

Supporting Information

How Do Electron Donating Substituents Affect the Electronic Structure, Molecular Topology, Vibrational Properties and Intra-/Intermolecular Interactions of Polyhalogenated Pyridines?

Enrico Benassi,^{1*} Tamara Vaganova,² Evgenij Malykhin,² and Haiyan Fan³

¹ Novosibirsk State University, Novosibirsk, 630090, Russia.

² Vorozhtsov Novosibirsk Institute of Organic Chemistry SB RAS, Novosibirsk, 630090, Russia.

³ Department of Chemistry, School of Sciences and Humanities, Nazarbayev University Nazarbayev University, Nursultan, 010000, Kazakhstan.

* Corresponding Author: ebenassi3@gmail.com

Index

A Synthesis of 2-hydroxy-3,5,6-trifluoropyridine (7)	p.	SI-2
B Optimised Geometries and Internal Coordinates of monomers	p.	SI-3
C Computed IR and Raman Spectra of monomers	p.	SI-35
D Composition of the vibrational normal modes as a function of the internal coordinates	p.	SI-151
E Optimised Geometries of aggregates	p.	SI-165
F Computed IR and Raman Spectra of aggregates	p.	SI-182
Table S1. Topological properties	p.	SI-227
Table S2. In-ring electron density transfer, orbital's occupancy and delocalisation energy.	p.	SI-231

A Synthesis of 2-hydroxy-3,5,6-trifluoropyridine (7)

2,3,5,6-Tetrafluoropyridine (8.3 g, 0.054 moles), sodium hydroxide (4.2 g., 0.11 moles), and water (100 ml) were stirred at 60-70 °C for 6 hr. The solution was acidified with concentrated hydrochloric acid (8 ml) and extracted with ether (3 x 70 ml). The ethereal extract was dried over MgSO₄ and solvent was evaporated. White solid thus obtained was sublimed at 50 °C (3 Torr) to yield 2-hydroxy-3,5,6-trifluoropyridine (6.6 g, 80%), mp 96-97 °C. ¹H NMR (acetone-d₆) δ: 7.82 (ddd, *J*_{HF}=7, *J*_{HF}=8, *J*_{HF}=8.5, H-4), 10.9 (br.s, OH). ¹⁹F NMR (acetone-d₆) δ: -94.8 (ddd, 1F, *J*_{HF}=7, *J*_{FF}=24, *J*_{FF}=30, F-6), -140.3 (dd, 1F, *J*_{HF}=8, *J*_{FF}=30, F-3), -150.2 (dd, 1F, *J*_{HF}=8.5, *J*_{FF}=24, F-5). High-resolution MS, found: *m/z* 149.0082 [M]⁺. Calculated for C₅H₂NOF₃ 149.0083.

B Optimised Geometries and Internal Coordinates of monomers

py-01_A_b3lyp

6	-0.008796	-1.197806	1.122857
6	0.009469	0.182080	1.185910
6	0.016013	0.928425	-0.000000
6	0.009469	0.182080	-1.185910
6	-0.008796	-1.197806	-1.122857
7	-0.019292	-1.878771	-0.000000
7	-0.005842	2.289435	-0.000000
1	0.183465	2.775845	0.860790
1	0.183465	2.775845	-0.860790
9	-0.014525	-1.893678	2.263153
9	0.025937	0.843150	2.362377
9	-0.014525	-1.893678	-2.263153
9	0.025937	0.843150	-2.362377

py-01_A_b3p86

6	-0.008658	-1.194657	1.119743
6	0.009439	0.182851	1.183736
6	0.016124	0.926837	-0.000000
6	0.009439	0.182851	-1.183736
6	-0.008658	-1.194657	-1.119743
7	-0.019113	-1.874201	-0.000000
7	-0.005371	2.283219	-0.000000
1	0.182986	2.769285	0.860377
1	0.182986	2.769285	-0.860377
9	-0.014394	-1.886385	2.253951
9	0.025796	0.840114	2.353156
9	-0.014394	-1.886385	-2.253951
9	0.025796	0.840114	-2.353156

py-01_A_b3pw91

6	-0.008574	-1.195898	1.120602
6	0.009145	0.183060	1.185004
6	0.015579	0.928204	-0.000000
6	0.009145	0.183060	-1.185004
6	-0.008574	-1.195898	-1.120602
7	-0.018830	-1.875834	0.000000
7	-0.007485	2.286326	-0.000000
1	0.184668	2.772272	0.859769
1	0.184668	2.772272	-0.859769
9	-0.014129	-1.889470	2.255654
9	0.025248	0.839823	2.356515
9	-0.014129	-1.889470	-2.255654
9	0.025248	0.839823	-2.356515

py-01_A_blyp

6	-0.008925	-1.209037	1.131875
6	0.008071	0.181674	1.195138
6	0.013424	0.936410	-0.000000
6	0.008071	0.181674	-1.195138
6	-0.008925	-1.209037	-1.131875
7	-0.019177	-1.896755	0.000000
7	-0.017871	2.309567	-0.000000
1	0.191638	2.796526	0.865156
1	0.191638	2.796526	-0.865156
9	-0.013319	-1.917999	2.288242
9	0.025335	0.853361	2.388160
9	-0.013319	-1.917999	-2.288242
9	0.025335	0.853361	-2.388160

py-01_A_bp86

6	-0.008391	-1.206143	1.129922
6	0.006556	0.183376	1.194147
6	0.010874	0.934901	0.000000
6	0.006556	0.183376	-1.194147
6	-0.008391	-1.206143	-1.129922
7	-0.017842	-1.892750	-0.000000
7	-0.024324	2.304040	0.000000
1	0.196591	2.787410	0.865357
1	0.196591	2.787410	-0.865357
9	-0.011586	-1.910618	2.279198
9	0.023464	0.852014	2.378555
9	-0.011586	-1.910618	-2.279198
9	0.023464	0.852014	-2.378555

py-01_A_bpw91

py-01_A_camb3lyp

6	-0.010182	-1.193934	1.117745
6	0.014974	0.180376	1.180456
6	0.026188	0.923832	-0.000000
6	0.014974	0.180376	-1.180456
6	-0.010182	-1.193934	-1.117745
7	-0.023588	-1.872698	0.000000
7	0.025023	2.278497	-0.000000
1	0.160589	2.773691	0.864452
1	0.160589	2.773691	-0.864452
9	-0.020544	-1.882881	2.253833
9	0.032341	0.837068	2.351884
9	-0.020544	-1.882881	-2.253833
9	0.032341	0.837068	-2.351884

py-01_A_mn15

6	-0.013900	-1.199145	1.121755
6	0.028364	0.178960	1.184523
6	0.051158	0.922189	-0.000000
6	0.028364	0.178960	-1.184523
6	-0.013900	-1.199145	-1.121755
7	-0.034767	-1.879525	0.000000
7	0.092737	2.277922	-0.000000
1	0.108301	2.785424	0.870471
1	0.108301	2.785424	-0.870471
9	-0.034851	-1.882257	2.257880
9	0.048510	0.835860	2.351514
9	-0.034851	-1.882257	-2.257880
9	0.048510	0.835860	-2.351514

py-01_A_o3lyp

6	-0.007192	-0.989076	1.122299
6	0.000574	0.393527	1.187854
6	0.001116	1.141259	-0.000000
6	0.000574	0.393527	-1.187854
6	-0.007192	-0.989076	-1.122299
7	-0.012656	-1.670352	0.000000
7	-0.041494	2.503639	-0.000000
1	0.179865	2.984736	0.854706
1	0.179865	2.984736	-0.854706
9	-0.007208	-1.687169	2.258483
9	0.012319	1.048085	2.363432
9	-0.007208	-1.687169	-2.258483
9	0.012319	1.048085	-2.363432

py-01_A_pbe0

6	-0.008291	-1.193621	1.119043
6	0.008371	0.183630	1.183516
6	0.014189	0.926652	-0.000000
6	0.008371	0.183630	-1.183516
6	-0.008291	-1.193621	-1.119043
7	-0.018061	-1.873126	-0.000000
7	-0.010300	2.282524	-0.000000
1	0.186987	2.765918	0.859431
1	0.186987	2.765918	-0.859431
9	-0.013183	-1.883633	2.250912
9	0.024191	0.838817	2.350872
9	-0.013183	-1.883633	-2.250912
9	0.024191	0.838817	-2.350872

py-01_A_pbe

6	-0.008567	-1.204652	1.128478
6	0.007286	0.183386	1.192784
6	0.011963	0.933916	-0.000000
6	0.007286	0.183386	-1.192784
6	-0.008567	-1.204652	-1.128478
7	-0.018376	-1.890003	-0.000000
7	-0.020513	2.300444	0.000000
1	0.193656	2.784822	0.865303
1	0.193656	2.784822	-0.865303
9	-0.012235	-1.907331	2.276552
9	0.024312	0.850732	2.375191
9	-0.012235	-1.907331	-2.276552
9	0.024312	0.850732	-2.375191

py-01_A_rtpss

6	-0.006924	-1.200119	1.125183
6	0.001352	0.184433	1.188624
6	0.002314	0.933971	-0.000000
6	0.001352	0.184433	-1.188624
6	-0.006924	-1.200119	-1.125183
7	-0.013707	-1.892930	-0.000000
7	-0.053940	2.304515	0.000000
1	0.217395	2.771756	0.858629
1	0.217395	2.771756	-0.858629
9	-0.005650	-1.901185	2.273421
9	0.017483	0.851472	2.372341
9	-0.005650	-1.901185	-2.273421
9	0.017483	0.851472	-2.372341

py-01_A_tpssh

6	-0.007816	-1.197787	1.122837
6	0.005578	0.183421	1.186590
6	0.009356	0.930877	-0.000000
6	0.005578	0.183421	-1.186590
6	-0.007816	-1.197787	-1.122837
7	-0.016498	-1.883916	0.000000
7	-0.030179	2.295378	-0.000000
1	0.200299	2.772740	0.858192
1	0.200299	2.772740	-0.858192
9	-0.010214	-1.896010	2.263767
9	0.021803	0.845602	2.364416
9	-0.010214	-1.896010	-2.263767
9	0.021803	0.845602	-2.364416

py-01_A_wb97xd

6	-0.008494	-1.194651	1.119009
6	0.009561	0.182845	1.182948

6	0.016619	0.926602	-0.000000
6	0.009561	0.182845	-1.182948
6	-0.008494	-1.194651	-1.119009
7	-0.018766	-1.875235	-0.000000
7	-0.004001	2.285076	-0.000000
1	0.182595	2.771634	0.859550
1	0.182595	2.771634	-0.859550
9	-0.014740	-1.885171	2.251263
9	0.025141	0.836257	2.353199
9	-0.014740	-1.885171	-2.251263
9	0.025141	0.836257	-2.353199

py-01_A_x3lyp

6	-0.009053	-1.197853	1.121791
6	0.010517	0.181505	1.185123
6	0.017959	0.928411	-0.000000
6	0.010517	0.181505	-1.185123
6	-0.009053	-1.197853	-1.121791
7	-0.020086	-1.878973	0.000000
7	-0.000821	2.288932	-0.000000
1	0.179620	2.777778	0.861105
1	0.179620	2.777778	-0.861105
9	-0.015653	-1.892368	2.261448
9	0.027032	0.840889	2.361236
9	-0.015653	-1.892368	-2.261448
9	0.027032	0.840889	-2.361236

py-04_A_b3lyp

6	-0.008220	-1.190665	1.120129
6	0.016005	0.186439	1.174559
6	0.024221	0.930856	-0.014840
6	0.012651	0.186424	-1.211093
6	-0.011727	-1.198053	-1.122470
7	-0.023171	-1.878164	-0.000305
7	0.018247	2.286884	0.016996
1	0.161201	2.758347	0.894230
1	0.165101	2.803126	-0.834346
9	-0.015780	-1.881921	2.262079
9	0.035314	0.852825	2.349307
9	-0.023715	-1.914056	-2.249749
17	0.030593	1.007512	-2.747141

py-04_A_b3p86

6	-0.008287	-1.187719	1.116568
6	0.016563	0.187067	1.172573
6	0.025286	0.929190	-0.014534
6	0.013344	0.187452	-1.208602

6	-0.011717	-1.194502	-1.119406
7	-0.023499	-1.873889	-0.000723
7	0.021388	2.280348	0.016364
1	0.159110	2.753312	0.892871
1	0.161855	2.795378	-0.836390
9	-0.016345	-1.875010	2.252288
9	0.035828	0.849560	2.340148
9	-0.024065	-1.905349	-2.241118
17	0.031259	1.003717	-2.732680

py-04_A_b3pw91

6	-0.008211	-1.188916	1.117443
6	0.016180	0.187276	1.173798
6	0.024598	0.930557	-0.014612
6	0.013010	0.187775	-1.210132
6	-0.011603	-1.195728	-1.120342
7	-0.023185	-1.875410	-0.000717
7	0.019109	2.283350	0.016591
1	0.160882	2.756166	0.892654
1	0.163870	2.798673	-0.835295
9	-0.016030	-1.878056	2.254002
9	0.035229	0.849309	2.343464
9	-0.023710	-1.908776	-2.242562
17	0.030580	1.003334	-2.736934

py-04_A_blyp

6	-0.007990	-1.201937	1.129427
6	0.013250	0.186048	1.183601
6	0.019033	0.938553	-0.015075
6	0.009831	0.186457	-1.221127
6	-0.011532	-1.208443	-1.131226
7	-0.021964	-1.895599	0.000191
7	0.000146	2.307324	0.017752
1	0.174000	2.777674	0.899289
1	0.178566	2.822778	-0.837744
9	-0.013082	-1.906230	2.287649
9	0.032993	0.863261	2.374663
9	-0.021238	-1.939072	-2.273852
17	0.028708	1.018742	-2.776190

py-04_A_bp86

6	-0.007666	-1.199610	1.126998
6	0.011836	0.187425	1.183482
6	0.016622	0.937034	-0.013716
6	0.008754	0.188278	-1.218315
6	-0.010986	-1.205227	-1.129512
7	-0.020871	-1.892104	-0.000560

