Frc consts --	0.1960	0.7391	0.2001
IR Inten --	23.2197	14.5588	46.8114

	10	11	12
	A	A	A
Frequencies --	479.7423	512.0697	534.2477
Red. masses --	2.2369	6.1893	14.3655
Frc consts --	0.3033	0.9562	2.4158
IR Inten --	55.2952	18.0962	24.7215

	13	14	15
	A	A	A
Frequencies --	544.3971	628.4376	765.5488
Red. masses --	10.0090	1.5228	7.7252
Frc consts --	1.7477	0.3543	2.6675
IR Inten --	38.1258	128.5357	105.2558

	16	17	18
	A	A	A
Frequencies --	798.0692	872.8894	957.6212
Red. masses --	1.1788	13.3421	4.9185
Frc consts --	0.4424	5.9895	2.6575

IR Inten -- 145.5744 233.5111 136.8327

	19	20	21
	A	A	A
Frequencies --	1031.2442	1127.7894	1146.6384
Red. masses --	1.2421	1.4189	3.3223
Frc consts --	0.7783	1.0633	2.5736
IR Inten --	18.0867	28.6475	305.3436

	22	23	24
	A	A	A
Frequencies --	1155.2079	1168.1377	1265.6359
Red. masses --	3.7943	1.4918	1.0879
Frc consts --	2.9833	1.1994	1.0267
IR Inten --	137.6582	91.2694	27.6282

	25	26	27
	A	A	A
Frequencies --	1343.7339	1385.5665	1436.1117
Red. masses --	2.6180	1.2986	1.3516
Frc consts --	2.7852	1.4689	1.6424
IR Inten --	215.2866	118.1359	149.6770

	28	29	30
	A	A	A
Frequencies --	1469.1989	1491.3417	1555.8546
Red. masses --	1.2295	1.1729	1.0983
Frc consts --	1.5636	1.5369	1.5664
IR Inten --	34.0594	42.9441	1.9724

	31	32	33
	A	A	A
Frequencies --	2843.7316	3092.0976	3162.3253
Red. masses --	1.0795	1.0558	1.1158
Frc consts --	5.1432	5.9477	6.5743
IR Inten --	1842.0382	33.3779	29.2026

	34	35	36
	A	A	A
Frequencies --	3635.4816	3713.9097	3742.0581
Red. masses --	1.0660	1.0661	1.0658
Frc consts --	8.3007	8.6639	8.7930
IR Inten --	422.4999	126.4908	64.2843

FA-MSA-W:

	1	2	3
	A	A	A
Frequencies --	84.5893	97.9134	120.6618
Red. masses --	7.0307	6.3622	6.7286
Frc consts --	0.0296	0.0359	0.0577
IR Inten --	4.8251	0.7879	6.2569

	4	5	6
	A	A	A
Frequencies --	144.0602	193.9651	222.5565
Red. masses --	3.6690	3.3036	1.0543
Frc consts --	0.0449	0.0732	0.0308
IR Inten --	0.4626	2.5777	0.2037
	7	8	9
	A	A	A
Frequencies --	238.1312	318.1264	347.6429
Red. masses --	3.3282	4.3349	4.3299
Frc consts --	0.1112	0.2585	0.3083
IR Inten --	31.4374	2.1984	38.5045
	10	11	12
	A	A	A
Frequencies --	462.8768	484.0384	493.9686
Red. masses --	6.1627	2.6332	8.7446
Frc consts --	0.7780	0.3635	1.2571
IR Inten --	6.4673	43.7490	17.0474
	13	14	15
	A	A	A
Frequencies --	511.9736	625.5322	729.0278
Red. masses --	6.6488	1.4692	5.7357
Frc consts --	1.0268	0.3387	1.7961
IR Inten --	27.7407	125.9605	23.6049
	16	17	18
	A	A	A
Frequencies --	836.7147	847.7005	949.0723
Red. masses --	1.4942	2.6987	2.3425
Frc consts --	0.6163	1.1426	1.2431
IR Inten --	141.9754	142.1205	46.2923
	19	20	21
	A	A	A
Frequencies --	998.3758	1002.6525	1015.9708
Red. masses --	1.4814	1.3390	1.5882
Frc consts --	0.8700	0.7931	0.9659
IR Inten --	95.6033	7.2510	27.1386
	22	23	24
	A	A	A
Frequencies --	1098.4267	1117.9453	1154.4671
Red. masses --	1.2844	8.3487	4.2587
Frc consts --	0.9130	6.1477	3.3442
IR Inten --	76.1012	159.5674	171.2474
	25	26	27
	A	A	A

Frequencies --	1260.8981	1292.0454	1367.0026
Red. masses --	1.3308	4.2425	1.1603
Frc consts --	1.2466	4.1728	1.2775
IR Inten --	34.5764	311.1846	114.6161

	28	29	30
	A	A	A
Frequencies --	1385.1942	1404.8108	1468.7807
Red. masses --	1.2090	1.1835	1.0509
Frc consts --	1.3668	1.3761	1.3358
IR Inten --	18.7450	51.5520	8.3131

	31	32	33
	A	A	A
Frequencies --	1471.9921	1477.0600	1496.9324
Red. masses --	1.1784	1.0433	1.1656
Frc consts --	1.5044	1.3411	1.5389
IR Inten --	12.0109	4.8392	51.7209

	34	35	36
	A	A	A
Frequencies --	1557.4167	2946.0578	3082.1865
Red. masses --	1.1000	1.0741	1.0563
Frc consts --	1.5721	5.4926	5.9125
IR Inten --	3.4602	1580.6380	36.2487

	37	38	39
	A	A	A
Frequencies --	3099.9101	3150.7848	3215.7685
Red. masses --	1.0297	1.1147	1.1062
Frc consts --	5.8301	6.5199	6.7401
IR Inten --	0.0035	36.1285	0.6051

	40	41	42
	A	A	A
Frequencies --	3221.9614	3576.4384	3736.7963
Red. masses --	1.1076	1.0670	1.0658
Frc consts --	6.7747	8.0408	8.7682
IR Inten --	0.3899	552.2782	62.7726

GL-SA-W:

	1	2	3
	A	A	A
Frequencies --	65.3576	88.2929	91.2510
Red. masses --	8.5958	5.4654	9.2927
Frc consts --	0.0216	0.0251	0.0456
IR Inten --	2.2118	3.6462	6.1051

	4	5	6
	A	A	A
Frequencies --	108.2175	124.6867	166.2608

Red. masses --	8.5752	8.4202	6.0343
Frc consts --	0.0592	0.0771	0.0983
IR Inten --	4.6050	1.9102	5.6749

	7	8	9
	A	A	A
Frequencies --	193.8176	339.3778	354.8473
Red. masses --	6.1956	2.9392	5.6230
Frc consts --	0.1371	0.1995	0.4172
IR Inten --	24.9521	18.8748	4.6514

	10	11	12
	A	A	A
Frequencies --	390.4703	413.0316	469.5301
Red. masses --	6.2261	3.3423	1.6163
Frc consts --	0.5593	0.3359	0.2099
IR Inten --	5.1299	3.4510	67.6571

	13	14	15
	A	A	A
Frequencies --	510.0719	531.1185	540.8308
Red. masses --	5.5165	7.6017	12.7988
Frc consts --	0.8456	1.2634	2.2057
IR Inten --	22.7165	57.3264	36.3163

	16	17	18
	A	A	A
Frequencies --	551.2906	621.6431	740.2431
Red. masses --	6.3228	1.2058	1.6902
Frc consts --	1.1322	0.2745	0.5457
IR Inten --	19.1107	87.5460	71.6469

	19	20	21
	A	A	A
Frequencies --	746.8000	778.6734	845.0555
Red. masses --	1.9634	7.1206	3.3001
Frc consts --	0.6451	2.5438	1.3885
IR Inten --	109.2321	106.0505	122.0667

	22	23	24
	A	A	A
Frequencies --	879.1860	948.2465	1018.9137
Red. masses --	7.7332	1.1072	1.9846
Frc consts --	3.5219	0.5866	1.2140
IR Inten --	212.5518	97.2172	62.4634

	25	26	27
	A	A	A
Frequencies --	1090.5200	1131.5816	1153.7384
Red. masses --	4.3618	4.7017	4.6794
Frc consts --	3.0562	3.5471	3.6699

IR Inten -- 15.5309 53.9021 358.4851

	28	29	30
	A	A	A
Frequencies --	1174.4865	1267.7969	1325.8532
Red. masses --	1.4133	1.3334	1.1108
Frc consts --	1.1486	1.2628	1.1505
IR Inten --	63.0652	77.4260	18.2882