7	-0.005785	2.301423	0.015721
1	0.179569	2.772053	0.895746
1	0.181794	2.809743	-0.843692
9	-0.011813	-1.899980	2.277706
9	0.031083	0.860772	2.366153
9	-0.019373	-1.928760	-2.266328
17	0.027556	1.018507	-2.756323

py-04_A_bpw91

py-04_A_camb3lyp

6	-0.011391	-1.185996	1.114590
6	0.030249	0.184760	1.167938
6	0.050487	0.925806	-0.016806
6	0.025803	0.184880	-1.207747
6	-0.015813	-1.193989	-1.117184
7	-0.034267	-1.871953	-0.000550
7	0.091426	2.274579	0.018170
1	0.107621	2.754374	0.901013
1	0.105957	2.806716	-0.834235
9	-0.029980	-1.869735	2.252460
9	0.052537	0.847946	2.337018
9	-0.039424	-1.903708	-2.239968
17	0.047515	0.995875	-2.737340

py-04_A_mn15

6	-0.011489	-1.190650	1.117883
6	0.030240	0.184900	1.171330
6	0.050463	0.925976	-0.017061
6	0.025803	0.184275	-1.210414
6	-0.015882	-1.198531	-1.121465
7	-0.034387	-1.878649	-0.001092
7	0.091478	2.279072	0.017522
1	0.107690	2.760432	0.903082
1	0.106043	2.812743	-0.837995
9	-0.029893	-1.868502	2.255925
9	0.052444	0.847174	2.336176
9	-0.039224	-1.900911	-2.245625
17	0.047434	0.992225	-2.730908

py-04_A_o3lyp

6	-0.007141	-1.190397	1.119013
6	0.012085	0.189360	1.175704
6	0.017073	0.934922	-0.015789
6	0.008974	0.189849	-1.214687
6	-0.010467	-1.197480	-1.122571

7	-0.019822	-1.877944	-0.000668
7	-0.005317	2.292318	0.017783
1	0.178185	2.756762	0.889740
1	0.183116	2.803173	-0.826923
9	-0.011570	-1.883779	2.256871
9	0.029643	0.849344	2.349254
9	-0.019295	-1.917054	-2.244222
17	0.025257	1.000480	-2.746147

py-04_A_pbe0

6	-0.007991	-1.186642	1.115682
6	0.015529	0.187891	1.172304
6	0.023492	0.929245	-0.014519
6	0.012400	0.188118	-1.208201
6	-0.011369	-1.193806	-1.118972
7	-0.022576	-1.872989	-0.000963
7	0.016649	2.279611	0.016146
1	0.162792	2.750498	0.891865
1	0.165805	2.792561	-0.835748
9	-0.015260	-1.872215	2.248995
9	0.034311	0.848124	2.337936
9	-0.022889	-1.902395	-2.238416
17	0.029826	1.001555	-2.728751

py-04_A_pbe

6	-0.007824	-1.197969	1.125261
6	0.012775	0.187574	1.181655
6	0.018230	0.936223	-0.014203
6	0.009625	0.188515	-1.217538
6	-0.011234	-1.203639	-1.128258
7	-0.021531	-1.889314	-0.000789
7	-0.000864	2.298024	0.015849
1	0.175717	2.769200	0.896202
1	0.178006	2.808190	-0.842995
9	-0.012591	-1.896422	2.274847
9	0.032171	0.859645	2.362300
9	-0.020367	-1.925292	-2.263880
17	0.028606	1.014820	-2.751093

py-04_A_rtpss

6	-0.006088	-1.193357	1.121945
6	0.005847	0.188829	1.176940
6	0.006504	0.936343	-0.014717
6	0.003061	0.189545	-1.214044
6	-0.009223	-1.199271	-1.124486
7	-0.016107	-1.892696	-0.000559
7	-0.039454	2.302023	0.015959

1	0.201243	2.754964	0.890617
1	0.208821	2.796491	-0.834565
9	-0.005081	-1.889621	2.271940
9	0.023974	0.861269	2.358641
9	-0.012610	-1.918646	-2.260806
17	0.019832	1.013680	-2.749507

py-04_A_tpssh

6	-0.007152	-1.191046	1.119799
6	0.011015	0.187588	1.175396
6	0.015380	0.933162	-0.014383
6	0.008086	0.188387	-1.211773
6	-0.010387	-1.197313	-1.122193
7	-0.019644	-1.883690	-0.000568
7	-0.010858	2.292491	0.016135
1	0.181581	2.756516	0.890224
1	0.186423	2.797819	-0.834368
9	-0.010597	-1.884731	2.262297
9	0.029651	0.855240	2.351245
9	-0.018140	-1.913981	-2.251025
17	0.025362	1.009114	-2.743427

py-04_A_wb97xd

6	-0.008551	-1.187445	1.115911
6	0.018319	0.186863	1.171592
6	0.028703	0.928774	-0.015400
6	0.014931	0.186786	-1.208188
6	-0.012057	-1.195231	-1.118525
7	-0.024545	-1.875255	-0.000476
7	0.030627	2.281330	0.017334
1	0.151954	2.755078	0.894765
1	0.156041	2.802241	-0.832861
9	-0.018226	-1.873157	2.249717
9	0.037498	0.846136	2.339776
9	-0.026081	-1.906068	-2.237430
17	0.032107	0.999502	-2.738856

py-04_A_x31yp

6	-0.008534	-1.190364	1.119007
6	0.017600	0.186028	1.173156
6	0.027133	0.930841	-0.015787
6	0.014112	0.185973	-1.211565
6	-0.012161	-1.198077	-1.121225
7	-0.024350	-1.878274	-0.000091
7	0.025968	2.286340	0.018279
1	0.155259	2.758597	0.897044
1	0.159216	2.807483	-0.832030

9	-0.017304	-1.879912	2.260516
9	0.037161	0.851393	2.347170
9	-0.025497	-1.913838	-2.247288
17	0.032116	1.003364	-2.749828

py-06_A_b31yp

6	0.004444	-1.194176	1.103969
6	-0.010818	0.189561	1.187501
6	-0.003257	0.906402	-0.010709
6	0.025273	0.191336	-1.196625
6	0.045494	-1.209956	-1.178167
7	0.028758	-1.870012	-0.016387
9	-0.011102	-1.900455	2.240360
9	-0.036715	0.817763	2.369310
9	0.028175	0.824494	-2.387678
7	0.124734	-1.929546	-2.340244
17	-0.030076	2.631115	-0.010220
1	-0.117784	-1.472309	-3.204184
1	-0.082704	-2.913234	-2.268100

py-06_A_b3p86

6	0.004448	-1.192236	1.100188
6	-0.010931	0.188911	1.184674
6	-0.003349	0.903687	-0.011609
6	0.025389	0.190203	-1.195763
6	0.045417	-1.208271	-1.175782
7	0.028785	-1.866476	-0.017705
9	-0.010900	-1.894583	2.230045
9	-0.036792	0.813885	2.359424
9	0.028469	0.819836	-2.379441
7	0.124179	-1.924846	-2.334224
17	-0.030019	2.616512	-0.011580
1	-0.117903	-1.467711	-3.197463
1	-0.082369	-2.907926	-2.261939

py-06_A_b3pw91

6	0.004397	-1.192751	1.100927
6	-0.011080	0.189806	1.186353
6	-0.003344	0.905785	-0.010990
6	0.025668	0.191877	-1.196880
6	0.045797	-1.208167	-1.177208
7	0.028943	-1.866743	-0.018110
9	-0.011086	-1.897479	2.231330
9	-0.037162	0.814567	2.362914
9	0.029107	0.823271	-2.381311
7	0.125792	-1.927243	-2.336128
17	-0.030018	2.620673	-0.010391

1	-0.120063	-1.472591	-3.199785
1	-0.082527	-2.910021	-2.261895

py-06_A_blyp

6	0.004390	-1.199633	1.114288
6	-0.010618	0.195474	1.200732
6	-0.003128	0.919928	-0.006641
6	0.025734	0.197829	-1.202512
6	0.046270	-1.214860	-1.187354
7	0.028676	-1.882370	-0.013994
9	-0.012322	-1.919324	2.267091
9	-0.036673	0.831606	2.399206
9	0.028025	0.842663	-2.410030
7	0.133681	-1.943946	-2.357524
17	-0.030755	2.663616	-0.005966
1	-0.122528	-1.487046	-3.227081
1	-0.086328	-2.932953	-2.281389

py-06_A_bp86

6	0.004757	-1.198490	1.111413
6	-0.011092	0.195085	1.198800
6	-0.003205	0.917199	-0.007950
6	0.027279	0.197048	-1.203307
6	0.048433	-1.213318	-1.185245
7	0.030187	-1.879989	-0.015584
9	-0.012439	-1.913810	2.256579
9	-0.038377	0.829005	2.388596
9	0.029953	0.838334	-2.402031
7	0.138186	-1.939178	-2.352342
17	-0.031993	2.646487	-0.007657
1	-0.127637	-1.480380	-3.218978
1	-0.089627	-2.927008	-2.273468

py-06_A_bpw91

py-06_A_camb3lyp

6	0.003814	-1.190391	1.099970
6	-0.010107	0.187210	1.181155
6	-0.003421	0.900918	-0.011834
6	0.022081	0.187352	-1.190876
6	0.040407	-1.208716	-1.172292
7	0.025836	-1.864757	-0.016012
9	-0.009550	-1.889755	2.231940
9	-0.033306	0.812050	2.358115
9	0.024692	0.813941	-2.378139
7	0.107274	-1.922008	-2.332177

17	-0.027148	2.616588	-0.012867
1	-0.103577	-1.461220	-3.201066
1	-0.072571	-2.910227	-2.267092

py-06_A_mn15

6	0.002932	-1.191136	1.107899
6	-0.008891	0.190869	1.188388
6	-0.003566	0.902519	-0.009965
6	0.017728	0.188723	-1.193219
6	0.033059	-1.211151	-1.172656
7	0.021299	-1.867533	-0.012376
9	-0.007873	-1.884594	2.239793
9	-0.028128	0.818028	2.360340
9	0.019626	0.814580	-2.376799
7	0.086231	-1.922454	-2.336510
17	-0.023536	2.609677	-0.012541
1	-0.084465	-1.457581	-3.214701
1	-0.059991	-2.918962	-2.278830

py-06_A_o3lyp

6	0.004553	-1.193956	1.101164
6	-0.011798	0.192100	1.189758
6	-0.003324	0.911491	-0.009936
6	0.027664	0.195904	-1.200195
6	0.048836	-1.207587	-1.180951
7	0.030578	-1.867667	-0.020117
9	-0.012192	-1.904421	2.231954
9	-0.039586	0.814865	2.369713
9	0.032322	0.831444	-2.384836
7	0.138716	-1.932882	-2.340631
17	-0.031281	2.627992	-0.007975
1	-0.132505	-1.485703	-3.199828
1	-0.087560	-2.910598	-2.259293

py-06_A_pbe0

6	0.004719	-1.192044	1.099262
6	-0.011300	0.188682	1.183915
6	-0.003385	0.902758	-0.012259
6	0.026449	0.189979	-1.196324
6	0.047136	-1.207912	-1.174899
7	0.030027	-1.865950	-0.018252
9	-0.011021	-1.892818	2.226546
9	-0.038179	0.812531	2.356219
9	0.029931	0.818307	-2.377204
7	0.127851	-1.923666	-2.333110
17	-0.030898	2.611861	-0.012288
1	-0.121897	-1.465902	-3.193376

1	-0.085009	-2.904841	-2.259406
py-06_A_pbe			
6	0.004672	-1.197554	1.109914
6	-0.010865	0.194498	1.197055
6	-0.003256	0.915458	-0.008555
6	0.026541	0.195726	-1.202379
6	0.047525	-1.213151	-1.183748
7	0.029629	-1.878155	-0.015586
9	-0.012197	-1.910933	2.253902
9	-0.037601	0.827848	2.384585
9	0.028994	0.835693	-2.399037
7	0.135179	-1.936690	-2.349422
17	-0.031557	2.639613	-0.008835
1	-0.124243	-1.476832	-3.216221
1	-0.088399	-2.924538	-2.272849
py-06_A_rtpss			
6	0.005897	-1.196065	1.105307
6	-0.011995	0.192196	1.191894
6	-0.003136	0.912497	-0.010020
6	0.031698	0.192600	-1.200052
6	0.055131	-1.211599	-1.182584
7	0.034796	-1.882903	-0.017466
9	-0.013885	-1.908131	2.249258
9	-0.043384	0.825302	2.380304
9	0.034622	0.832931	-2.397708
7	0.161307	-1.935900	-2.350971
17	-0.036410	2.636626	-0.011078
1	-0.145789	-1.474241	-3.201058
1	-0.104429	-2.912326	-2.267003
py-06_A_tpssh			
6	0.004951	-1.193995	1.103289
6	-0.011342	0.190916	1.189090
6	-0.003236	0.909063	-0.010280
6	0.028013	0.192206	-1.197901
6	0.049599	-1.209641	-1.179959
7	0.031202	-1.874049	-0.017576
9	-0.012425	-1.903265	2.239796
9	-0.039467	0.820217	2.371681
9	0.030900	0.828405	-2.389156
7	0.141935	-1.932024	-2.343222
17	-0.032683	2.629273	-0.010563
1	-0.130679	-1.474964	-3.200601
1	-0.092342	-2.911156	-2.265771

py-06_A_wb97xd

6	0.004247	-1.191807	1.099798
6	-0.011374	0.188698	1.183501
6	-0.003344	0.903921	-0.011372
6	0.025843	0.191248	-1.194721
6	0.045831	-1.207122	-1.174713
7	0.029182	-1.866259	-0.018704
9	-0.010914	-1.893972	2.226856
9	-0.037629	0.810538	2.358800
9	0.029899	0.819140	-2.377893
7	0.123902	-1.925406	-2.334607
17	-0.029533	2.621306	-0.010583
1	-0.121411	-1.471314	-3.197703
1	-0.080275	-2.907986	-2.259836

py-06_A_x31yp

6	0.004225	-1.193552	1.103417
6	-0.010635	0.189659	1.187098
6	-0.003314	0.906673	-0.010362
6	0.024375	0.191104	-1.195483
6	0.044033	-1.210070	-1.177409
7	0.027840	-1.869411	-0.016148
9	-0.010795	-1.898569	2.239048
9	-0.035754	0.816103	2.368648
9	0.027322	0.822973	-2.386028
7	0.121486	-1.929139	-2.339437
17	-0.029240	2.631560	-0.010211
1	-0.114849	-1.472407	-3.205116
1	-0.080270	-2.913941	-2.269192

py-08_A_b31yp

6	0.005165	-1.199319	1.106567
6	-0.013010	0.185759	1.178394
6	-0.006352	0.903261	-0.010199
6	0.024559	0.187314	-1.186221
6	0.048341	-1.215252	-1.179532
7	0.031942	-1.872486	-0.016524
9	-0.010147	-1.909919	2.241904
9	-0.041629	0.821077	2.364707
9	0.025551	0.826532	-2.382961
7	0.132539	-1.935959	-2.342985
1	-0.123754	-1.477301	-3.202399
1	-0.084161	-2.917741	-2.270680
1	-0.025184	1.985020	-0.011248

py-08_A_b3p86

6	0.005169	-1.198086	1.102879
6	-0.013087	0.184490	1.175869
6	-0.006430	0.899094	-0.011027
6	0.024695	0.185727	-1.185596
6	0.048310	-1.214157	-1.177356
7	0.031982	-1.869301	-0.017918
9	-0.009973	-1.905283	2.231348
9	-0.041611	0.815442	2.355343
9	0.025760	0.820289	-2.375139
7	0.132006	-1.932070	-2.336986
1	-0.123639	-1.473419	-3.195703
1	-0.084013	-2.913191	-2.264528
1	-0.025308	1.981450	-0.012360

py-08_A_b3pw91

6	0.005100	-1.198647	1.103777
6	-0.013246	0.185335	1.177691
6	-0.006395	0.900573	-0.010305
6	0.024989	0.187476	-1.186730
6	0.048656	-1.213954	-1.179006
7	0.032103	-1.869320	-0.018392
9	-0.010152	-1.908522	2.232600
9	-0.042005	0.817566	2.358285
9	0.026407	0.825501	-2.376211
7	0.133507	-1.934567	-2.338984
1	-0.125863	-1.478628	-3.198209
1	-0.084006	-2.915422	-2.264381
1	-0.025234	1.983594	-0.011311

py-08_A_blyp

6	0.005073	-1.204250	1.117502
6	-0.012658	0.192337	1.190861
6	-0.006217	0.916710	-0.006192
6	0.024593	0.194249	-1.191167
6	0.048331	-1.219809	-1.188752
7	0.031367	-1.884063	-0.013789
9	-0.011167	-1.928236	2.269050
9	-0.041321	0.838862	2.392798
9	0.024787	0.847909	-2.403690
7	0.139849	-1.949575	-2.360085
1	-0.126973	-1.490795	-3.225647
1	-0.086544	-2.937277	-2.284846
1	-0.025257	2.004923	-0.007219

py-08_A_bp86

6	0.005439	-1.204128	1.114482
6	-0.013140	0.191170	1.188890

6	-0.006448	0.913114	-0.007433
6	0.025933	0.192802	-1.191845
6	0.050412	-1.219252	-1.186583
7	0.032870	-1.882600	-0.015415
9	-0.011219	-1.923908	2.258265
9	-0.042881	0.832600	2.383287
9	0.026274	0.839950	-2.396732
7	0.144056	-1.945654	-2.354815
1	-0.131389	-1.484656	-3.217446
1	-0.089663	-2.932252	-2.277179
1	-0.026385	2.003798	-0.008648

py-08_A_bpw91

py-08_A_camb3lyp

6	0.004608	-1.195823	1.102193
6	-0.012355	0.182944	1.172645
6	-0.006241	0.897378	-0.011380
6	0.022206	0.183055	-1.181383
6	0.044384	-1.214133	-1.173751
7	0.029631	-1.867681	-0.016469
9	-0.008991	-1.899786	2.233126
9	-0.038622	0.813023	2.354694
9	0.023220	0.814071	-2.374757
7	0.117626	-1.929119	-2.335137
1	-0.111900	-1.467237	-3.198923
1	-0.076223	-2.914732	-2.268837
1	-0.023480	1.979024	-0.013197

py-08_A_mn15

6	0.003856	-1.196592	1.109712
6	-0.011117	0.186716	1.179987
6	-0.006011	0.899961	-0.009705
6	0.018835	0.184495	-1.184143
6	0.038403	-1.216747	-1.173856
7	0.025823	-1.870669	-0.012876
9	-0.007839	-1.894515	2.240700
9	-0.033932	0.813242	2.359589
9	0.019388	0.808878	-2.376373
7	0.099906	-1.929691	-2.339398
1	-0.095620	-1.463132	-3.211752
1	-0.066455	-2.923107	-2.280387
1	-0.021375	1.982145	-0.012674

py-08_A_o3lyp

6	0.005199	-1.200193	1.104646
---	----------	-----------	----------

6	-0.014008	0.187394	1.181232
6	-0.006378	0.903869	-0.008977
6	0.026701	0.191536	-1.189783
6	0.051194	-1.213427	-1.183351
7	0.033451	-1.869699	-0.020444
9	-0.011050	-1.916506	2.233334
9	-0.044419	0.822219	2.363118
9	0.029265	0.838679	-2.377100
7	0.145217	-1.940525	-2.343688
1	-0.137680	-1.492503	-3.198891
1	-0.087766	-2.916732	-2.261980
1	-0.025865	1.986872	-0.009291

py-08_A_pbe0

6	0.005449	-1.198165	1.101758
6	-0.013532	0.184044	1.175095
6	-0.006563	0.898215	-0.011633
6	0.025682	0.185395	-1.186165
6	0.050045	-1.213999	-1.176464
7	0.033282	-1.869075	-0.018573
9	-0.010031	-1.903754	2.227695
9	-0.043076	0.812763	2.352616
9	0.027159	0.817772	-2.373268
7	0.135643	-1.931135	-2.335886
1	-0.127688	-1.472060	-3.191598
1	-0.086462	-2.910330	-2.261801
1	-0.026048	1.981313	-0.012951

py-08_A_pbe

6	0.005363	-1.203379	1.112920
6	-0.012887	0.190480	1.187251
6	-0.006424	0.910859	-0.008066
6	0.025228	0.191396	-1.191093
6	0.049517	-1.219299	-1.185064
7	0.032300	-1.880942	-0.015428
9	-0.011005	-1.921186	2.255515
9	-0.042053	0.830296	2.379782
9	0.025423	0.836192	-2.394297
7	0.141030	-1.943366	-2.351828
1	-0.127963	-1.481283	-3.214683
1	-0.088528	-2.929985	-2.276535
1	-0.026138	2.001201	-0.009649

py-08_A_rtpss

6	0.006670	-1.201599	1.107783
6	-0.014305	0.188244	1.181372
6	-0.007022	0.911887	-0.009729

6	0.029895	0.188122	-1.188281
6	0.056910	-1.217531	-1.183436
7	0.037650	-1.886024	-0.017261
9	-0.012250	-1.917622	2.250736
9	-0.048219	0.824987	2.376820
9	0.030323	0.830530	-2.394598
7	0.166601	-1.942109	-2.353188
1	-0.149003	-1.478383	-3.199220
1	-0.103557	-2.917487	-2.270381
1	-0.029831	1.997971	-0.011791

py-08_A_tpssh

6	0.005679	-1.199483	1.105948
6	-0.013572	0.186892	1.179501
6	-0.006644	0.906560	-0.009802
6	0.026836	0.187964	-1.187006
6	0.051942	-1.215234	-1.181341
7	0.034204	-1.876659	-0.017662
9	-0.011179	-1.913475	2.241120
9	-0.044303	0.821851	2.367670
9	0.027523	0.828693	-2.385121
7	0.148526	-1.938748	-2.345797
1	-0.135317	-1.480171	-3.198922
1	-0.092755	-2.916281	-2.268485
1	-0.027081	1.989077	-0.011279

py-08_A_wb97xd

6	0.004982	-1.197556	1.102249
6	-0.013707	0.184089	1.174856
6	-0.006415	0.899798	-0.010675
6	0.025550	0.186877	-1.184811
6	0.049348	-1.212526	-1.176556
7	0.032795	-1.869105	-0.019274
9	-0.010122	-1.904855	2.227999
9	-0.042863	0.813794	2.353862
9	0.027714	0.822067	-2.372549
7	0.133092	-1.932789	-2.337747
1	-0.128758	-1.477868	-3.195795
1	-0.082730	-2.912926	-2.261507
1	-0.025026	1.981985	-0.011227

py-08_A_x31yp

6	0.004943	-1.198592	1.106168
6	-0.012809	0.185842	1.178371
6	-0.006302	0.903034	-0.009836
6	0.023838	0.187148	-1.185478
6	0.047040	-1.215174	-1.178996

7	0.031081	-1.871556	-0.016350
9	-0.009927	-1.908350	2.240542
9	-0.040693	0.819912	2.363995
9	0.024940	0.825667	-2.381218
7	0.129683	-1.935727	-2.342280
1	-0.121195	-1.477741	-3.203416
1	-0.082126	-2.918489	-2.271559
1	-0.024613	1.985012	-0.011117

py-10_A_b3lyp

6	-0.011520	-1.190750	1.119587
6	0.020615	0.191029	1.200034
6	0.036036	0.934775	-0.000000
6	0.020615	0.191029	-1.200034
6	-0.011520	-1.190750	-1.119587
7	-0.028065	-1.877239	0.000000
7	0.051330	2.286493	-0.000000
1	0.135349	2.788107	0.867801
1	0.135349	2.788107	-0.867801
9	-0.026836	-1.902522	2.248356
9	-0.026836	-1.902522	-2.248356
17	0.042472	1.012539	-2.737333
17	0.042472	1.012539	2.737333

py-10_A_b3p86

6	-0.011902	-1.187344	1.116051
6	0.022480	0.191918	1.197684
6	0.039494	0.932959	-0.000000
6	0.022480	0.191918	-1.197684
6	-0.011902	-1.187344	-1.116051
7	-0.029437	-1.873211	0.000000
7	0.061060	2.279538	-0.000000
1	0.127417	2.781581	0.868789
1	0.127417	2.781581	-0.868789
9	-0.028611	-1.894048	2.239157
9	-0.028611	-1.894048	-2.239157
17	0.044789	1.008669	-2.722555
17	0.044789	1.008669	2.722555

py-10_A_b3pw91

6	-0.011872	-1.188560	1.117010
6	0.022301	0.192190	1.199187
6	0.039137	0.934262	-0.000000
6	0.022301	0.192190	-1.199187
6	-0.011872	-1.188560	-1.117010
7	-0.029299	-1.874648	0.000000
7	0.059951	2.282274	-0.000000

1	0.128453	2.784921	0.868239
1	0.128453	2.784921	-0.868239
9	-0.028488	-1.897478	2.240618
9	-0.028488	-1.897478	-2.240618
17	0.044442	1.008403	-2.726708
17	0.044442	1.008403	2.726708

py-10_A_blyp

6	-0.010714	-1.201226	1.128569
6	0.015695	0.191011	1.209878
6	0.026609	0.942163	-0.000000
6	0.015695	0.191011	-1.209878
6	-0.010714	-1.201226	-1.128569
7	-0.025055	-1.894278	0.000000
7	0.022652	2.307133	-0.000000
1	0.157246	2.806605	0.872249
1	0.157246	2.806605	-0.872249
9	-0.021988	-1.927593	2.272944
9	-0.021988	-1.927593	-2.272944
17	0.037390	1.024114	-2.765859
17	0.037390	1.024114	2.765859

py-10_A_bp86

6	-0.010378	-1.198556	1.126396
6	0.014740	0.192503	1.207904
6	0.024549	0.940572	-0.000000
6	0.014740	0.192503	-1.207904
6	-0.010378	-1.198556	-1.126396
7	-0.024235	-1.891261	0.000000
7	0.017710	2.300691	-0.000000
1	0.160803	2.796818	0.874370
1	0.160803	2.796818	-0.874370
9	-0.020639	-1.918322	2.264559
9	-0.020639	-1.918322	-2.264559
17	0.036193	1.022975	-2.746730
17	0.036193	1.022975	2.746730

py-10_A_bpw91

py-10_A_camb3lyp

6	-0.013381	-1.185312	1.113890
6	0.027674	0.190813	1.195369
6	0.049741	0.930502	-0.000000
6	0.027674	0.190813	-1.195369
6	-0.013381	-1.185312	-1.113890
7	-0.033817	-1.870287	0.000000