	31	32	33
	A	A	A
Frequencies --	1349.3242	1400.9304	1422.9381
Red. masses --	3.6670	1.1828	1.1763
Frc consts --	3.9336	1.3677	1.4033
IR Inten --	274.6390	17.9177	14.4790

	34	35	36
	A	A	A
Frequencies --	1473.4172	1514.2505	1786.0077
Red. masses --	1.2193	1.5307	10.2044
Frc consts --	1.5596	2.0679	19.1780
IR Inten --	172.6453	49.4177	83.6634

	37	38	39
	A	A	A
Frequencies --	2985.5977	3035.9797	3092.9752
Red. masses --	1.0767	1.0897	1.0858
Frc consts --	5.6545	5.9177	6.1200
IR Inten --	1786.4034	32.6505	17.0489

	40	41	42
	A	A	A
Frequencies --	3614.6262	3622.6880	3711.8682
Red. masses --	1.0663	1.0651	1.0661
Frc consts --	8.2081	8.2356	8.6542
IR Inten --	625.8090	28.3855	129.7650

GL-MSA-W:

	1	2	3
	A	A	A
Frequencies --	58.2610	83.0343	87.3513
Red. masses --	7.6917	5.9897	7.7157
Frc consts --	0.0154	0.0243	0.0347
IR Inten --	2.0148	1.8121	3.4994

	4	5	6
	A	A	A
Frequencies --	103.4144	121.9797	148.5392
Red. masses --	7.4543	5.9969	6.0884
Frc consts --	0.0470	0.0526	0.0791
IR Inten --	6.4137	7.0203	18.2244

	7	8	9
	A	A	A
Frequencies --	175.0516	228.5132	320.0336
Red. masses --	3.6718	1.0501	4.0264
Frc consts --	0.0663	0.0323	0.2430
IR Inten --	6.5033	0.6974	8.2777
	10	11	12
	A	A	A
Frequencies --	325.7964	352.4932	409.6528
Red. masses --	4.2589	3.9367	3.2362
Frc consts --	0.2663	0.2882	0.3200
IR Inten --	9.5937	4.9696	3.8916
	13	14	15
	A	A	A
Frequencies --	461.8648	491.7236	509.9108
Red. masses --	6.7058	7.6522	3.9609
Frc consts --	0.8428	1.0901	0.6068
IR Inten --	10.4374	33.8699	47.6854
	16	17	18
	A	A	A
Frequencies --	524.9688	557.9892	728.4824
Red. masses --	1.9001	3.3337	5.3845
Frc consts --	0.3085	0.6115	1.6836
IR Inten --	33.2969	61.2112	27.0894
	19	20	21
	A	A	A
Frequencies --	749.6714	825.7369	832.9213
Red. masses --	3.5825	1.3122	4.2482
Frc consts --	1.1862	0.5272	1.7365
IR Inten --	50.0689	54.8371	141.8607
	22	23	24
	A	A	A
Frequencies --	859.4784	913.7375	1002.7237
Red. masses --	2.5279	1.1312	1.3649
Frc consts --	1.1002	0.5565	0.8085
IR Inten --	133.6675	94.8855	2.8612
	25	26	27
	A	A	A
Frequencies --	1013.4716	1024.3246	1091.4459
Red. masses --	1.5294	1.8182	5.4226
Frc consts --	0.9255	1.1240	3.8059
IR Inten --	24.6616	55.4817	14.5884
	28	29	30
	A	A	A

Frequencies --	1115.6983	1142.3637	1279.0384
Red. masses --	4.3103	5.5523	1.6879
Frc consts --	3.1612	4.2691	1.6269
IR Inten --	144.3660	200.6582	94.3017

	31	32	33
	A	A	A
Frequencies --	1292.3314	1330.8984	1359.5756
Red. masses --	3.7989	1.1419	1.1466
Frc consts --	3.7382	1.1917	1.2488
IR Inten --	200.4484	89.1502	96.9129

	34	35	36
	A	A	A
Frequencies --	1393.9271	1405.9947	1445.7973
Red. masses --	1.2184	1.1870	1.1209
Frc consts --	1.3949	1.3825	1.3805
IR Inten --	28.5595	10.5814	51.8021

	37	38	39
	A	A	A
Frequencies --	1468.8700	1476.0270	1512.8414
Red. masses --	1.0466	1.0433	1.5030
Frc consts --	1.3305	1.3392	2.0267
IR Inten --	3.9883	5.9943	48.4620

	40	41	42
	A	A	A
Frequencies --	1789.4499	3020.0696	3083.2826
Red. masses --	10.2623	1.0893	1.0807
Frc consts --	19.3612	5.8538	6.0531
IR Inten --	89.2324	76.8444	425.4197

	43	44	45
	A	A	A
Frequencies --	3096.6657	3099.7513	3214.7362
Red. masses --	1.0757	1.0316	1.1062
Frc consts --	6.0777	5.8398	6.7357
IR Inten --	1109.9266	46.5958	0.7458

	46	47	48
	A	A	A
Frequencies --	3222.1665	3548.2620	3677.7418
Red. masses --	1.1077	1.0670	1.0651
Frc consts --	6.7757	7.9152	8.4881
IR Inten --	0.4045	790.9470	82.7905

MG-SA-W:

	1	2	3
	A	A	A
Frequencies --	58.6410	72.9235	91.5468

Red. masses --	4.7875	6.6125	8.1451
Frc consts --	0.0097	0.0207	0.0402
IR Inten --	1.3364	3.3855	5.0876
	4	5	6
	A	A	A
Frequencies --	101.9191	108.2777	138.1833
Red. masses --	7.5326	5.5801	5.1547
Frc consts --	0.0461	0.0385	0.0580
IR Inten --	1.6655	4.6449	0.5205
	7	8	9
	A	A	A
Frequencies --	162.1962	187.3190	291.3487
Red. masses --	1.2225	9.7009	4.1907
Frc consts --	0.0189	0.2006	0.2096
IR Inten --	0.3163	31.8086	0.7188
	10	11	12
	A	A	A
Frequencies --	337.9974	345.8072	389.6197
Red. masses --	2.9813	3.6767	6.5052
Frc consts --	0.2007	0.2590	0.5818
IR Inten --	18.6315	3.7352	5.3788
	13	14	15
	A	A	A
Frequencies --	426.4982	468.6293	509.2649
Red. masses --	4.2516	1.6425	5.7981
Frc consts --	0.4557	0.2125	0.8860
IR Inten --	1.8632	69.5749	18.3994
	16	17	18
	A	A	A
Frequencies --	531.8634	538.0746	543.0943
Red. masses --	8.6132	7.2191	7.4631
Frc consts --	1.4355	1.2315	1.2969
IR Inten --	42.7268	46.1500	18.1487
	19	20	21
	A	A	A
Frequencies --	586.7823	659.4907	681.6127
Red. masses --	3.8669	2.1059	1.5001
Frc consts --	0.7845	0.5396	0.4106
IR Inten --	21.1851	22.5014	80.2222
	22	23	24
	A	A	A
Frequencies --	739.5389	777.9327	819.5565
Red. masses --	1.1959	7.3162	2.4632
Frc consts --	0.3854	2.6087	0.9748

IR Inten --	150.8310	109.9728	19.9145
	25	26	27
	A	A	A
Frequencies --	877.3149	964.5150	982.7969
Red. masses --	11.9417	1.1154	2.2575
Frc consts --	5.4153	0.6113	1.2847
IR Inten --	262.0559	91.5271	40.7385
	28	29	30
	A	A	A
Frequencies --	1046.4161	1067.9144	1126.9524
Red. masses --	1.8253	3.9561	6.4289
Frc consts --	1.1776	2.6582	4.8106
IR Inten --	26.2163	81.3190	42.5282
	31	32	33
	A	A	A
Frequencies --	1152.2849	1174.6775	1223.2621
Red. masses --	5.1255	1.4000	1.5920
Frc consts --	4.0097	1.1382	1.4036
IR Inten --	370.1318	63.2110	7.8744
	34	35	36
	A	A	A
Frequencies --	1277.7779	1330.4815	1349.2557
Red. masses --	1.6863	1.1158	3.8959
Frc consts --	1.6221	1.1638	4.1787
IR Inten --	152.5776	14.2740	263.3392
	37	38	39
	A	A	A
Frequencies --	1409.7415	1420.1597	1476.2899
Red. masses --	1.3243	1.1794	1.2121
Frc consts --	1.5506	1.4015	1.5565
IR Inten --	39.5119	13.6749	162.7561
	40	41	42
	A	A	A
Frequencies --	1486.8366	1489.2082	1519.9349
Red. masses --	1.0632	1.0550	1.5344
Frc consts --	1.3848	1.3785	2.0886
IR Inten --	22.9012	19.9750	49.5888
	43	44	45
	A	A	A
Frequencies --	1781.9977	2936.5546	3068.2821
Red. masses --	10.4480	1.0776	1.0368
Frc consts --	19.5477	5.4749	5.7508
IR Inten --	91.6076	1963.7295	0.4221
	46	47	48