7	0.089919	2.277287	-0.000000
1	0.105035	2.783738	0.868051
1	0.105035	2.783738	-0.868051
9	-0.034421	-1.890495	2.238227
9	-0.034421	-1.890495	-2.238227
17	0.051902	1.002925	-2.725559
17	0.051902	1.002925	2.725559

py-10_A_mn15

6	-0.013500	-1.190012	1.117362
6	0.027663	0.190420	1.197439
6	0.049755	0.931289	-0.000000
6	0.027663	0.190420	-1.197439
6	-0.013500	-1.190012	-1.117362
7	-0.034007	-1.877699	0.000000
7	0.090051	2.282607	-0.000000
1	0.105209	2.790947	0.871080
1	0.105209	2.790947	-0.871080
9	-0.034302	-1.887583	2.243294
9	-0.034302	-1.887583	-2.243294
17	0.051761	0.998549	-2.718800
17	0.051761	0.998549	2.718800

py-10_A_o3lyp

6	1.211540	-0.000841	1.119117
6	-0.173274	-0.001379	1.202850
6	-0.917465	-0.004762	-0.000000
6	-0.173274	-0.001379	-1.202850
6	1.211540	-0.000841	-1.119117
7	1.898339	-0.001592	0.000000
7	-2.269802	-0.034567	-0.000000
1	-2.768615	0.090722	0.862625
1	-2.768615	0.090722	-0.862625
9	1.926897	0.001569	2.242336
9	1.926897	0.001569	-2.242336
17	-0.985334	0.002895	-2.734739
17	-0.985334	0.002895	2.734739

py-10_A_pbe0

6	-0.011686	-1.186649	1.115463
6	0.021824	0.192590	1.197251
6	0.038238	0.933216	-0.000000
6	0.021824	0.192590	-1.197251
6	-0.011686	-1.186649	-1.115463
7	-0.028833	-1.872488	0.000000
7	0.057619	2.278625	-0.000000
1	0.130137	2.779532	0.868192

1	0.130137	2.779532	-0.868192
9	-0.027804	-1.891112	2.236212
9	-0.027804	-1.891112	-2.236212
17	0.043747	1.006381	-2.718695
17	0.043747	1.006381	2.718695

py-10_A_pbe

6	-0.013705	-1.197475	1.124795
6	0.027700	0.191675	1.206805
6	0.049969	0.938792	-0.000000
6	0.027700	0.191675	-1.206805
6	-0.013705	-1.197475	-1.124795
7	-0.034320	-1.889140	0.000000
7	0.090349	2.293627	-0.000000
1	0.105487	2.801253	0.877151
1	0.105487	2.801253	-0.877151
9	-0.035091	-1.915005	2.261932
9	-0.035091	-1.915005	-2.261932
17	0.052340	1.018332	-2.741211
17	0.052340	1.018332	2.741211

py-10_A_rtpss

6	-0.008414	-1.192457	1.120998
6	0.008043	0.194066	1.202601
6	0.012291	0.940222	-0.000000
6	0.008043	0.194066	-1.202601
6	-0.008414	-1.192457	-1.120998
7	-0.018618	-1.892415	0.000000
7	-0.021424	2.301475	-0.000000
1	0.189994	2.782828	0.867112
1	0.189994	2.782828	-0.867112
9	-0.012796	-1.907322	2.259050
9	-0.012796	-1.907322	-2.259050
17	0.026778	1.018665	-2.738861
17	0.026778	1.018665	2.738861

py-10_A_tpssh

6	-0.009918	-1.190530	1.118942
6	0.014502	0.192637	1.200830
6	0.024099	0.936826	-0.000000
6	0.014502	0.192637	-1.200830
6	-0.009918	-1.190530	-1.118942
7	-0.023361	-1.883379	0.000000
7	0.015135	2.291377	-0.000000
1	0.162400	2.784492	0.866925
1	0.162400	2.784492	-0.866925
9	-0.019888	-1.902930	2.249299

9	-0.019888	-1.902930	-2.249299
17	0.034699	1.014338	-2.733051
17	0.034699	1.014338	2.733051

py-10_A_wb97xd

6	-1.209774	-0.000035	1.115254
6	0.169683	0.000126	1.197046
6	0.911079	0.000212	0.000000
6	0.169683	0.000126	-1.197046
6	-1.209774	-0.000035	-1.115254
7	-1.897070	-0.000115	-0.000000
7	2.259349	0.000369	0.000000
1	2.766424	0.000429	0.867137
1	2.766424	0.000429	-0.867137
9	-1.916350	-0.000117	2.235561
9	-1.916350	-0.000117	-2.235561
17	0.983533	0.000220	-2.728344
17	0.983533	0.000220	2.728344

py-10_A_x31yp

6	-0.012180	-1.190372	1.118238
6	0.023105	0.190777	1.199867
6	0.040918	0.934776	-0.000000
6	0.023105	0.190777	-1.199867
6	-0.012180	-1.190372	-1.118238
7	-0.030091	-1.877227	0.000000
7	0.064763	2.286069	-0.000000
1	0.124918	2.790656	0.867884
1	0.124918	2.790656	-0.867884
9	-0.029579	-1.901518	2.246017
9	-0.029579	-1.901518	-2.246017
17	0.045672	1.009068	-2.739000
17	0.045672	1.009068	2.739000

py-14_A_b31yp

6	0.000365	-1.195764	1.121960
6	-0.012915	0.189579	1.189190
6	-0.020757	0.906842	-0.009375
6	-0.014568	0.167273	-1.193583
6	-0.001222	-1.214183	-1.128775
7	0.006059	-1.878778	0.000972
9	0.007928	-1.888840	2.260816
9	-0.018204	0.834517	2.358735
9	0.004643	-1.916103	-2.262750
9	-0.021963	0.840453	-2.363145
8	-0.033643	2.247637	0.012665
1	-0.037638	2.589065	-0.891640

py-14_A_b3p86

6	0.000334	-1.192817	1.118655
6	-0.012919	0.189927	1.187827
6	-0.020742	0.905321	-0.008474
6	-0.014575	0.168194	-1.190865
6	-0.001254	-1.210670	-1.126225
7	0.006012	-1.873967	0.000505
9	0.007858	-1.882387	2.251176
9	-0.018172	0.830548	2.351152
9	0.004576	-1.908443	-2.254158
9	-0.021951	0.840057	-2.352266
8	-0.033572	2.240143	0.011421
1	-0.037512	2.575791	-0.893679

py-14_A_b3pw91

6	0.000344	-1.193754	1.119607
6	-0.012923	0.190382	1.188739
6	-0.020755	0.906672	-0.008960
6	-0.014578	0.168411	-1.192533
6	-0.001243	-1.211916	-1.127043
7	0.006027	-1.875440	0.000635
9	0.007885	-1.885026	2.253048
9	-0.018181	0.831717	2.353502
9	0.004607	-1.911716	-2.255697
9	-0.021948	0.839365	-2.356263
8	-0.033599	2.242998	0.012205
1	-0.037551	2.580005	-0.892170

py-14_A_blyp

6	0.000463	-1.205206	1.131670
6	-0.012921	0.191179	1.200183
6	-0.020838	0.915341	-0.008555
6	-0.014586	0.168479	-1.202305
6	-0.001139	-1.223604	-1.137533
7	0.006213	-1.894737	0.001509
9	0.008166	-1.911598	2.286098
9	-0.018302	0.846788	2.384693
9	0.004844	-1.938978	-2.287140
9	-0.022117	0.854389	-2.387628
8	-0.033874	2.271906	0.015887
1	-0.037825	2.607739	-0.901811

py-14_A_bp86

6	0.000440	-1.202898	1.129376
6	-0.012929	0.192026	1.200366

6	-0.020828	0.914394	-0.006910
6	-0.014603	0.170298	-1.200106
6	-0.001172	-1.220246	-1.136055
7	0.006175	-1.890820	0.000897
9	0.008101	-1.905589	2.276471
9	-0.018274	0.843322	2.377843
9	0.004772	-1.930715	-2.278924
9	-0.022123	0.856106	-2.375725
8	-0.033806	2.264749	0.014414
1	-0.037669	2.591072	-0.906576

py-14_A_bpw91

6	0.000426	-1.201654	1.128248
6	-0.012930	0.192015	1.198940
6	-0.020822	0.913798	-0.007486
6	-0.014601	0.170158	-1.199675
6	-0.001179	-1.219223	-1.135043
7	0.006150	-1.888252	0.000885
9	0.008090	-1.904663	2.274301
9	-0.018271	0.842825	2.375614
9	0.004769	-1.930302	-2.276692
9	-0.022101	0.853810	-2.375265
8	-0.033788	2.262915	0.014638
1	-0.037659	2.590271	-0.903397

py-14_A_camb31yp

6	0.000321	-1.191725	1.116941
6	-0.012904	0.187996	1.183780
6	-0.020714	0.902378	-0.009121
6	-0.014553	0.166153	-1.188022
6	-0.001258	-1.209963	-1.123867
7	0.005996	-1.872282	0.000766
9	0.007820	-1.878421	2.251453
9	-0.018148	0.827869	2.349056
9	0.004543	-1.904946	-2.253815
9	-0.021904	0.835119	-2.352091
8	-0.033543	2.237115	0.010746
1	-0.037573	2.582405	-0.890755

py-14_A_mn15

6	0.000362	-1.195487	1.121260
6	-0.012905	0.188582	1.189056
6	-0.020720	0.903108	-0.007750
6	-0.014561	0.166795	-1.190958
6	-0.001229	-1.213493	-1.128192
7	0.006042	-1.877033	0.000845
9	0.007810	-1.877105	2.255503

9	-0.018134	0.826611	2.351236
9	0.004522	-1.903060	-2.257972
9	-0.021928	0.837901	-2.349511
8	-0.033559	2.238509	0.007298
1	-0.037615	2.586370	-0.895746

py-14_A_o3lyp

6	0.000362	-1.195491	1.121366
6	-0.012936	0.191946	1.190601
6	-0.020792	0.910400	-0.010599
6	-0.014591	0.169340	-1.196983
6	-0.001220	-1.214430	-1.128755
7	0.006061	-1.879041	0.000846
9	0.007943	-1.890812	2.256215
9	-0.018213	0.835269	2.357279
9	0.004678	-1.919318	-2.258237
9	-0.021931	0.836837	-2.365686
8	-0.033662	2.249850	0.015919
1	-0.037616	2.587148	-0.886896

py-14_A_pbe0

6	0.000326	-1.192094	1.117765
6	-0.012923	0.190239	1.187111
6	-0.020742	0.905301	-0.008686
6	-0.014579	0.168637	-1.190790
6	-0.001261	-1.209934	-1.125485
7	0.006007	-1.873411	0.000415
9	0.007831	-1.879818	2.248140
9	-0.018163	0.829388	2.348546
9	0.004554	-1.905854	-2.251251
9	-0.021927	0.837646	-2.350656
8	-0.033554	2.238324	0.011878
1	-0.037486	2.573274	-0.891917

py-14_A_pbe

6	0.000426	-1.201615	1.127832
6	-0.012928	0.191782	1.198773
6	-0.020818	0.913413	-0.007036
6	-0.014601	0.170221	-1.198879
6	-0.001182	-1.218861	-1.134703
7	0.006150	-1.888252	0.000776
9	0.008069	-1.902503	2.273735
9	-0.018265	0.842118	2.374277
9	0.004743	-1.927545	-2.276391
9	-0.022104	0.854282	-2.372750
8	-0.033774	2.261383	0.014748
1	-0.037631	2.587274	-0.905313

py-14_A_rtpss

6	0.000392	-1.198383	1.124233
6	-0.012924	0.191101	1.196078
6	-0.020801	0.911685	-0.005792
6	-0.014593	0.169839	-1.194107
6	-0.001213	-1.215435	-1.131803
7	0.006191	-1.892492	0.000468
9	0.008026	-1.898281	2.270228
9	-0.018239	0.839351	2.374119
9	0.004696	-1.922474	-2.273779
9	-0.022125	0.856835	-2.367716
8	-0.033773	2.261228	0.013157
1	-0.037553	2.578724	-0.910018

py-14_A_tpssh

6	0.000364	-1.195689	1.121841
6	-0.012923	0.190661	1.192078
6	-0.020773	0.908654	-0.007627
6	-0.014581	0.168654	-1.193223
6	-0.001228	-1.213653	-1.129424
7	0.006104	-1.883436	0.000618
9	0.007959	-1.892063	2.260903
9	-0.018209	0.835422	2.363738
9	0.004662	-1.918115	-2.263881
9	-0.022035	0.848006	-2.361876
8	-0.033686	2.252078	0.011897
1	-0.037568	2.581179	-0.899975

py-14_A_wb97xd

6	0.000329	-1.192209	1.117975
6	-0.012924	0.190226	1.185229
6	-0.020742	0.905495	-0.010347
6	-0.014572	0.167649	-1.191657
6	-0.001253	-1.211236	-1.125252
7	0.006025	-1.875386	0.000809
9	0.007840	-1.880047	2.249042
9	-0.018171	0.829756	2.348064
9	0.004573	-1.908134	-2.251222
9	-0.021877	0.832828	-2.355279
8	-0.033565	2.239249	0.013129
1	-0.037578	2.583507	-0.885420

py-14_A_x3lyp

6	0.000360	-1.195365	1.120997
6	-0.012913	0.189397	1.188319

6	-0.020755	0.906651	-0.009713
6	-0.014564	0.166881	-1.193149
6	-0.001223	-1.214097	-1.127859
7	0.006057	-1.878534	0.001022
9	0.007910	-1.887158	2.259204
9	-0.018192	0.833106	2.357262
9	0.004634	-1.915005	-2.261006
9	-0.021944	0.838545	-2.362143
8	-0.033634	2.246714	0.012593
1	-0.037651	2.590563	-0.890459

py-15_A_b31yp

6	-0.002516	-1.214035	1.100148
6	-0.003441	0.171008	1.166950
6	-0.003828	0.889496	-0.020252
6	-0.003269	0.183618	-1.207489
6	-0.002342	-1.214988	-1.180221
7	-0.001989	-1.877482	-0.032378
9	-0.002124	-1.928888	2.229033
9	-0.003950	0.803818	2.351453
9	-0.003609	0.831768	-2.383361
1	-0.001186	-2.841318	-2.118740
1	-0.004547	1.971474	-0.016100
8	-0.001797	-1.899367	-2.337420

py-15_A_b3p86

6	-0.002514	-1.213174	1.096170
6	-0.003439	0.169383	1.164565
6	-0.003825	0.885328	-0.020734
6	-0.003268	0.182856	-1.206809
6	-0.002342	-1.213142	-1.178806
7	-0.001989	-1.873918	-0.034259
9	-0.002127	-1.925078	2.218044
9	-0.003947	0.797579	2.342514
9	-0.003607	0.827230	-2.375615
1	-0.001193	-2.834654	-2.106802
1	-0.004546	1.967916	-0.016300
8	-0.001801	-1.895221	-2.330347

py-15_A_b3pw91

6	-0.002514	-1.213817	1.097339
6	-0.003440	0.170157	1.166106
6	-0.003826	0.886414	-0.020579
6	-0.003268	0.183642	-1.208064
6	-0.002341	-1.213875	-1.179971
7	-0.001989	-1.874629	-0.034174
9	-0.002126	-1.927873	2.219859

9	-0.003949	0.800085	2.344951
9	-0.003609	0.830089	-2.377595
1	-0.001191	-2.836955	-2.107904
1	-0.004547	1.969656	-0.016135
8	-0.001799	-1.897790	-2.332211

py-15_A_blyp

6	-0.002511	-1.219898	1.109738
6	-0.003445	0.176888	1.177071
6	-0.003836	0.901929	-0.018636
6	-0.003272	0.189545	-1.215013
6	-0.002336	-1.220582	-1.189930
7	-0.001979	-1.890442	-0.031251
9	-0.002115	-1.947146	2.254673
9	-0.003965	0.820680	2.377073
9	-0.003620	0.850002	-2.405993
1	-0.001172	-2.863235	-2.130560
1	-0.004561	1.990380	-0.014553
8	-0.001786	-1.913016	-2.360997

py-15_A_bp86

6	-0.002510	-1.220112	1.106099
6	-0.003444	0.175355	1.175421
6	-0.003834	0.898566	-0.019198
6	-0.003272	0.189598	-1.215619
6	-0.002337	-1.218778	-1.189528
7	-0.001980	-1.888091	-0.033928
9	-0.002117	-1.944137	2.242939
9	-0.003960	0.813532	2.368441
9	-0.003618	0.845357	-2.398966
1	-0.001178	-2.856763	-2.115104
1	-0.004560	1.989515	-0.014456
8	-0.001790	-1.908936	-2.354481

py-15_A_bpw91

py-15_A_camb3lyp

6	-0.002515	-1.210696	1.095300
6	-0.003438	0.167985	1.161468
6	-0.003824	0.884160	-0.020874
6	-0.003267	0.180644	-1.202353
6	-0.002343	-1.212437	-1.174849
7	-0.001991	-1.872018	-0.032904
9	-0.002131	-1.919664	2.219636
9	-0.003945	0.795169	2.341844
9	-0.003604	0.822257	-2.374467

1	-0.001193	-2.834128	-2.116300
1	-0.004544	1.966013	-0.016824
8	-0.001803	-1.892180	-2.328055

py-15_A_mn15

6	-0.002515	-1.212505	1.100345
6	-0.003440	0.170780	1.167192
6	-0.003826	0.886605	-0.020048
6	-0.003268	0.183412	-1.206956
6	-0.002342	-1.213450	-1.178129
7	-0.001989	-1.874081	-0.032498
9	-0.002133	-1.916597	2.224062
9	-0.003945	0.793580	2.345526
9	-0.003603	0.821075	-2.376753
1	-0.001189	-2.838861	-2.123347
1	-0.004546	1.968941	-0.016064
8	-0.001802	-1.893794	-2.331709

py-15_A_o3lyp

6	-0.002514	-1.215448	1.099609
6	-0.003442	0.172238	1.169413
6	-0.003828	0.888803	-0.020315
6	-0.003269	0.185214	-1.210897
6	-0.002340	-1.216034	-1.182365
7	-0.001987	-1.877192	-0.033896
9	-0.002121	-1.934198	2.223009
9	-0.003953	0.805947	2.349116
9	-0.003613	0.836028	-2.381042
1	-0.001190	-2.839675	-2.108176
1	-0.004548	1.972023	-0.016085
8	-0.001795	-1.902602	-2.336751

py-15_A_pbe0

6	-0.002514	-1.213109	1.095316
6	-0.003439	0.168999	1.164241
6	-0.003825	0.884545	-0.020980
6	-0.003268	0.182601	-1.206891
6	-0.002342	-1.213011	-1.178030
7	-0.001990	-1.873568	-0.034589
9	-0.002128	-1.923576	2.214747
9	-0.003945	0.795152	2.340298
9	-0.003606	0.824644	-2.373898
1	-0.001195	-2.831618	-2.104018
1	-0.004545	1.967882	-0.016473
8	-0.001802	-1.893836	-2.328100

py-15_A_pbe			
6	-0.002511	-1.219409	1.104462
6	-0.003443	0.174636	1.173987
6	-0.003833	0.896546	-0.019437
6	-0.003271	0.188635	-1.214573
6	-0.002338	-1.218339	-1.188224
7	-0.001981	-1.886181	-0.034097
9	-0.002118	-1.941628	2.240039
9	-0.003958	0.810902	2.365314
9	-0.003616	0.842189	-2.396367
1	-0.001180	-2.853104	-2.112899
1	-0.004558	1.987152	-0.014833
8	-0.001792	-1.906295	-2.351751

py-15_A_rtpss			
6	-0.002513	-1.216829	1.100761
6	-0.003442	0.172924	1.169782
6	-0.003834	0.898087	-0.019741
6	-0.003270	0.187026	-1.210843
6	-0.002340	-1.215414	-1.185266
7	-0.001978	-1.890484	-0.034732
9	-0.002120	-1.937890	2.236660
9	-0.003955	0.806936	2.364022
9	-0.003614	0.839181	-2.395419
1	-0.001183	-2.849412	-2.108329
1	-0.004557	1.984473	-0.015135
8	-0.001794	-1.903493	-2.350138

py-15_A_tpssh			
6	-0.002514	-1.214689	1.099389
6	-0.003441	0.171644	1.167847
6	-0.003830	0.892394	-0.020107
6	-0.003269	0.185240	-1.209113
6	-0.002341	-1.214263	-1.182388
7	-0.001984	-1.881622	-0.034057
9	-0.002123	-1.933128	2.227956
9	-0.003952	0.804305	2.354361
9	-0.003612	0.835259	-2.386142
1	-0.001187	-2.843522	-2.109966
1	-0.004550	1.975163	-0.015639
8	-0.001796	-1.901677	-2.340520

py-15_A_wb97xd			
6	-0.002515	-1.212413	1.096602
6	-0.003439	0.169137	1.163846
6	-0.003825	0.885493	-0.020985
6	-0.003268	0.182121	-1.205409

6	-0.002342	-1.213542	-1.176791
7	-0.001989	-1.875085	-0.033499
9	-0.002128	-1.923496	2.216681
9	-0.003947	0.797323	2.340774
9	-0.003606	0.824607	-2.374096
1	-0.001194	-2.832425	-2.111102
1	-0.004546	1.967894	-0.016614
8	-0.001801	-1.894508	-2.327786

py-15_A_x3lyp

6	-0.002515	-1.213439	1.099796
6	-0.003440	0.170950	1.166731
6	-0.003828	0.889059	-0.020179
6	-0.003268	0.183131	-1.206841
6	-0.002341	-1.215132	-1.179296
7	-0.001988	-1.876895	-0.031999
9	-0.002127	-1.927244	2.227902
9	-0.003951	0.802711	2.350426
9	-0.003609	0.830189	-2.381954
1	-0.001188	-2.840856	-2.120471
1	-0.004548	1.971246	-0.016308
8	-0.001798	-1.898615	-2.336185

C Computed IR and Raman Spectra of monomers

py-01_A_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	121.1486	0.1571	0.0095	0.0031
2	A'	155.2360	0.1423	0.7224	0.2124
3	A'	205.9105	0.2096	1.2733	0.4193
4	A''	275.2808	0.1927	4.7534	0.8068
5	A'	279.8887	0.6705	3.6680	0.4590
6	A'	304.1893	0.0693	247.0842	2.6784
7	A''	312.1516	0.5373	0.2449	0.2142
8	A'	341.7527	0.8863	10.8012	0.6900
9	A'	349.6120	0.8659	13.3973	0.2714
10	A''	409.3057	0.2133	2.2807	1.8928
11	A''	463.8763	1.7095	0.3018	4.4188
12	A''	468.6353	0.2258	3.0396	1.1515
13	A'	485.6509	1.6575	2.4597	6.7591
14	A'	610.0419	2.1482	5.4495	20.5494
15	A'	641.5894	2.7634	6.6897	0.5312
16	A''	673.2523	3.2385	0.0002	0.0036
17	A'	696.2458	4.2833	3.1958	12.9488
18	A''	718.6331	1.9866	0.4396	0.1445
19	A'	729.0306	3.7063	6.3473	0.9167
20	A''	910.8158	2.0816	132.6775	0.0106
21	A'	1116.0109	6.7575	208.4489	0.2468
22	A''	1124.2619	3.2926	74.1090	0.5424
23	A''	1182.4631	2.1859	60.8039	0.6953
24	A'	1281.3574	8.9366	51.5451	6.8237
25	A''	1374.1834	8.8427	18.5998	14.4976
26	A'	1431.7483	14.4633	32.4286	5.2358
27	A''	1504.6276	15.7129	616.0222	3.4541
28	A'	1551.8845	8.1319	93.4046	0.6159
29	A'	1637.3949	2.3591	9.6409	1.0300
30	A''	1645.7640	15.2573	7.4103	0.6915
31	A'	1681.8658	7.8911	385.5952	22.6396
32	A'	3605.9928	8.0087	101.3733	139.1222
33	A''	3722.4729	9.0191	69.6063	36.3667

py-01_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	121.4599	0.1579	0.0093	0.0025
2	A'	155.7929	0.1448	0.6142	0.2163
3	A'	207.8240	0.2080	1.7732	0.4184
4	A''	268.7647	0.1786	4.7283	0.8028
5	A'	277.3286	0.6479	3.9160	0.4228

6	A'	298.4697	0.0662	250.7054	2.6848
7	A''	312.4535	0.5543	0.2204	0.1993
8	A'	344.1652	0.9311	8.0332	0.6404
9	A'	351.9124	0.9353	10.3165	0.2812
10	A''	411.2850	0.1995	2.4911	1.8383
11	A''	464.0786	1.7994	0.2166	4.4016
12	A''	470.6430	0.2418	2.8523	1.0522
13	A'	484.1555	1.6528	2.4265	6.4232
14	A'	613.5067	2.1882	4.7962	19.6868
15	A'	642.6813	2.7419	6.2723	0.4818
16	A''	673.9396	3.2400	0.0008	0.0024
17	A'	700.6421	4.3321	2.3164	13.3685
18	A''	721.9370	1.9698	0.2980	0.1643
19	A'	723.3743	3.6572	6.3975	0.9131
20	A''	921.6553	1.9876	118.2858	0.0045
21	A'	1129.0946	6.8810	202.9800	0.2164
22	A''	1138.4543	2.6194	91.1772	0.2388
23	A''	1195.4515	2.7705	39.1735	0.9550
24	A'	1298.2151	8.7239	53.9320	6.4712
25	A''	1405.8512	10.1083	19.8792	14.0818
26	A'	1452.0882	14.8772	32.8393	5.1045
27	A''	1527.8465	16.3708	639.2009	3.4273
28	A'	1571.1960	5.9075	75.9793	0.3805
29	A'	1638.1385	2.3901	47.6697	1.7277
30	A''	1669.4777	16.3374	8.4809	0.6355
31	A'	1701.6005	12.1372	369.4589	20.7681
32	A'	3624.8754	8.0944	104.7465	136.3516
33	A''	3744.7601	9.1273	73.2643	35.2028

py-01_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	120.8821	0.1564	0.0095	0.0027
2	A'	155.0818	0.1401	0.7048	0.2131
3	A'	208.4518	0.2157	1.4989	0.4177
4	A''	270.8829	0.1822	4.7299	0.8014
5	A'	278.3074	0.6873	2.9667	0.3849
6	A'	302.9842	0.0682	250.4260	2.6557
7	A''	312.8090	0.5565	0.2313	0.2007
8	A'	344.2816	0.9216	8.9068	0.6506
9	A'	351.7402	0.9017	11.9876	0.2862
10	A''	410.4500	0.1895	2.7516	1.7989
11	A''	463.0925	1.7957	0.2205	4.4146
12	A''	469.2963	0.2518	2.7979	1.1126
13	A'	482.9860	1.6384	2.5149	6.4794
14	A'	611.7028	2.1715	4.9526	19.8427
15	A'	642.6348	2.7412	6.4300	0.4955
16	A''	675.0586	3.2513	0.0009	0.0026