	A	A	A
Frequencies --	3088.2699	3148.3307	3196.8286
Red. masses --	1.0849	1.0981	1.1044
Frc consts --	6.0962	6.4132	6.6501
IR Inten --	16.5598	1.9613	4.0183
	49	50	51
	A	A	A
Frequencies --	3560.4191	3613.3177	3713.1027
Red. masses --	1.0646	1.0665	1.0661
Frc consts --	7.9516	8.2037	8.6599
IR Inten --	163.5490	550.7053	128.8614

MG-MSA-W:

	1	2	3
	A	A	A
Frequencies --	55.5941	70.0381	85.1823
Red. masses --	4.9627	5.4283	7.4400
Frc consts --	0.0090	0.0157	0.0318
IR Inten --	1.6181	1.2092	3.6202
	4	5	6
	A	A	A
Frequencies --	92.0456	107.2856	137.9170
Red. masses --	6.3853	5.5250	4.6957
Frc consts --	0.0319	0.0375	0.0526
IR Inten --	3.3650	5.4861	1.1340
	7	8	9
	A	A	A
Frequencies --	151.2541	158.5515	229.5896
Red. masses --	5.2386	1.1843	1.0538
Frc consts --	0.0706	0.0175	0.0327
IR Inten --	24.1336	1.0088	0.7116
	10	11	12
	A	A	A
Frequencies --	286.1927	322.7572	337.5574
Red. masses --	3.8865	4.1998	3.8123
Frc consts --	0.1876	0.2578	0.2559
IR Inten --	1.3503	3.0598	4.7270
	13	14	15
	A	A	A
Frequencies --	346.3401	411.5695	460.8506
Red. masses --	4.7740	3.3159	7.0430
Frc consts --	0.3374	0.3309	0.8813
IR Inten --	16.0011	2.2227	8.7760
	16	17	18
	A	A	A

Frequencies --	492.7088	513.4034	540.7971
Red. masses --	8.5889	6.5722	4.5300
Frc consts --	1.2285	1.0207	0.7806
IR Inten --	25.0781	44.4535	6.8313

	19	20	21
	A	A	A
Frequencies --	587.6922	592.7637	669.8724
Red. masses --	2.0503	1.7613	3.5214
Frc consts --	0.4172	0.3646	0.9310
IR Inten --	24.5375	83.5129	22.9798

	22	23	24
	A	A	A
Frequencies --	730.4992	812.1649	827.7891
Red. masses --	5.2675	1.8515	1.5749
Frc consts --	1.6561	0.7196	0.6358
IR Inten --	36.0799	25.7906	77.0079

	25	26	27
	A	A	A
Frequencies --	849.5105	911.8733	982.8129
Red. masses --	3.5283	1.1286	2.1728
Frc consts --	1.5002	0.5529	1.2365
IR Inten --	185.5190	92.3001	44.0364

	28	29	30
	A	A	A
Frequencies --	1002.4909	1015.8179	1046.6552
Red. masses --	1.3689	1.4295	1.8463
Frc consts --	0.8105	0.8691	1.1917
IR Inten --	3.5348	23.0972	20.4636

	31	32	33
	A	A	A
Frequencies --	1076.3209	1109.8318	1138.6310
Red. masses --	4.3938	6.7482	6.5977
Frc consts --	2.9990	4.8972	5.0397
IR Inten --	52.5509	159.7531	213.4110

	34	35	36
	A	A	A
Frequencies --	1219.0547	1282.3367	1295.8747
Red. masses --	1.6617	2.6983	2.8600
Frc consts --	1.4550	2.6143	2.8298
IR Inten --	14.6737	213.9214	133.6390

	37	38	39
	A	A	A
Frequencies --	1336.3971	1369.4369	1394.9151
Red. masses --	1.1293	1.1487	1.2067

Frc consts --	1.1883	1.2692	1.3834
IR Inten --	71.2560	75.9926	32.6955

	40	41	42
	A	A	A
Frequencies --	1408.7137	1440.9627	1469.2603
Red. masses --	1.3632	1.1166	1.0467
Frc consts --	1.5939	1.3660	1.3313
IR Inten --	56.4367	48.9693	4.0507

	43	44	45
	A	A	A
Frequencies --	1475.9874	1488.1210	1489.4655
Red. masses --	1.0434	1.0619	1.0521
Frc consts --	1.3393	1.3855	1.3753
IR Inten --	5.8746	19.6020	14.5806

	46	47	48
	A	A	A
Frequencies --	1519.7981	1783.6674	3054.5964
Red. masses --	1.5193	10.5673	1.0734
Frc consts --	2.0676	19.8081	5.9011
IR Inten --	45.6106	95.2994	1730.6234

	49	50	51
	A	A	A
Frequencies --	3067.2852	3082.5962	3099.4850
Red. masses --	1.0372	1.0846	1.0298
Frc consts --	5.7492	6.0724	5.8287
IR Inten --	1.1504	70.7610	0.2661

	52	53	54
	A	A	A
Frequencies --	3147.9513	3195.5205	3214.4340
Red. masses --	1.0981	1.1044	1.1062
Frc consts --	6.4114	6.6445	6.7344
IR Inten --	2.4384	4.6476	0.5560

	55	56	57
	A	A	A
Frequencies --	3221.9994	3550.3413	3614.2839
Red. masses --	1.1076	1.0672	1.0646
Frc consts --	6.7748	7.9260	8.1940
IR Inten --	0.3110	840.1364	97.7226

FA-SA-A:

	1	2	3
	A	A	A
Frequencies --	83.3261	95.1607	130.5600
Red. masses --	8.3188	5.1504	8.4205
Frc consts --	0.0340	0.0275	0.0846

IR Inten --	4.9521	13.9004	5.2420
	4	5	6
	A	A	A
Frequencies --	190.2245	222.4035	282.1812
Red. masses --	2.8107	4.7346	3.3575
Frc consts --	0.0599	0.1380	0.1575
IR Inten --	9.6611	15.9390	86.5587
	7	8	9
	A	A	A
Frequencies --	337.9498	384.1974	424.1416
Red. masses --	1.6243	8.7594	1.6043
Frc consts --	0.1093	0.7618	0.1700
IR Inten --	125.3178	2.7284	10.7877
	10	11	12
	A	A	A
Frequencies --	453.4678	511.7129	539.3924
Red. masses --	2.4967	1.8553	9.8823
Frc consts --	0.3025	0.2862	1.6940
IR Inten --	29.4542	23.8085	20.2861
	13	14	15
	A	A	A
Frequencies --	565.2870	584.1442	749.5052
Red. masses --	9.3553	11.8344	16.9561
Frc consts --	1.7613	2.3792	5.6121
IR Inten --	35.9111	90.4202	224.2720
	16	17	18
	A	A	A
Frequencies --	834.6838	953.9305	965.0826
Red. masses --	3.1370	1.0895	1.1041
Frc consts --	1.2877	0.5841	0.6059
IR Inten --	10.5852	93.4200	26.3668
	19	20	21
	A	A	A
Frequencies --	987.4969	1068.5363	1087.3967
Red. masses --	11.8891	4.4306	2.2926
Frc consts --	6.8308	2.9805	1.5972
IR Inten --	348.4544	134.6868	234.5396
	22	23	24
	A	A	A
Frequencies --	1160.2083	1185.4366	1245.1888
Red. masses --	1.3868	1.2937	2.8181
Frc consts --	1.0998	1.0711	2.5744
IR Inten --	127.6783	30.6339	98.0831
	25	26	27