17	A'	698.6725	4.3101	2.4919	13.2953
18	A''	721.6131	1.9805	0.3077	0.1619
19	A'	725.4078	3.6731	6.1539	0.8736
20	A''	919.5529	2.0135	121.5420	0.0052
21	A'	1125.1047	6.8473	203.6958	0.2175
22	A''	1135.2316	2.7577	86.7287	0.3042
23	A''	1192.2621	2.5807	43.6996	0.9160
24	A'	1293.4847	8.7725	53.2335	6.4115
25	A''	1400.5165	9.8766	17.8134	14.3565
26	A'	1447.1749	14.7899	31.6520	5.2263
27	A''	1522.5597	16.1890	636.7020	3.3502
28	A'	1566.6539	6.5334	82.6004	0.4573
29	A'	1638.1981	2.3325	36.5751	1.5684
30	A''	1664.9005	16.1916	8.8062	0.6197
31	A'	1696.9928	11.2077	370.2649	21.2593
32	A'	3623.5567	8.0888	101.8533	136.8991
33	A''	3742.7775	9.1166	71.0024	35.4971

py-01_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	113.8493	0.1390	0.0106	0.0044
2	A'	148.1183	0.1225	1.1976	0.2081
3	A'	196.3512	0.2110	0.6111	0.4795
4	A''	267.1616	0.1819	4.5236	0.8905
5	A'	270.0221	0.7374	1.2536	0.3760
6	A''	300.1563	0.4862	0.4371	0.2553
7	A'	321.6877	0.2128	48.3528	0.8566
8	A'	330.8643	0.4783	26.3950	1.0360
9	A'	343.0208	0.1295	190.7277	1.3547
10	A''	392.0903	0.2177	2.1200	1.9138
11	A''	445.2673	1.6537	0.2657	5.0106
12	A''	452.6159	0.1957	3.6154	1.0722
13	A'	465.5840	1.4975	3.7726	8.7878
14	A'	582.2795	1.9027	7.8582	22.7360
15	A'	607.1573	2.4946	6.7558	0.4522
16	A''	633.7474	2.8658	0.0000	0.0074
17	A'	661.7353	3.8605	3.9923	13.4565
18	A'	685.6366	3.2316	3.7285	1.0104
19	A''	689.4988	1.8914	0.8253	0.1875
20	A''	864.8157	2.0763	153.0023	0.0154
21	A''	1060.1933	4.7432	46.6248	1.3419
22	A'	1062.4082	6.2688	202.7762	0.4105
23	A''	1132.9029	1.5590	92.9350	0.8807
24	A'	1208.4934	8.2228	48.0728	7.5315
25	A''	1342.6896	8.1067	54.9006	11.0970
26	A'	1348.5824	12.8178	27.0635	5.3896
27	A''	1424.1929	14.1568	534.7412	5.0734

28	A'	1481.8248	9.5418	70.7441	0.3772
29	A''	1560.8425	13.0189	4.3882	0.6071
30	A'	1580.6083	3.0927	25.4650	2.5694
31	A'	1615.5445	3.3999	321.1307	16.2606
32	A'	3500.9610	7.5475	83.8968	156.0271
33	A''	3612.1086	8.4859	57.9286	40.2332

py-01_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	113.8310	0.1388	0.0117	0.0036
2	A'	148.8628	0.1191	1.3087	0.2059
3	A'	197.3872	0.2155	0.7325	0.4695
4	A''	260.7395	0.1668	4.5297	0.8690
5	A'	267.6872	0.7297	1.2676	0.3229
6	A''	300.5287	0.5022	0.3957	0.2263
7	A'	324.3224	0.3270	22.2917	0.6242
8	A'	334.6737	0.6874	10.2390	0.7269
9	A'	354.9390	0.1110	235.0024	1.7099
10	A''	392.0124	0.1914	2.7682	1.8380
11	A''	445.6644	1.5766	0.2894	4.7915
12	A''	451.4550	0.2177	3.5137	1.2409
13	A'	465.5067	1.4673	4.3700	8.1859
14	A'	587.8695	1.9451	7.2878	21.9933
15	A'	606.4075	2.4957	5.7965	0.3602
16	A''	631.8399	2.8430	0.0007	0.0043
17	A'	667.4816	3.8994	2.9791	13.4479
18	A'	674.8646	3.1642	3.9582	1.4977
19	A''	692.6165	1.8834	0.5232	0.2142
20	A''	878.6745	1.9900	136.6000	0.0043
21	A'	1077.0428	6.4153	196.3953	0.3385
22	A''	1081.9448	3.7083	59.1857	0.8709
23	A''	1143.1959	1.7630	70.7176	1.2896
24	A'	1228.6860	8.0353	50.1267	7.1722
25	A'	1374.0484	13.3631	29.4450	5.3147
26	A''	1375.1460	9.3319	64.4144	10.4384
27	A''	1448.6269	14.8421	558.1221	5.1857
28	A'	1505.0005	7.5987	62.4708	0.4646
29	A'	1580.1884	2.1790	8.1628	0.9989
30	A''	1585.3726	14.1256	4.7406	0.5435
31	A'	1629.6020	7.5697	345.1951	16.4105
32	A'	3508.1054	7.5803	82.2580	155.6779
33	A''	3622.3962	8.5321	59.6587	39.6527

py-01_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A''	113.6655	0.1385	0.0112	0.0036
2	A'	148.5303	0.1191	1.2747	0.2073
3	A'	198.9849	0.2190	0.7269	0.4664
4	A''	263.7737	0.1718	4.5411	0.8655
5	A'	269.6103	0.7392	1.2365	0.3205
6	A''	302.2521	0.5090	0.4085	0.2303
7	A'	325.4438	0.2588	36.1569	0.7166
8	A'	335.5837	0.5889	17.0231	0.8415
9	A'	350.7153	0.1205	213.9889	1.5119
10	A''	394.2078	0.1879	2.8227	1.8126
11	A''	446.5543	1.6495	0.2441	4.8176
12	A''	453.5589	0.2236	3.3750	1.1410
13	A'	466.1146	1.4815	4.0759	8.0819
14	A'	589.0955	1.9670	7.1522	21.6562
15	A'	609.8299	2.5125	6.0704	0.3735
16	A''	637.3117	2.8934	0.0008	0.0050
17	A'	669.1310	3.9362	2.9931	13.8603
18	A'	682.7295	3.2226	3.7950	1.0654
19	A''	695.4531	1.9008	0.5466	0.2122
20	A''	881.0650	2.0159	138.6780	0.0055
21	A'	1079.5194	6.4638	198.2352	0.3204
22	A''	1083.4936	3.8179	58.5873	0.8934
23	A''	1146.0744	1.7448	72.5733	1.2383
24	A'	1231.4924	8.1214	49.9708	6.9847
25	A'	1378.0163	13.4389	28.1318	5.2531
26	A''	1380.1213	9.3644	60.2615	10.5914
27	A''	1452.4535	14.8753	560.3840	5.0686
28	A'	1509.6001	7.8643	64.1069	0.4422
29	A'	1587.9081	2.2279	5.7695	0.9700
30	A''	1590.8645	14.2996	5.4228	0.5307
31	A'	1635.0217	7.1309	346.6666	16.6146
32	A'	3529.9566	7.6750	82.7426	151.8501
33	A''	3644.5529	8.6373	59.3104	38.9004

py-01_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	124.8634	0.1667	0.0050	0.0033
2	A'	152.9919	0.2044	14.4348	0.7470
3	A'	199.5219	0.0341	132.2548	2.0908
4	A'	218.1563	0.0983	113.4945	2.2504
5	A''	274.0403	0.1909	4.8444	0.8410
6	A'	281.3434	0.7953	2.5549	0.1702
7	A''	314.9528	0.5538	0.1762	0.2110
8	A'	347.0799	0.9509	1.9524	0.5463
9	A'	353.7450	1.0832	4.1465	0.2666
10	A''	420.2029	0.2468	1.0614	1.8414

11	A''	469.9667	1.9435	0.1617	4.3461
12	A''	481.6190	0.2158	1.8384	0.6990
13	A'	490.5729	1.7347	1.3837	5.8724
14	A'	619.8654	2.2817	3.6641	18.6360
15	A'	659.8086	2.8698	6.9209	0.7151
16	A''	694.0986	3.4474	0.0000	0.0023
17	A'	708.9709	4.4264	2.0650	13.6725
18	A''	726.8621	1.9380	0.3782	0.0950
19	A'	755.2952	3.9901	8.3637	0.9700
20	A''	925.7115	1.9582	113.4349	0.0198
21	A'	1139.6865	6.9208	211.8543	0.2553
22	A''	1142.7266	2.4529	107.3897	0.2500
23	A''	1200.6268	3.3096	32.1055	0.4618
24	A'	1312.3340	8.9541	51.8064	5.7553
25	A''	1365.2462	8.8586	9.4957	19.1928
26	A'	1466.5552	14.9972	31.6178	5.2165
27	A''	1543.2750	16.6431	641.4301	3.2243
28	A'	1580.4214	5.5298	91.7634	1.7095
29	A'	1650.0578	2.4450	85.3009	3.0896
30	A''	1690.7032	16.9024	12.8951	0.7001
31	A'	1717.7375	14.3630	387.4468	26.4643
32	A'	3636.5919	8.1435	124.2901	128.4402
33	A''	3755.9665	9.1927	83.5050	32.8547

py-01_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	125.8587	0.1695	0.0113	0.0020
2	A'	159.7851	0.1392	1.0102	0.2174
3	A'	210.3104	0.2245	1.2784	0.4074
4	A''	271.6849	0.1878	4.6193	0.7697
5	A'	279.3273	0.7230	2.2611	0.3311
6	A''	314.5881	0.5549	0.1064	0.1891
7	A'	315.4460	0.0770	249.8028	2.8348
8	A'	348.1459	0.8268	17.9298	0.7163
9	A'	357.0964	0.7751	22.3520	0.3856
10	A''	409.1635	0.1587	4.2434	1.7324
11	A''	466.1116	0.3054	2.9100	0.8925
12	A''	468.9836	1.8540	0.0065	4.6709
13	A'	488.5760	1.6332	2.7978	5.8239
14	A'	620.7320	2.2136	4.4349	17.6341
15	A'	649.2458	2.7946	5.3002	0.4497
16	A''	684.6359	3.3447	0.0017	0.0020
17	A'	712.7655	4.4504	2.5017	14.1106
18	A''	726.4237	2.0130	0.1381	0.1142
19	A'	734.2393	3.8229	8.7459	0.7991
20	A''	940.2765	1.9431	104.0718	0.0032
21	A'	1144.6360	6.8368	199.0185	0.2615

22	A''	1156.5639	2.1133	103.9272	0.1074
23	A''	1224.7471	4.3202	16.4147	0.4522
24	A'	1329.7887	8.8045	47.8200	5.0287
25	A''	1361.6972	8.7371	5.0127	18.5490
26	A'	1485.2849	15.5035	33.6175	5.5863
27	A''	1560.0485	17.2078	664.0677	2.5907
28	A'	1586.2543	5.0926	93.1315	2.9121
29	A'	1646.8747	2.5143	99.7049	5.1320
30	A''	1701.5465	17.1990	8.8846	0.5295
31	A'	1723.6744	15.2898	341.9702	26.0169
32	A'	3625.4764	8.0989	119.8449	138.1796
33	A''	3746.4365	9.1364	83.3974	35.5446

py-01_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	54.3203	0.0027	192.1148	0.0016
2	A''	123.2981	0.1620	0.0000	0.0020
3	A'	164.7170	0.0479	38.2020	0.2665
4	A'	210.0757	0.3798	8.2099	0.4183
5	A''	265.8684	0.1809	4.8725	0.9200
6	A'	272.4408	0.7562	1.8880	0.1520
7	A''	308.9818	0.5305	0.1136	0.2697
8	A'	344.5024	0.9345	1.8738	0.4719
9	A'	350.9061	1.0745	3.7256	0.3076
10	A''	419.4222	0.2658	0.0000	2.0067
11	A''	458.2015	1.8497	0.0853	4.5576
12	A'	476.3732	1.6369	1.3989	5.7202
13	A''	482.5935	0.2028	0.0000	0.2467
14	A'	614.0374	2.2985	2.4498	17.6734
15	A'	655.7532	2.8960	6.1504	0.2066
16	A''	681.0567	3.3158	0.0000	0.0011
17	A'	701.7527	4.3161	0.7224	15.8282
18	A''	715.2744	1.7934	0.3663	0.1124
19	A'	743.4726	3.8901	9.1192	0.2321
20	A''	921.7550	1.6633	86.1074	0.0066
21	A''	1131.6088	1.9658	135.0934	0.0108
22	A'	1138.9870	6.8118	209.0131	0.2211
23	A''	1206.8120	5.7354	8.9053	0.6747
24	A'	1315.4586	8.1165	52.4701	6.2258
25	A''	1373.5503	10.4223	12.5718	17.1098
26	A'	1476.8791	15.1759	38.5378	5.3654
27	A''	1554.3672	17.2831	684.8730	2.9920
28	A'	1571.5616	2.8909	34.1096	0.3242
29	A'	1628.6333	3.6937	187.6789	5.6390
30	A''	1689.1421	17.7637	11.6546	0.7525
31	A'	1712.5938	17.3786	364.2349	24.1882
32	A'	3650.1131	8.2034	130.8141	134.7891

33 A" 3779.6795 9.3134 86.9416 35.2463

py-01_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A"	119.0734	0.1518	0.0267	0.0021
2	A'	154.2202	0.1042	2.4177	0.1967
3	A'	209.4650	0.2915	0.9144	0.3663
4	A"	277.6214	0.1889	4.2158	0.7052
5	A'	282.5171	0.8224	1.1976	0.2113
6	A"	313.4107	0.5745	0.1369	0.1499
7	A'	339.8822	0.7400	1.1863	0.5202
8	A'	349.6813	1.0727	1.9936	0.2343
9	A"	376.5401	0.0997	13.5450	1.0190
10	A"	451.8069	0.6786	2.0402	2.0301
11	A"	463.8974	1.9143	0.0117	5.0646
12	A'	483.4157	1.7460	1.0922	5.5519
13	A'	546.8429	0.4494	113.7990	3.1585
14	A'	572.8840	0.6256	140.9395	3.7347
15	A'	606.5109	1.9234	9.2833	15.2739
16	A"	617.1452	2.7007	0.0114	0.0097
17	A'	623.7772	0.9439	75.9035	8.9494
18	A'	704.0987	4.0569	9.9596	14.1617
19	A"	714.8973	2.1803	0.1214	0.1121
20	A"	929.5656	2.3395	125.4968	0.0078
21	A'	1112.3659	6.3808	188.7423	0.3874
22	A"	1150.7549	3.7307	42.2041	0.1739
23	A"	1218.3619	1.8874	51.8542	0.6627
24	A'	1297.1032	8.8713	35.1448	3.9614
25	A'	1445.3510	15.0366	36.2247	7.3167
26	A"	1461.2817	11.4317	56.6797	15.2733
27	A"	1529.5699	16.4132	573.9400	5.4456
28	A'	1569.5787	9.8953	71.1289	4.6758
29	A'	1646.1958	2.1885	10.8992	0.8073
30	A"	1670.9924	15.4123	0.7007	0.4650
31	A'	1708.3873	9.1845	276.8780	36.3028
32	A'	3604.7541	8.0167	78.5645	164.0025
33	A"	3723.5775	8.9971	57.5151	36.6030

py-01_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A"	118.3569	0.1501	0.0123	0.0035
2	A'	153.0159	0.1204	1.5063	0.1890
3	A'	208.2920	0.2475	0.6431	0.4267
4	A"	279.1765	0.1971	4.5619	0.7756