	A	A	A
Frequencies --	1286.1674	1346.0626	1457.1826
Red. masses --	6.2723	1.1320	1.2050
Frc consts --	6.1132	1.2085	1.5075
IR Inten --	526.1407	9.4293	22.0143
	28	29	30
	A	A	A
Frequencies --	1527.0273	1548.8351	1576.2254
Red. masses --	1.1836	1.1039	1.1349
Frc consts --	1.6262	1.5602	1.6612
IR Inten --	49.4801	16.3887	92.9947
	31	32	33
	A	A	A
Frequencies --	1656.3740	1708.8092	2206.8788
Red. masses --	1.0339	1.0460	1.1359
Frc consts --	1.6712	1.7995	3.2593
IR Inten --	8.7842	25.4038	2310.3511
	34	35	36
	A	A	A
Frequencies --	3093.0096	3168.4355	3292.1608
Red. masses --	1.0566	1.1150	1.0685
Frc consts --	5.9554	6.5951	6.8231
IR Inten --	54.1760	25.8676	1047.0706
	37	38	39
	A	A	A
Frequencies --	3464.1402	3556.0694	3735.4882
Red. masses --	1.0513	1.0940	1.0660
Frc consts --	7.4333	8.1509	8.7638
IR Inten --	48.2204	55.9559	103.1558

FA-MSA-A:

	1	2	3
	A	A	A
Frequencies --	62.0068	89.4747	94.2218
Red. masses --	4.4752	6.2006	4.8753
Frc consts --	0.0101	0.0292	0.0255
IR Inten --	243.7355	5.1550	13.5188
	4	5	6
	A	A	A
Frequencies --	139.2588	207.5282	230.2916
Red. masses --	5.4239	3.3936	1.0789
Frc consts --	0.0620	0.0861	0.0337
IR Inten --	5.0263	48.0120	7.2236
	7	8	9
	A	A	A

Frequencies --	235.0752	297.7503	328.9279
Red. masses --	2.1632	3.3782	4.2953
Frc consts --	0.0704	0.1765	0.2738
IR Inten --	132.1891	32.0831	19.4921

	10	11	12
	A	A	A
Frequencies --	411.7616	471.8895	498.2108
Red. masses --	1.4539	6.5754	10.0698
Frc consts --	0.1452	0.8627	1.4726
IR Inten --	7.4917	11.3585	14.0584

	13	14	15
	A	A	A
Frequencies --	515.3962	540.5786	747.9898
Red. masses --	5.7118	2.3778	6.4579
Frc consts --	0.8939	0.4094	2.1288
IR Inten --	14.5806	0.2588	31.2855

	16	17	18
	A	A	A
Frequencies --	770.6552	887.1085	933.7904
Red. masses --	1.0765	8.0756	2.6100
Frc consts --	0.3767	3.7444	1.3409
IR Inten --	92.0334	279.6448	33.5144

	19	20	21
	A	A	A
Frequencies --	990.8368	999.0141	1002.9191
Red. masses --	1.1889	1.3570	1.4186
Frc consts --	0.6877	0.7979	0.8407
IR Inten --	43.1361	3.2146	144.5940

	22	23	24
	A	A	A
Frequencies --	1057.2923	1105.1776	1170.0610
Red. masses --	3.0542	4.6634	1.7008
Frc consts --	2.0116	3.3559	1.3719
IR Inten --	42.8827	222.9834	83.3060

	25	26	27
	A	A	A
Frequencies --	1223.5905	1263.2206	1325.0891
Red. masses --	1.9287	5.3154	1.1241
Frc consts --	1.7013	4.9974	1.1629
IR Inten --	10.3257	270.0370	102.7649

	28	29	30
	A	A	A
Frequencies --	1356.4142	1384.6142	1456.5797
Red. masses --	1.1172	1.2212	1.1983

Frc consts --	1.2111	1.3794	1.4979
IR Inten --	53.3499	0.7747	330.3280
	31	32	33
	A	A	A
Frequencies --	1469.1550	1476.7363	1507.9453
Red. masses --	1.0457	1.0499	1.1621
Frc consts --	1.3298	1.3489	1.5570
IR Inten --	5.3415	5.8577	70.3243
	34	35	36
	A	A	A
Frequencies --	1560.0787	1571.4310	1608.2159
Red. masses --	1.1140	1.1482	1.0694
Frc consts --	1.5974	1.6705	1.6296
IR Inten --	122.3999	618.8465	13.1544
	37	38	39
	A	A	A
Frequencies --	1671.3195	3063.0430	3098.4323
Red. masses --	1.1403	1.0569	1.0298
Frc consts --	1.8767	5.8423	5.8251
IR Inten --	2456.3200	37.2993	0.1269
	40	41	42
	A	A	A
Frequencies --	3124.0857	3213.3829	3219.7450
Red. masses --	1.1131	1.1062	1.1074
Frc consts --	6.4008	6.7296	6.7637
IR Inten --	27.7042	0.0967	0.0411
	43	44	45
	A	A	A
Frequencies --	3477.4044	3547.5218	3576.9038
Red. masses --	1.0503	1.0679	1.0931
Frc consts --	7.4831	7.9184	8.2402
IR Inten --	6.1996	551.1431	21.1435

GL-SA-A:

	1	2	3
	A	A	A
Frequencies --	60.9586	82.2504	100.7675
Red. masses --	9.2261	5.7552	9.2497
Frc consts --	0.0202	0.0229	0.0553
IR Inten --	8.9775	8.5675	3.7722
	4	5	6
	A	A	A
Frequencies --	120.8008	136.2753	187.0987
Red. masses --	4.2042	4.4834	6.7525
Frc consts --	0.0361	0.0491	0.1393

IR Inten -- 7.9493 8.6292 15.9558

	7	8	9
	A	A	A
Frequencies --	223.1336	310.6429	343.5694
Red. masses --	8.4315	3.9308	2.1267
Frc consts --	0.2473	0.2235	0.1479
IR Inten --	19.5061	107.9178	67.0292

	10	11	12
	A	A	A
Frequencies --	394.8686	411.3334	432.1506
Red. masses --	2.7601	2.1165	2.4220
Frc consts --	0.2536	0.2110	0.2665
IR Inten --	11.4070	2.6031	36.7022

	13	14	15
	A	A	A
Frequencies --	454.2516	493.5872	532.7402
Red. masses --	1.8202	2.7108	8.7812
Frc consts --	0.2213	0.3891	1.4684
IR Inten --	48.5192	3.3624	6.0559

	16	17	18
	A	A	A
Frequencies --	563.0624	574.3825	650.4490
Red. masses --	12.5760	13.4027	3.7911
Frc consts --	2.3491	2.6052	0.9450
IR Inten --	22.1834	121.5131	5.6370

	19	20	21
	A	A	A
Frequencies --	715.2335	788.4885	951.2618
Red. masses --	15.2666	3.3856	1.1093
Frc consts --	4.6014	1.2402	0.5914
IR Inten --	226.9004	9.0557	63.7728

	22	23	24
	A	A	A
Frequencies --	975.9918	987.9526	1045.1350
Red. masses --	1.6899	9.6451	1.9345
Frc consts --	0.9484	5.5467	1.2450
IR Inten --	3.2144	200.5925	90.2199

	25	26	27
	A	A	A
Frequencies --	1075.2552	1122.2500	1155.9227
Red. masses --	4.0868	2.8990	1.3343
Frc consts --	2.7839	2.1512	1.0504
IR Inten --	88.6676	172.8589	52.0467

	28	29	30

	A	A	A
Frequencies --	1167.6510	1256.8099	1294.1706
Red. masses --	1.5510	2.0707	7.1669
Frc consts --	1.2459	1.9271	7.0724
IR Inten --	136.6092	92.5223	557.4862
	31	32	33
	A	A	A
Frequencies --	1374.2360	1395.3669	1427.9183
Red. masses --	1.2745	1.2784	1.2271
Frc consts --	1.4181	1.4665	1.4742
IR Inten --	36.2542	11.2614	47.5032
	34	35	36
	A	A	A
Frequencies --	1537.4630	1569.4187	1645.0587
Red. masses --	1.2480	1.1902	1.0669
Frc consts --	1.7380	1.7272	1.7012
IR Inten --	55.0579	122.5237	29.5076
	37	38	39
	A	A	A
Frequencies --	1691.2321	1787.9224	2420.9399
Red. masses --	1.0447	9.2284	1.1116
Frc consts --	1.7606	17.3810	3.8387
IR Inten --	27.1550	77.1045	1841.6059
	40	41	42
	A	A	A
Frequencies --	3029.1473	3063.1994	3198.3738
Red. masses --	1.0901	1.0847	1.0699
Frc consts --	5.8931	5.9969	6.4482
IR Inten --	34.1345	35.8280	1298.2449
	43	44	45
	A	A	A
Frequencies --	3454.8395	3539.1057	3733.7115
Red. masses --	1.0525	1.0927	1.0660
Frc consts --	7.4019	8.0638	8.7557
IR Inten --	71.8906	71.8125	98.0686