5	A'	281.6149	0.8070	1.1173	0.2613
6	A''	313.5578	0.5544	0.3261	0.2065
7	A'	338.7227	0.3186	28.0313	0.6906
8	A'	348.0466	0.7588	10.8833	0.6727
9	A'	367.9584	0.1238	239.4330	1.7479
10	A''	404.5442	0.1618	4.2940	1.6275
11	A''	458.7257	1.7068	0.2878	4.4332
12	A''	462.6453	0.2903	3.0164	1.5211
13	A'	478.4131	1.5142	4.5664	7.1056
14	A'	605.2698	2.0652	6.4813	20.9294
15	A'	636.0590	2.7436	6.5047	0.5267
16	A''	673.3670	3.2372	0.0007	0.0038
17	A'	690.1994	4.2046	3.3326	12.4827
18	A''	718.3034	2.0406	0.3200	0.1669
19	A'	726.7595	3.6727	4.7767	0.8051
20	A''	913.6076	2.1178	133.9472	0.0029
21	A'	1110.7340	6.7246	199.8006	0.2791
22	A''	1125.0001	3.3633	67.1590	0.5843
23	A''	1185.2329	2.0544	59.1750	1.0133
24	A'	1276.7210	8.7488	51.6345	6.2451
25	A''	1402.7363	9.6187	18.4866	13.6873
26	A'	1430.5196	14.5415	29.8589	5.9510
27	A''	1504.1092	15.6599	640.0537	3.3201
28	A'	1551.9656	8.2464	87.4989	0.3026
29	A'	1634.8228	2.3307	8.2338	1.2738
30	A''	1647.6817	15.6435	7.6331	0.5038
31	A'	1682.4506	7.9350	354.0776	20.0668
32	A'	3622.7473	8.0878	89.8212	146.5305
33	A''	3739.9375	9.0952	62.1642	37.3716

py-01_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	122.5868	0.1607	0.0105	0.0026
2	A'	157.2942	0.1402	0.8015	0.2033
3	A'	209.5370	0.2196	1.5138	0.4004
4	A''	271.4959	0.1837	4.6860	0.7679
5	A'	279.2586	0.7366	1.9928	0.3230
6	A'	311.6980	0.0731	247.3312	2.6484
7	A''	314.6487	0.5564	0.2224	0.1907
8	A'	347.7339	0.8782	13.1518	0.7060
9	A'	355.3640	0.8498	15.8506	0.2894
10	A''	413.1388	0.1884	3.0398	1.7715
11	A''	466.5112	1.7938	0.2341	4.3069
12	A''	472.1596	0.2610	2.9341	1.2156
13	A'	487.0139	1.6510	2.6549	6.1996
14	A'	618.7860	2.2257	4.7800	19.2822
15	A'	648.3547	2.8081	6.1055	0.5116

16	A''	683.1434	3.3326	0.0007	0.0024
17	A'	706.3156	4.3977	2.3405	13.2636
18	A''	726.7614	2.0032	0.2276	0.1548
19	A'	734.1041	3.7762	6.6704	0.8664
20	A''	930.8619	2.0020	115.9032	0.0034
21	A'	1138.4830	6.9592	201.6232	0.2265
22	A''	1149.4720	2.4853	93.5870	0.1739
23	A''	1207.1928	3.0366	32.9981	0.9176
24	A'	1311.7308	8.7655	53.5040	6.1136
25	A''	1412.9216	10.2578	14.9209	14.9705
26	A'	1469.7534	15.2466	33.6490	5.4786
27	A''	1543.9578	16.7102	654.8449	3.1781
28	A'	1583.7714	5.3554	74.3087	0.6498
29	A'	1646.7859	2.4937	62.7511	2.3785
30	A''	1687.2406	16.8209	9.3362	0.5970
31	A'	1716.1383	13.3607	363.5773	21.5770
32	A'	3640.8725	8.1672	104.5785	136.6677
33	A''	3761.5152	9.2081	73.6457	35.0032

py-01_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	114.2558	0.1397	0.0115	0.0038
2	A'	149.4335	0.1232	1.1323	0.2053
3	A'	197.9133	0.2125	0.8126	0.4662
4	A''	262.7573	0.1719	4.4547	0.8636
5	A'	268.2932	0.7304	1.2446	0.3104
6	A''	301.5858	0.4981	0.4436	0.2364
7	A'	324.5135	0.1959	58.7065	0.8931
8	A'	335.2669	0.4737	28.3962	1.0314
9	A'	346.5645	0.1413	177.7874	1.2730
10	A''	395.4647	0.2022	2.5007	1.8369
11	A''	446.5283	1.6910	0.2014	4.8581
12	A''	456.0459	0.2124	3.5544	1.0860
13	A'	466.0064	1.4954	3.7740	8.0781
14	A'	590.4460	1.9891	6.8866	21.5615
15	A'	610.1022	2.5181	6.1949	0.4167
16	A''	639.0003	2.9126	0.0002	0.0057
17	A'	670.1911	3.9466	2.6741	13.8486
18	A'	686.1647	3.2501	3.6000	1.0612
19	A''	694.8202	1.8855	0.5276	0.2095
20	A''	883.1856	1.9750	133.9704	0.0031
21	A'	1083.1282	6.5114	196.2806	0.3801
22	A''	1087.0514	3.4937	64.2204	0.7204
23	A''	1146.4235	1.8321	65.9038	1.4220
24	A'	1235.6895	7.9891	49.8219	6.8949
25	A'	1382.9630	13.5262	28.4337	5.7502
26	A''	1388.7318	9.7598	68.7644	10.3597

27	A''	1457.8499	15.0555	561.6850	5.2669
28	A'	1514.9493	6.7379	57.7924	0.4981
29	A'	1582.7599	2.1702	16.7435	1.0769
30	A''	1596.4067	14.6038	5.7958	0.4789
31	A'	1638.8431	9.0726	344.9994	16.2399
32	A'	3523.8169	7.6482	86.4116	155.5341
33	A''	3639.1447	8.6125	61.9359	38.8579

py-01_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	116.5497	0.1455	0.0184	0.0031
2	A'	152.7203	0.1138	2.2262	0.1885
3	A'	198.9842	0.2304	0.6716	0.4299
4	A''	253.1947	0.1594	4.4253	0.7511
5	A'	261.3602	0.7001	1.3814	0.2780
6	A''	298.0177	0.4705	0.3972	0.2000
7	A'	328.6815	0.6466	2.4294	0.5315
8	A'	336.9368	0.9865	1.3262	0.4044
9	A''	390.2659	0.1659	5.0399	1.7460
10	A''	447.0615	0.7851	1.3707	3.3554
11	A'	447.6296	0.1896	233.1162	0.4898
12	A''	449.2047	0.3008	3.3587	2.7956
13	A'	471.3505	0.5666	66.5040	9.8975
14	A'	594.2316	1.7435	12.7860	22.4177
15	A'	608.3925	2.6596	3.6218	0.3413
16	A''	634.7317	2.8670	0.0023	0.0041
17	A'	671.6190	3.2469	3.7108	1.5543
18	A'	675.3661	3.8642	6.7737	12.5356
19	A''	693.9233	1.9635	0.2723	0.2425
20	A''	890.4683	2.1776	146.1883	0.0039
21	A'	1084.9662	6.3648	194.6765	0.2525
22	A''	1097.9802	4.9863	37.9474	1.1339
23	A''	1165.8922	1.6049	80.4913	0.9252
24	A'	1238.9594	8.3107	48.8852	6.7381
25	A''	1388.0856	9.1311	70.9641	10.3078
26	A'	1388.7022	13.7726	27.3367	5.3127
27	A''	1468.8260	15.2648	555.2322	5.3278
28	A'	1522.0063	9.6548	72.8852	0.1882
29	A''	1608.9137	13.8096	1.9037	0.6814
30	A'	1618.3738	2.4807	6.0756	1.3375
31	A'	1659.2834	5.3790	317.1994	18.3250
32	A'	3512.4582	7.6028	59.0740	160.3810
33	A''	3623.6169	8.5276	45.5129	44.8291

py-01_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	119.3575	0.1526	0.0135	0.0030
2	A'	154.7647	0.1241	1.5969	0.1910
3	A'	205.2331	0.2375	0.6964	0.4241
4	A''	260.7787	0.1690	4.6272	0.7691
5	A'	269.5571	0.7421	1.2967	0.2714
6	A''	305.5542	0.5130	0.2761	0.1993
7	A'	336.0649	0.4644	11.1567	0.5728
8	A'	343.2860	0.9132	3.7728	0.4831
9	A'	381.8577	0.1184	271.5917	2.0802
10	A''	403.7560	0.1849	3.7692	1.7976
11	A''	456.6918	1.6004	0.3153	4.4607
12	A''	461.8605	0.2502	3.7094	1.3463
13	A'	477.5136	1.4803	5.7573	7.4038
14	A'	604.2804	2.0080	7.3344	21.4138
15	A'	628.6306	2.6807	5.7154	0.3901
16	A''	658.1121	3.0840	0.0019	0.0034
17	A'	688.2221	4.1683	3.6212	12.7971
18	A'	703.0695	3.4549	5.4774	1.0155
19	A''	709.1778	1.9894	0.2886	0.2000
20	A''	906.6245	2.1318	135.6520	0.0055
21	A'	1106.0898	6.6366	202.5370	0.2283
22	A''	1120.9610	3.9326	55.9367	0.7380
23	A''	1181.0227	1.8988	69.2937	0.8356
24	A'	1268.0818	8.7420	50.5922	6.7599
25	A''	1392.2385	9.2745	33.8046	12.7201
26	A'	1419.4101	14.3354	30.1171	5.2833
27	A''	1497.1716	15.6941	608.1663	4.0729
28	A'	1546.3654	9.1424	88.3065	0.2910
29	A''	1638.6039	14.8449	4.2695	0.6372
30	A'	1638.6317	2.4289	3.5370	1.0717
31	A'	1680.9681	6.5390	357.0570	20.5549
32	A'	3579.2138	7.8934	81.4624	148.4050
33	A''	3695.5805	8.8804	58.8983	40.2326

py-01_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	123.1724	0.1626	0.0089	0.0029
2	A'	156.6844	0.1470	0.5273	0.2185
3	A'	211.0534	0.2077	2.2303	0.3827
4	A''	277.8597	0.1948	4.6362	0.7930
5	A'	281.8454	0.1699	71.4689	1.8012
6	A'	288.8055	0.0834	194.1360	1.8034
7	A''	317.1108	0.5729	0.1788	0.1856
8	A'	346.8636	0.9690	6.1800	0.5843
9	A'	355.6618	1.0133	7.8050	0.2738

10	A"	411.5693	0.1697	3.1597	1.6096
11	A"	468.5343	0.8054	1.1075	2.9217
12	A"	469.6136	0.3575	1.4944	2.5994
13	A'	488.9950	1.6809	2.1461	5.9404
14	A'	617.3039	2.2182	4.4602	19.1043
15	A'	652.3131	2.8074	6.0913	0.5586
16	A"	687.5050	3.3755	0.0010	0.0018
17	A'	706.2606	4.4039	2.8345	13.3667
18	A"	729.4316	2.0166	0.2498	0.1070
19	A'	738.9702	3.8336	7.8219	0.8302
20	A"	928.3833	2.0333	121.5653	0.0132
21	A'	1136.0870	6.9102	207.8841	0.2558
22	A"	1146.1219	2.5979	93.5539	0.3320
23	A"	1203.7875	2.9256	36.4514	0.4793
24	A'	1308.9572	8.9735	52.1087	5.5179
25	A"	1374.7734	8.8547	6.3823	18.7944
26	A'	1463.9580	15.0710	31.7419	5.2283
27	A"	1540.2725	16.4786	656.5601	3.0599
28	A'	1579.4790	6.3553	98.5878	1.9805
29	A'	1652.8965	2.3675	55.0073	2.2743
30	A"	1690.3136	16.8211	11.9379	0.6880
31	A'	1716.3413	12.5866	380.1028	25.5585
32	A'	3647.7412	8.1985	101.6622	129.4530
33	A"	3768.3682	9.2435	70.9923	33.5130

py-01_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A"	122.0249	0.1594	0.0087	0.0032
2	A'	155.5970	0.1513	0.5348	0.2256
3	A'	207.0440	0.2018	1.6651	0.4206
4	A"	273.8891	0.1901	4.7566	0.8181
5	A'	278.7722	0.3870	18.3516	0.8232
6	A'	290.1034	0.0660	239.9517	2.5935
7	A"	312.1688	0.5430	0.2261	0.2123
8	A'	342.7760	0.9500	5.3271	0.6309
9	A'	349.8045	0.9626	8.7617	0.2780
10	A"	411.2320	0.2167	2.0727	1.8931
11	A"	464.2630	1.8160	0.2252	4.4966
12	A"	470.7360	0.2241	2.8821	1.0379
13	A'	484.8558	1.6703	2.1795	6.6870
14	A'	609.5512	2.1485	5.0317	20.5370
15	A'	644.8804	2.7696	7.0549	0.5895
16	A"	676.9327	3.2745	0.0001	0.0035
17	A'	696.9936	4.2975	3.0012	12.8307
18	A"	719.7219	1.9762	0.4130	0.1391
19	A'	733.2082	3.7418	6.3676	0.9448
20	A"	912.4235	2.0582	129.0852	0.0115