GL-MSA-A:

	1	2	3
	A	A	A
Frequencies --	81.1860	94.6272	114.5327
Red. masses --	6.0981	9.3228	6.7535
Frc consts --	0.0237	0.0492	0.0522
IR Inten --	2.9700	1.7946	2.5795
	4	5	6
	A	A	A

Frequencies --	146.9108	155.7127	198.3768
Red. masses --	6.3389	5.4854	3.4068
Frc consts --	0.0806	0.0784	0.0790
IR Inten --	4.4295	14.2517	16.6389
	7	8	9
	A	A	A
Frequencies --	237.8701	260.1784	281.7108
Red. masses --	2.6900	1.2448	3.1087
Frc consts --	0.0897	0.0496	0.1454
IR Inten --	55.7165	10.5232	17.2264
	10	11	12
	A	A	A
Frequencies --	310.2288	338.7952	381.6710
Red. masses --	4.0403	4.1424	2.1996
Frc consts --	0.2291	0.2801	0.1888
IR Inten --	0.0714	4.1184	7.8530
	13	14	15
	A	A	A
Frequencies --	454.3187	474.4496	498.1736
Red. masses --	3.1321	2.9856	8.0658
Frc consts --	0.3809	0.3960	1.1794
IR Inten --	19.1219	7.7464	26.3802
	16	17	18
	A	A	A
Frequencies --	515.1738	568.1993	628.2416
Red. masses --	7.2939	2.7212	3.2866
Frc consts --	1.1406	0.5176	0.7643
IR Inten --	41.7850	5.6328	9.7759
	19	20	21
	A	A	A
Frequencies --	742.0296	805.1135	827.9429
Red. masses --	6.2747	1.2676	2.5519
Frc consts --	2.0356	0.4841	1.0307
IR Inten --	23.8037	64.7156	17.1472
	22	23	24
	A	A	A
Frequencies --	881.9906	992.0550	1003.4264
Red. masses --	5.7639	1.3019	1.4318
Frc consts --	2.6417	0.7549	0.8494
IR Inten --	239.2129	54.0302	15.3865
	25	26	27
	A	A	A
Frequencies --	1017.2805	1034.8129	1080.4054
Red. masses --	1.3923	1.8323	4.0212

Frc consts --	0.8489	1.1560	2.7655
IR Inten --	19.7666	16.6120	91.4943
	28	29	30
	A	A	A
Frequencies --	1113.7719	1142.6819	1197.8661
Red. masses --	3.5477	1.9342	1.6155
Frc consts --	2.5929	1.4880	1.3658
IR Inten --	152.4375	36.4600	188.7148
	31	32	33
	A	A	A
Frequencies --	1256.7746	1295.9270	1350.6306
Red. masses --	1.1408	10.1350	1.3002
Frc consts --	1.0617	10.0284	1.3974
IR Inten --	4.6596	399.9027	3.0277
	34	35	36
	A	A	A
Frequencies --	1389.2358	1391.4076	1415.6352
Red. masses --	1.3417	1.2796	1.3293
Frc consts --	1.5257	1.4596	1.5696
IR Inten --	9.7862	11.7667	2.2732
	37	38	39
	A	A	A
Frequencies --	1472.6116	1476.4293	1495.6673
Red. masses --	1.0435	1.0449	1.1549
Frc consts --	1.3333	1.3420	1.5222
IR Inten --	3.9817	5.3092	67.7680
	40	41	42
	A	A	A
Frequencies --	1523.3341	1602.0216	1780.5591
Red. masses --	1.1345	1.1073	9.7291
Frc consts --	1.5511	1.6744	18.1735
IR Inten --	53.1286	64.8564	72.9957
	43	44	45
	A	A	A
Frequencies --	2268.5448	3014.5157	3032.4833
Red. masses --	1.1080	1.0890	1.0832
Frc consts --	3.3595	5.8306	5.8686
IR Inten --	2751.2969	40.0656	35.8564
	46	47	48
	A	A	A
Frequencies --	3092.5191	3207.4237	3213.8883
Red. masses --	1.0298	1.1062	1.1073
Frc consts --	5.8025	6.7047	6.7387
IR Inten --	1.2480	0.9804	0.8611

	49	50	51
	A	A	A
Frequencies --	3493.3707	3551.3519	3597.2061
Red. masses --	1.0501	1.0665	1.0935
Frc consts --	7.5501	7.9252	8.3371
IR Inten --	9.5487	485.1055	28.6112

MG-SA-A:

	1	2	3
	A	A	A
Frequencies --	61.3704	70.6864	83.0646
Red. masses --	5.4339	5.6062	6.3155
Frc consts --	0.0121	0.0165	0.0257
IR Inten --	5.2764	4.1253	9.1554

	4	5	6
	A	A	A
Frequencies --	100.9995	122.9125	173.4726
Red. masses --	9.3529	5.2344	3.4469
Frc consts --	0.0562	0.0466	0.0611
IR Inten --	3.0499	9.2534	6.0832

	7	8	9
	A	A	A
Frequencies --	182.3142	215.9025	277.1788
Red. masses --	1.2394	9.6125	3.6442
Frc consts --	0.0243	0.2640	0.1650
IR Inten --	0.8582	45.0918	36.2352

	10	11	12
	A	A	A
Frequencies --	335.5614	374.3352	391.8845
Red. masses --	2.2637	3.0429	2.3400
Frc consts --	0.1502	0.2512	0.2117
IR Inten --	14.3105	113.8123	3.5719

	13	14	15
	A	A	A
Frequencies --	400.6965	419.9260	451.7221
Red. masses --	2.2298	2.2607	1.8826
Frc consts --	0.2109	0.2349	0.2263
IR Inten --	9.7771	18.9934	41.8114

	16	17	18
	A	A	A
Frequencies --	474.9990	531.4257	549.1480
Red. masses --	3.1557	9.3987	5.5522
Frc consts --	0.4195	1.5639	0.9865
IR Inten --	5.4445	5.8885	10.1081

	19	20	21

	A	A	A
Frequencies --	568.2918	572.3910	636.7675
Red. masses --	9.1309	13.3548	2.9320
Frc consts --	1.7374	2.5779	0.7004
IR Inten --	17.2676	119.5944	6.5902
	22	23	24
	A	A	A
Frequencies --	713.7190	784.9704	895.9600
Red. masses --	16.6691	2.6288	3.1386
Frc consts --	5.0028	0.9544	1.4845
IR Inten --	226.4842	9.3191	3.1966
	25	26	27
	A	A	A
Frequencies --	947.8202	989.4819	1001.6327
Red. masses --	1.0914	9.7916	1.6584
Frc consts --	0.5777	5.6483	0.9803
IR Inten --	58.9208	168.3734	21.4115
	28	29	30
	A	A	A
Frequencies --	1040.8531	1075.2429	1113.2204
Red. masses --	1.6411	3.3480	2.7138
Frc consts --	1.0475	2.2806	1.9815
IR Inten --	25.8412	51.1214	273.8464
	31	32	33
	A	A	A
Frequencies --	1151.5467	1163.2231	1226.0887
Red. masses --	1.3520	1.5358	2.8825
Frc consts --	1.0563	1.2244	2.5530
IR Inten --	68.2556	128.7904	120.3118
	34	35	36
	A	A	A
Frequencies --	1271.8818	1292.4141	1377.5890
Red. masses --	1.9702	6.8394	1.4110
Frc consts --	1.8778	6.7309	1.5777
IR Inten --	38.0589	548.7847	34.2633
	37	38	39
	A	A	A
Frequencies --	1410.9232	1423.8705	1480.2714
Red. masses --	1.3053	1.2759	1.0556
Frc consts --	1.5310	1.5240	1.3628
IR Inten --	62.3746	11.0417	25.3456
	40	41	42
	A	A	A
Frequencies --	1486.7192	1533.7116	1564.2448

Red. masses --	1.0513	1.2193	1.2272
Frc consts --	1.3691	1.6898	1.7692
IR Inten --	14.9243	75.9888	101.5727
	43	44	45
	A	A	A
Frequencies --	1642.6493	1692.8174	1780.9712
Red. masses --	1.0611	1.0439	9.8237
Frc consts --	1.6870	1.7624	18.3586
IR Inten --	18.1471	23.1348	88.6740
	46	47	48
	A	A	A
Frequencies --	2521.7457	3069.7997	3071.8005
Red. masses --	1.1033	1.0544	1.0659
Frc consts --	4.1337	5.8541	5.9260
IR Inten --	1709.6407	16.2787	23.7236
	49	50	51
	A	A	A
Frequencies --	3148.1515	3193.5690	3201.6896
Red. masses --	1.0975	1.0718	1.1033
Frc consts --	6.4087	6.4406	6.6632
IR Inten --	0.5472	1318.7613	40.7198
	52	53	54
	A	A	A
Frequencies --	3451.7659	3537.2961	3735.7186
Red. masses --	1.0534	1.0919	1.0660
Frc consts --	7.3951	8.0496	8.7652
IR Inten --	78.5463	71.0484	95.8870

FA-SA-MA:

	1	2	3
	A	A	A
Frequencies --	79.2109	84.1892	111.6283
Red. masses --	5.8695	8.3758	5.3771
Frc consts --	0.0217	0.0350	0.0395
IR Inten --	6.5225	1.2494	7.9874
	4	5	6
	A	A	A
Frequencies --	135.0350	179.1524	206.9884
Red. masses --	2.8219	1.9411	1.6055
Frc consts --	0.0303	0.0367	0.0405
IR Inten --	1.8971	1.5789	17.9303
	7	8	9
	A	A	A
Frequencies --	228.3829	275.7475	299.1373
Red. masses --	4.1036	2.6549	2.3545

Frc consts --	0.1261	0.1189	0.1241
IR Inten --	4.5257	19.5362	32.1641
	10	11	12
	A	A	A
Frequencies --	325.9885	385.3354	446.8578
Red. masses --	1.6096	11.3681	2.9331
Frc consts --	0.1008	0.9945	0.3451
IR Inten --	132.7429	4.1772	27.8295
	13	14	15
	A	A	A
Frequencies --	471.7485	539.4237	560.4006
Red. masses --	4.7550	10.2746	12.4933
Frc consts --	0.6235	1.7615	2.3117
IR Inten --	2.2943	25.6347	56.8267
	16	17	18
	A	A	A
Frequencies --	579.3795	747.9665	882.1727
Red. masses --	14.6915	16.8036	3.0739
Frc consts --	2.9057	5.5388	1.4094
IR Inten --	67.7883	229.0203	25.6795
	19	20	21
	A	A	A
Frequencies --	900.9585	940.2912	995.9175
Red. masses --	1.0805	1.0886	13.7299
Frc consts --	0.5168	0.5671	8.0235
IR Inten --	45.8654	96.0093	284.3810
	22	23	24
	A	A	A
Frequencies --	1025.8192	1067.2159	1088.1685
Red. masses --	1.4805	2.5852	4.6986
Frc consts --	0.9179	1.7348	3.2780
IR Inten --	7.5481	64.0035	277.4153
	25	26	27
	A	A	A
Frequencies --	1156.4400	1164.1770	1205.1869
Red. masses --	1.4933	2.2016	1.3116
Frc consts --	1.1767	1.7580	1.1224
IR Inten --	149.4853	52.8212	43.6533
	28	29	30
	A	A	A
Frequencies --	1231.2406	1278.8299	1331.4435
Red. masses --	2.6467	5.9677	1.2457
Frc consts --	2.3639	5.7502	1.3011
IR Inten --	67.3205	497.3263	3.7105

	31	32	33
	A	A	A
Frequencies --	1393.4800	1452.0057	1477.9326
Red. masses --	1.2177	1.1744	1.1816
Frc consts --	1.3931	1.4588	1.5207
IR Inten --	11.0060	24.8481	2.9553

	34	35	36
	A	A	A
Frequencies --	1518.6330	1520.4315	1524.5765
Red. masses --	1.1402	1.0464	1.0577
Frc consts --	1.5493	1.4252	1.4485
IR Inten --	59.9092	8.3095	11.0859

	37	38	39
	A	A	A
Frequencies --	1545.4882	1619.5504	1661.8575
Red. masses --	1.1029	1.1133	1.0605
Frc consts --	1.5520	1.7205	1.7256
IR Inten --	19.2267	22.0064	38.5574

	40	41	42
	A	A	A
Frequencies --	2478.8121	3083.9894	3096.0213
Red. masses --	1.1099	1.0554	1.0324
Frc consts --	4.0181	5.9142	5.8306
IR Inten --	1972.2273	42.9250	8.4739

	43	44	45
	A	A	A
Frequencies --	3158.2782	3198.0492	3209.4837
Red. masses --	1.1147	1.1071	1.1067
Frc consts --	6.5511	6.6715	6.7164
IR Inten --	19.2606	3.2394	1.0475

	46	47	48
	A	A	A
Frequencies --	3310.8663	3508.0777	3750.2967
Red. masses --	1.0683	1.0756	1.0660
Frc consts --	6.8995	7.7991	8.8337
IR Inten --	1012.9790	45.7380	103.2002

FA-MSA-MA:

	1	2	3
	A	A	A
Frequencies --	99.5291	107.5880	126.1285
Red. masses --	6.5351	5.8018	6.4490
Frc consts --	0.0381	0.0396	0.0604
IR Inten --	4.4658	8.9220	9.4212

	4	5	6

	A	A	A
Frequencies --	142.4336	196.2905	225.2957
Red. masses --	3.2316	3.2776	2.4576
Frc consts --	0.0386	0.0744	0.0735
IR Inten --	5.0718	4.1180	13.4615
	7	8	9
	A	A	A
Frequencies --	230.1559	244.1013	275.2832
Red. masses --	1.2815	1.0532	2.5530
Frc consts --	0.0400	0.0370	0.1140
IR Inten --	13.7168	0.1699	38.4508
	10	11	12
	A	A	A
Frequencies --	308.5699	339.9572	364.0447
Red. masses --	2.3396	3.9719	4.5972
Frc consts --	0.1312	0.2705	0.3590
IR Inten --	4.6774	10.5409	31.2398
	13	14	15
	A	A	A
Frequencies --	465.8716	504.5401	509.0289
Red. masses --	4.9947	9.3435	9.4915
Frc consts --	0.6387	1.4014	1.4490
IR Inten --	6.2559	15.2611	16.7824
	16	17	18
	A	A	A
Frequencies --	544.1688	760.9793	862.5638
Red. masses --	6.8515	6.5942	3.1248
Frc consts --	1.1954	2.2499	1.3698
IR Inten --	111.3187	68.8615	33.3078
	19	20	21
	A	A	A
Frequencies --	900.1274	914.8368	978.2104
Red. masses --	1.1274	1.0930	2.1850
Frc consts --	0.5382	0.5390	1.2319
IR Inten --	86.2093	40.5918	125.8032
	22	23	24
	A	A	A
Frequencies --	991.1169	1004.3542	1027.5976
Red. masses --	1.4131	3.3645	1.5253
Frc consts --	0.8178	1.9996	0.9490
IR Inten --	4.9783	174.0657	4.9481
	25	26	27
	A	A	A
Frequencies --	1054.4287	1094.3651	1161.6778

Red. masses --	2.1500	5.7922	3.0954
Frc consts --	1.4084	4.0871	2.4612
IR Inten --	47.1676	301.1758	38.3857
	28	29	30
	A	A	A
Frequencies --	1174.4127	1218.7649	1229.9426
Red. masses --	3.7284	1.4000	2.5470
Frc consts --	3.0298	1.2253	2.2701
IR Inten --	280.0845	8.2245	90.8802
	31	32	33
	A	A	A
Frequencies --	1334.8733	1380.5427	1391.9666
Red. masses --	1.2428	1.2296	1.2013
Frc consts --	1.3047	1.3807	1.3714
IR Inten --	0.2282	8.4775	10.1435
	34	35	36
	A	A	A
Frequencies --	1450.9509	1471.7316	1475.7659
Red. masses --	1.1465	1.0465	1.0484
Frc consts --	1.4221	1.3355	1.3453
IR Inten --	14.5642	3.9277	6.1564
	37	38	39
	A	A	A
Frequencies --	1481.1453	1521.0315	1527.6451
Red. masses --	1.1737	1.0433	1.0853
Frc consts --	1.5171	1.4221	1.4922
IR Inten --	5.2315	6.9191	40.0044
	40	41	42
	A	A	A
Frequencies --	1537.3073	1554.0909	1573.8605
Red. masses --	1.0920	1.0952	1.1493
Frc consts --	1.5205	1.5585	1.6773
IR Inten --	29.0578	33.7107	11.8082
	43	44	45
	A	A	A
Frequencies --	1696.3344	2565.3698	3087.8470
Red. masses --	1.0588	1.1047	1.0424
Frc consts --	1.7951	4.2833	5.8562
IR Inten --	82.1157	1527.5350	8.8298
	46	47	48
	A	A	A
Frequencies --	3090.1299	3094.6161	3164.6115
Red. masses --	1.0449	1.0300	1.1152
Frc consts --	5.8785	5.8117	6.5805

IR Inten --	60.5338	1.7224	12.6226
	49	50	51
	A	A	A
Frequencies --	3195.5964	3203.5314	3209.5362
Red. masses --	1.1076	1.1075	1.1062
Frc consts --	6.6638	6.6964	6.7137
IR Inten --	2.6163	1.9411	0.5227
	52	53	54
	A	A	A
Frequencies --	3211.6795	3292.3571	3503.7058
Red. masses --	1.1066	1.0696	1.0758
Frc consts --	6.7250	6.8313	7.7808
IR Inten --	0.4860	880.8586	44.6537

GL-SA-MA:

	1	2	3
	A	A	A
Frequencies --	65.2753	82.8055	91.7339
Red. masses --	7.8120	6.9382	7.3438
Frc consts --	0.0196	0.0280	0.0364
IR Inten --	9.1324	0.0529	2.4817
	4	5	6
	A	A	A
Frequencies --	104.7361	130.4404	150.0454
Red. masses --	5.1447	3.7256	2.3913
Frc consts --	0.0333	0.0373	0.0317
IR Inten --	6.2227	10.8540	2.5008
	7	8	9
	A	A	A
Frequencies --	182.8207	192.5029	226.1156
Red. masses --	7.0891	1.2850	7.5154
Frc consts --	0.1396	0.0281	0.2264
IR Inten --	12.6979	8.8906	21.4471
	10	11	12
	A	A	A
Frequencies --	289.9912	324.0854	345.6229
Red. masses --	3.2662	2.7475	2.3967
Frc consts --	0.1618	0.1700	0.1687
IR Inten --	5.4257	23.8571	101.7594
	13	14	15
	A	A	A
Frequencies --	402.2580	434.3072	460.0892
Red. masses --	7.8961	3.6587	1.8252
Frc consts --	0.7528	0.4066	0.2276
IR Inten --	5.3506	27.1083	45.2695

	16	17	18
	A	A	A
Frequencies --	530.9376	560.0007	565.0915
Red. masses --	10.1189	10.5197	9.4133
Frc consts --	1.6806	1.9437	1.7710
IR Inten --	13.0724	23.7986	78.1638

	19	20	21
	A	A	A
Frequencies --	586.4812	664.6268	718.7700
Red. masses --	5.4460	3.0949	15.2750
Frc consts --	1.1037	0.8055	4.6495
IR Inten --	41.1547	0.6576	217.6144

	22	23	24
	A	A	A
Frequencies --	751.2969	928.5292	962.8441
Red. masses --	3.5325	1.1940	2.5830
Frc consts --	1.1748	0.6065	1.4109
IR Inten --	18.0197	38.9247	5.6202

	25	26	27
	A	A	A
Frequencies --	982.9676	1010.4937	1052.7916
Red. masses --	4.2489	1.3257	2.4439
Frc consts --	2.4188	0.7975	1.5960
IR Inten --	74.3896	212.6617	14.8897

	28	29	30
	A	A	A
Frequencies --	1063.0057	1097.1059	1140.3468
Red. masses --	3.1213	3.1761	1.7519
Frc consts --	2.0780	2.2524	1.3422
IR Inten --	87.1108	122.7231	83.0177

	31	32	33
	A	A	A
Frequencies --	1171.6601	1204.7472	1240.3491
Red. masses --	1.5784	1.4751	1.9640
Frc consts --	1.2767	1.2614	1.7803
IR Inten --	174.1678	9.0052	67.4354

	34	35	36
	A	A	A
Frequencies --	1289.7940	1347.1797	1379.8100
Red. masses --	6.8925	1.3792	1.2545
Frc consts --	6.7557	1.4748	1.4072
IR Inten --	535.1308	29.4898	5.9030

	37	38	39
	A	A	A

Frequencies --	1397.9850	1427.5977	1481.5810
Red. masses --	1.1880	1.2385	1.1712
Frc consts --	1.3680	1.4872	1.5147
IR Inten --	26.6800	38.3982	0.7638

	40	41	42
	A	A	A
Frequencies --	1504.7367	1522.6957	1525.2246
Red. masses --	1.1567	1.0484	1.0825
Frc consts --	1.5431	1.4322	1.4838
IR Inten --	20.4209	19.1131	26.9058

	43	44	45
	A	A	A
Frequencies --	1563.4032	1677.2653	1785.1460
Red. masses --	1.2698	1.0738	9.3018
Frc consts --	1.8286	1.7799	17.4649
IR Inten --	53.7916	55.9334	66.2285

	46	47	48
	A	A	A
Frequencies --	2687.5731	3030.3478	3049.4065
Red. masses --	1.0980	1.0901	1.0837
Frc consts --	4.6727	5.8978	5.9372
IR Inten --	1341.4578	35.0451	52.1005

	49	50	51
	A	A	A
Frequencies --	3111.1095	3141.7641	3212.5871
Red. masses --	1.0320	1.0707	1.1077
Frc consts --	5.8851	6.2270	6.7359
IR Inten --	6.9616	1456.6344	4.8789

	52	53	54
	A	A	A
Frequencies --	3242.8445	3454.6780	3734.0145
Red. masses --	1.1062	1.0749	1.0659
Frc consts --	6.8538	7.5581	8.7564
IR Inten --	2.7867	82.1755	97.0923

MG-SA-MA:

	1	2	3
	A	A	A
Frequencies --	54.0329	83.7476	87.6559
Red. masses --	10.7056	7.0711	7.3963
Frc consts --	0.0184	0.0292	0.0335
IR Inten --	0.6070	1.5824	3.6008

	4	5	6
	A	A	A
Frequencies --	108.9031	114.6070	150.7751

Red. masses --	3.9568	4.5370	4.3819
Frc consts --	0.0276	0.0351	0.0587
IR Inten --	2.2777	8.1735	1.7234
	7	8	9
	A	A	A
Frequencies --	180.7309	191.2905	203.8618
Red. masses --	1.0957	3.3387	1.7821
Frc consts --	0.0211	0.0720	0.0436
IR Inten --	1.4295	15.2278	2.5628
	10	11	12
	A	A	A
Frequencies --	223.8718	268.6351	284.5935
Red. masses --	2.1475	3.1598	1.9339
Frc consts --	0.0634	0.1343	0.0923
IR Inten --	16.6361	62.8847	27.7689
	13	14	15
	A	A	A
Frequencies --	294.5798	357.5940	396.6018
Red. masses --	3.0327	3.9467	4.4259
Frc consts --	0.1551	0.2974	0.4102
IR Inten --	59.7504	12.6577	18.4522
	16	17	18
	A	A	A
Frequencies --	418.5474	444.4931	482.1560
Red. masses --	3.2321	2.9277	4.5310
Frc consts --	0.3336	0.3408	0.6206
IR Inten --	16.6851	13.2900	2.5152
	19	20	21
	A	A	A
Frequencies --	546.2630	555.3338	566.2777
Red. masses --	13.1390	10.0734	3.8287
Frc consts --	2.3100	1.8303	0.7234
IR Inten --	10.1103	116.7773	7.5862
	22	23	24
	A	A	A
Frequencies --	573.2151	628.2274	753.7979
Red. masses --	14.6850	3.1850	17.0455
Frc consts --	2.8429	0.7406	5.7065
IR Inten --	24.8307	5.4204	224.8365
	25	26	27
	A	A	A
Frequencies --	797.1677	884.6904	942.5076
Red. masses --	2.4906	2.1879	1.4124
Frc consts --	0.9325	1.0089	0.7392

IR Inten --	13.5728	12.8486	12.1818
	28	29	30
	A	A	A
Frequencies --	989.7655	996.7203	1019.4772
Red. masses --	1.2156	6.3031	1.7146
Frc consts --	0.7016	3.6893	1.0500
IR Inten --	52.6082	323.3116	1.1820
	31	32	33
	A	A	A
Frequencies --	1039.3289	1060.2621	1089.6845
Red. masses --	2.1703	2.6006	6.0968
Frc consts --	1.3813	1.7225	4.2654
IR Inten --	13.3993	38.7637	283.9487
	34	35	36
	A	A	A
Frequencies --	1137.3702	1151.3561	1183.2931
Red. masses --	1.4020	2.1682	1.4872
Frc consts --	1.0686	1.6934	1.2269
IR Inten --	132.3796	109.7512	7.6146
	37	38	39
	A	A	A
Frequencies --	1223.9142	1254.6029	1290.0207
Red. masses --	2.6113	1.5608	4.8335
Frc consts --	2.3046	1.4475	4.7392
IR Inten --	71.1822	64.8851	441.5457
	40	41	42
	A	A	A
Frequencies --	1331.4747	1369.4673	1405.4630
Red. masses --	1.5020	1.2749	1.3731
Frc consts --	1.5688	1.4087	1.5980
IR Inten --	35.5429	6.8246	34.6401
	43	44	45
	A	A	A
Frequencies --	1410.0997	1474.9434	1484.8269
Red. masses --	1.5838	1.1725	1.0704
Frc consts --	1.8555	1.5029	1.3904
IR Inten --	26.1669	1.6118	12.9369
	46	47	48
	A	A	A
Frequencies --	1495.9804	1518.1154	1524.4281
Red. masses --	1.0558	1.0752	1.0691
Frc consts --	1.3921	1.4600	1.4638
IR Inten --	14.3199	29.3479	8.4088
	49	50	51

	A	A	A
Frequencies --	1532.3429	1586.7490	1671.4137
Red. masses --	1.0927	1.1273	1.0613
Frc consts --	1.5117	1.6722	1.7468
IR Inten --	46.4541	55.6757	18.3989
	52	53	54
	A	A	A
Frequencies --	1776.4415	2588.9268	3070.9063
Red. masses --	10.8099	1.1024	1.0451
Frc consts --	20.0990	4.3533	5.8068
IR Inten --	90.5132	1614.7754	1.4387
	55	56	57
	A	A	A
Frequencies --	3073.0554	3098.5164	3155.7351
Red. masses --	1.0738	1.0319	1.0982
Frc consts --	5.9748	5.8370	6.4438
IR Inten --	50.2986	9.0579	2.4755
	58	59	60
	A	A	A
Frequencies --	3197.1609	3202.8188	3215.9663
Red. masses --	1.1048	1.1070	1.1069
Frc consts --	6.6539	6.6906	6.7451
IR Inten --	2.3643	2.2581	0.3539
	61	62	63
	A	A	A
Frequencies --	3250.7932	3444.1929	3744.0656
Red. masses --	1.0695	1.0745	1.0662
Frc consts --	6.6593	7.5101	8.8059
IR Inten --	1038.0211	72.9693	120.5679

MG-MSA-MA:

	1	2	3
	A	A	A
Frequencies --	55.8464	87.8874	94.9769
Red. masses --	7.7490	4.6296	5.7742
Frc consts --	0.0142	0.0211	0.0307
IR Inten --	2.3521	3.5430	2.1907
	4	5	6
	A	A	A
Frequencies --	115.4119	125.6575	154.3867
Red. masses --	4.1319	4.7601	3.0537
Frc consts --	0.0324	0.0443	0.0429
IR Inten --	1.5455	8.9745	5.1193
	7	8	9
	A	A	A

Frequencies --	168.2253	195.1649	199.8551
Red. masses --	1.1036	3.4537	2.0877
Frc consts --	0.0184	0.0775	0.0491
IR Inten --	0.2520	15.7319	1.6138

	10	11	12
	A	A	A
Frequencies --	220.7375	257.3699	269.9108
Red. masses --	1.6540	1.0977	3.2883
Frc consts --	0.0475	0.0428	0.1411
IR Inten --	9.8133	3.5242	39.2285

	13	14	15
	A	A	A
Frequencies --	295.1558	330.3611	356.5829
Red. masses --	3.7393	4.5754	4.6621
Frc consts --	0.1919	0.2942	0.3493
IR Inten --	19.8714	17.1184	10.7972

	16	17	18
	A	A	A
Frequencies --	363.4400	433.5576	487.5429
Red. masses --	4.0965	2.8209	4.5745
Frc consts --	0.3188	0.3124	0.6407
IR Inten --	19.5984	12.2543	8.2317

	19	20	21
	A	A	A
Frequencies --	510.5353	530.3306	535.5457
Red. masses --	9.1816	6.8828	8.5390
Frc consts --	1.4100	1.1405	1.4430
IR Inten --	26.3654	32.9101	92.5628

	22	23	24
	A	A	A
Frequencies --	568.0764	632.6382	756.4016
Red. masses --	3.7138	3.1782	6.7609
Frc consts --	0.7061	0.7494	2.2791
IR Inten --	9.3616	5.6062	33.9847

	25	26	27
	A	A	A
Frequencies --	802.4521	888.6281	943.0980
Red. masses --	2.4625	2.0551	1.4633
Frc consts --	0.9342	0.9562	0.7668
IR Inten --	7.8218	5.0448	5.9546

	28	29	30
	A	A	A
Frequencies --	967.5770	983.3417	1002.0782
Red. masses --	2.8964	2.5893	1.3041

Frc consts --	1.5976	1.4751	0.7715
IR Inten --	193.3262	141.4125	33.7891
	31	32	33
	A	A	A
Frequencies --	1010.4498	1018.5641	1033.7522
Red. masses --	1.4362	1.7391	2.0643
Frc consts --	0.8640	1.0631	1.2998
IR Inten --	70.3791	1.2231	103.6298
	34	35	36
	A	A	A
Frequencies --	1059.2935	1070.0117	1149.4335
Red. masses --	2.6621	2.3204	2.2391
Frc consts --	1.7600	1.5653	1.7430
IR Inten --	146.4357	67.3472	96.1366
	37	38	39
	A	A	A
Frequencies --	1186.2563	1222.7024	1238.7483
Red. masses --	1.5034	2.6198	2.8134
Frc consts --	1.2465	2.3076	2.5436
IR Inten --	20.3901	64.7437	279.6224
	40	41	42
	A	A	A
Frequencies --	1254.7564	1331.7354	1365.5283
Red. masses --	2.7710	1.4703	1.2817
Frc consts --	2.5704	1.5363	1.4081
IR Inten --	271.4187	32.5754	6.1266
	43	44	45
	A	A	A
Frequencies --	1380.8948	1403.3368	1410.9851
Red. masses --	1.2286	1.3571	1.5902
Frc consts --	1.3803	1.5747	1.8653
IR Inten --	14.0135	43.5278	15.5679
	46	47	48
	A	A	A
Frequencies --	1473.3846	1474.3593	1476.1279
Red. masses --	1.1510	1.0600	1.0497
Frc consts --	1.4722	1.3576	1.3477
IR Inten --	2.8160	3.3336	4.1443
	49	50	51
	A	A	A
Frequencies --	1483.9213	1497.1365	1519.8138
Red. masses --	1.0697	1.0548	1.0437
Frc consts --	1.3878	1.3930	1.4204
IR Inten --	11.1846	12.2973	11.3570

	52	53	54
	A	A	A
Frequencies --	1530.5372	1538.5443	1622.0726
Red. masses --	1.0534	1.1392	1.1101
Frc consts --	1.4539	1.5888	1.7210
IR Inten --	2.9122	81.8996	35.0822

	55	56	57
	A	A	A
Frequencies --	1673.9153	1773.2583	2315.8830
Red. masses --	1.0640	10.6492	1.1271
Frc consts --	1.7566	19.7293	3.5615
IR Inten --	24.2651	87.5078	2072.7708

	58	59	60
	A	A	A
Frequencies --	3061.6184	3073.9533	3087.9972
Red. masses --	1.0829	1.0354	1.0302
Frc consts --	5.9805	5.7646	5.7882
IR Inten --	78.8666	7.5502	2.4124

	61	62	63
	A	A	A
Frequencies --	3095.5229	3159.9394	3181.8649
Red. masses --	1.0324	1.0990	1.0716
Frc consts --	5.8284	6.4654	6.3924
IR Inten --	12.9489	3.5141	1022.1144

	64	65	66
	A	A	A
Frequencies --	3195.1351	3197.6894	3200.3385
Red. masses --	1.1034	1.1064	1.1064
Frc consts --	6.6370	6.6655	6.6764
IR Inten --	56.3210	8.1333	1.0220

	67	68	69
	A	A	A
Frequencies --	3206.2588	3215.0661	3467.8766
Red. masses --	1.1060	1.1066	1.0741
Frc consts --	6.6989	6.7392	7.6103
IR Inten --	0.7083	0.1791	53.5531