21	A'	1117.8115	6.7670	208.5771	0.2527
22	A''	1126.5917	3.1646	78.5008	0.4955
23	A''	1184.0334	2.2823	57.5359	0.7070
24	A'	1283.5049	8.9646	52.0769	6.7042
25	A''	1374.6867	8.9129	16.9182	14.8661
26	A'	1432.7161	14.4679	31.0056	5.3800
27	A''	1508.9744	15.8011	621.5049	3.3440
28	A'	1553.7883	8.0193	97.4158	0.7119
29	A'	1639.6665	2.3299	13.6965	1.0951
30	A''	1650.5685	15.4801	8.2468	0.6486
31	A'	1685.5249	8.4984	388.4405	23.1376
32	A'	3610.1697	8.0274	105.4152	138.7867
33	A''	3727.0479	9.0426	71.6316	36.1719

py-01_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	121.1489	0.1571	0.0095	0.0031
2	A	155.2360	0.1423	0.7224	0.2124
3	A	205.9109	0.2096	1.2735	0.4193
4	A	275.2810	0.1927	4.7532	0.8068
5	A	279.8886	0.6706	3.6669	0.4590
6	A	304.1891	0.0693	247.0850	2.6783
7	A	312.1516	0.5373	0.2449	0.2142
8	A	341.7529	0.8863	10.8023	0.6900
9	A	349.6120	0.8659	13.3973	0.2714
10	A	409.3056	0.2133	2.2809	1.8927
11	A	463.8762	1.7096	0.3017	4.4189
12	A	468.6354	0.2258	3.0398	1.1514
13	A	485.6508	1.6575	2.4596	6.7591
14	A	610.0413	2.1482	5.4495	20.5493
15	A	641.5892	2.7634	6.6894	0.5311
16	A	673.2524	3.2385	0.0002	0.0036
17	A	696.2457	4.2833	3.1958	12.9487
18	A	718.6329	1.9866	0.4396	0.1445
19	A	729.0303	3.7063	6.3475	0.9167
20	A	910.8152	2.0816	132.6779	0.0106
21	A	1116.0097	6.7575	208.4495	0.2468
22	A	1124.2605	3.2926	74.1095	0.5425
23	A	1182.4631	2.1859	60.8034	0.6953
24	A	1281.3575	8.9366	51.5454	6.8236
25	A	1374.1835	8.8427	18.5995	14.4977
26	A	1431.7468	14.4633	32.4281	5.2358
27	A	1504.6273	15.7129	616.0224	3.4541
28	A	1551.8835	8.1320	93.4068	0.6160
29	A	1637.3945	2.3590	9.6408	1.0301
30	A	1645.7646	15.2573	7.4100	0.6915
31	A	1681.8651	7.8910	385.5911	22.6395

32	A	3605.9928	8.0087	101.3728	139.1219
33	A	3722.4729	9.0191	69.6058	36.3667

py-01_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	125.8598	0.1695	0.0113	0.0020
2	A	159.7886	0.1393	1.0104	0.2173
3	A	210.3348	0.2250	1.2560	0.4075
4	A	271.7043	0.1877	4.6299	0.7687
5	A	279.3328	0.7248	2.2222	0.3288
6	A	314.5899	0.5544	0.1078	0.1889
7	A	315.8313	0.0773	249.3016	2.8310
8	A	348.1625	0.8235	18.1481	0.7189
9	A	357.1117	0.7706	22.6630	0.3877
10	A	409.1921	0.1589	4.2313	1.7340
11	A	466.1241	0.3054	2.9085	0.8906
12	A	468.9850	1.8492	0.0059	4.6735
13	A	488.5755	1.6330	2.8011	5.8250
14	A	620.7333	2.2136	4.4372	17.6333
15	A	649.2530	2.7943	5.3047	0.4500
16	A	684.6377	3.3447	0.0017	0.0020
17	A	712.7652	4.4503	2.5021	14.1100
18	A	726.4458	2.0138	0.1380	0.1140
19	A	734.2429	3.8229	8.7438	0.8000
20	A	940.3234	1.9440	104.1374	0.0033
21	A	1144.6385	6.8370	199.0153	0.2614
22	A	1156.6197	2.1139	103.8379	0.1080
23	A	1224.7679	4.3154	16.4490	0.4514
24	A	1329.7902	8.8052	47.8236	5.0291
25	A	1361.7043	8.7338	5.0088	18.5486
26	A	1485.2855	15.5036	33.6197	5.5862
27	A	1560.0484	17.2073	664.0657	2.5906
28	A	1586.2663	5.0948	93.1527	2.9133
29	A	1646.8945	2.5138	99.6781	5.1306
30	A	1701.5486	17.1977	8.8839	0.5295
31	A	1723.6744	15.2892	341.9931	26.0179
32	A	3625.4886	8.0990	119.8497	138.1787
33	A	3746.4450	9.1364	83.3984	35.5440

py-01_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.0733	0.1518	0.0267	0.0021
2	A	154.2205	0.1042	2.4177	0.1967
3	A	209.4647	0.2915	0.9144	0.3663

4	A	277.6216	0.1889	4.2158	0.7052
5	A	282.5170	0.8224	1.1976	0.2113
6	A	313.4106	0.5745	0.1369	0.1499
7	A	339.8824	0.7400	1.1863	0.5202
8	A	349.6811	1.0727	1.9936	0.2343
9	A	376.5387	0.0997	13.5452	1.0190
10	A	451.8077	0.6787	2.0401	2.0301
11	A	463.8975	1.9143	0.0117	5.0645
12	A	483.4159	1.7460	1.0922	5.5519
13	A	546.8447	0.4493	113.8093	3.1587
14	A	572.8851	0.6257	140.9273	3.7346
15	A	606.5112	1.9234	9.2830	15.2740
16	A	617.1460	2.7007	0.0113	0.0097
17	A	623.7784	0.9439	75.9059	8.9495
18	A	704.0988	4.0569	9.9599	14.1616
19	A	714.8976	2.1803	0.1214	0.1121
20	A	929.5659	2.3395	125.4968	0.0078
21	A	1112.3662	6.3808	188.7422	0.3874
22	A	1150.7561	3.7307	42.2040	0.1739
23	A	1218.3619	1.8874	51.8540	0.6627
24	A	1297.1029	8.8713	35.1448	3.9614
25	A	1445.3514	15.0366	36.2254	7.3167
26	A	1461.2820	11.4317	56.6806	15.2731
27	A	1529.5715	16.4132	573.9404	5.4457
28	A	1569.5785	9.8954	71.1285	4.6759
29	A	1646.1957	2.1885	10.8995	0.8073
30	A	1670.9930	15.4123	0.7007	0.4651
31	A	1708.3875	9.1846	276.8770	36.3025
32	A	3604.7548	8.0167	78.5639	164.0022
33	A	3723.5781	8.9971	57.5148	36.6032

py-04_A_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.1305	0.1025	0.0516	0.0667
2	A	137.6134	0.1611	0.9949	0.2410
3	A	206.0069	0.1198	10.4911	0.7313
4	A	221.5454	0.4412	3.0693	1.4333
5	A	231.6403	0.0422	219.0687	3.7512
6	A	289.5173	0.4551	3.0652	0.2279
7	A	312.9588	0.3167	2.0169	0.5306
8	A	318.2922	0.7036	0.0182	0.3087
9	A	335.1389	0.9324	1.7220	1.9821
10	A	395.4141	0.4003	3.3715	0.9694
11	A	406.7245	1.2025	1.9430	6.2303
12	A	476.0406	1.7701	1.6070	5.5234
13	A	487.7920	0.1710	2.9452	0.3171
14	A	609.5810	2.0565	3.5335	26.6390

15	A	632.2165	3.6210	7.2324	3.7027
16	A	651.0255	2.8342	5.5162	1.1777
17	A	681.1572	3.2913	0.6166	0.1958
18	A	700.1902	1.7272	1.0575	0.2760
19	A	747.3593	3.8919	10.0429	1.4339
20	A	845.3686	2.7091	105.3062	1.6324
21	A	1077.8826	5.1532	58.9120	1.3028
22	A	1115.3780	3.8147	105.3200	0.8566
23	A	1126.7593	1.8688	122.4006	0.7531
24	A	1240.6852	6.3332	47.3254	4.5753
25	A	1364.7266	8.6138	25.4371	20.8829
26	A	1425.6369	13.9289	72.5921	5.9177
27	A	1474.8422	12.9610	370.3528	3.7498
28	A	1528.8933	6.9388	198.8710	1.2218
29	A	1627.0475	8.0581	41.5652	5.9316
30	A	1632.2167	3.2958	4.6957	0.7744
31	A	1669.6384	5.7076	459.0927	17.8075
32	A	3607.3532	8.0132	93.7924	124.1166
33	A	3727.2989	9.0461	74.0960	28.2605

py-04_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.7985	0.1062	0.0739	0.0694
2	A	137.6185	0.1727	2.2877	0.2936
3	A	206.2001	0.0624	49.4543	1.1986
4	A	218.4518	0.1400	50.8488	2.8079
5	A	220.0999	0.0663	129.5782	2.0151
6	A	284.9209	0.3708	3.2840	0.2479
7	A	311.1508	0.3336	1.7277	0.3538
8	A	320.3551	0.7084	0.0362	0.2944
9	A	336.6349	1.0176	1.5244	1.9930
10	A	398.2606	0.3898	3.0517	0.9212
11	A	409.1335	1.2300	1.8301	5.8314
12	A	475.3578	1.7596	1.6245	5.2561
13	A	490.9982	0.1753	2.6143	0.2913
14	A	612.5072	2.0962	3.2268	25.9579
15	A	635.9133	3.6733	5.6126	3.9046
16	A	653.7602	2.8398	5.2625	1.1647
17	A	683.5005	3.3056	0.4519	0.2036
18	A	702.3394	1.7061	0.9962	0.3088
19	A	745.5846	3.8788	10.2733	1.3489
20	A	856.5287	2.6187	96.2470	1.6321
21	A	1091.7487	3.8512	61.5942	1.4938
22	A	1125.2830	2.1988	94.3575	1.0243
23	A	1137.0497	3.5895	120.6914	0.2631
24	A	1257.1490	6.7294	46.3148	4.6776
25	A	1396.1293	9.8772	28.1354	20.1813

26	A	1444.7740	14.0751	73.5722	5.5967
27	A	1495.9679	12.6318	363.3220	3.8024
28	A	1546.9150	5.2846	197.5167	0.8976
29	A	1632.5264	2.6143	61.7654	2.8890
30	A	1652.2805	15.1957	30.3096	3.3413
31	A	1687.7748	10.2355	448.9383	17.1865
32	A	3623.2165	8.0857	96.2375	121.1226
33	A	3747.4311	9.1438	79.0393	27.7509

py-04_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.2508	0.1039	0.0586	0.0681
2	A	137.1612	0.1668	1.7283	0.2752
3	A	207.4174	0.0742	36.9047	1.0176
4	A	219.0143	0.2727	16.0539	1.9368
5	A	221.9761	0.0497	178.5045	2.9443
6	A	286.1650	0.3789	3.2710	0.2519
7	A	311.3200	0.3360	1.7489	0.3738
8	A	320.6087	0.7051	0.0431	0.2945
9	A	336.3232	0.9945	1.5489	2.0083
10	A	398.3605	0.3724	3.1779	0.9512
11	A	408.1948	1.2213	1.8548	5.8194
12	A	474.2498	1.7472	1.6342	5.2834
13	A	488.5071	0.1761	2.7139	0.2988
14	A	610.6257	2.0827	3.2594	26.0741
15	A	634.2839	3.6542	5.8069	3.8523
16	A	653.7196	2.8349	5.4439	1.0623
17	A	684.3302	3.3162	0.4668	0.1985
18	A	701.9921	1.7119	0.9739	0.3027
19	A	747.2646	3.8910	9.9883	1.2708
20	A	854.1207	2.6376	97.9629	1.6419
21	A	1088.5472	4.1788	62.5403	1.4201
22	A	1122.8722	2.3844	92.4334	1.0814
23	A	1133.5902	2.9736	123.2987	0.3194
24	A	1252.6586	6.6258	46.1646	4.6381
25	A	1390.7432	9.6682	25.7288	20.4653
26	A	1439.7663	13.9849	72.4014	5.7500
27	A	1491.1989	12.7595	366.1797	3.7456
28	A	1542.8940	5.6881	200.7989	0.9465
29	A	1632.2799	2.5978	50.1124	3.0580
30	A	1647.8828	14.5599	29.3680	3.1077
31	A	1683.4244	9.2319	450.9331	17.4388
32	A	3622.9309	8.0844	94.2068	121.8671
33	A	3746.4065	9.1383	76.6778	27.9204

py-04_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	92.6062	0.0884	0.0934	0.0596
2	A	131.9323	0.1213	0.3978	0.1812
3	A	197.6287	0.1865	0.8466	0.7462
4	A	211.9804	0.4532	0.5954	1.3058
5	A	277.9828	0.1599	56.2183	0.7939
6	A	282.8615	0.0734	171.5167	2.7555
7	A	300.0529	0.2992	2.4135	0.7820
8	A	305.3504	0.6929	0.4549	0.3608
9	A	319.6376	0.7500	1.7844	2.5480
10	A	378.4980	0.3797	4.2663	0.9152
11	A	388.1658	1.0537	3.1802	7.8134
12	A	456.2309	1.6258	2.2851	6.8914
13	A	469.4314	0.1581	3.8937	0.4677
14	A	581.8931	1.8420	5.0642	29.0149
15	A	599.2823	3.2095	9.4631	4.2008
16	A	614.5684	2.5439	5.2958	0.9499
17	A	641.4242	2.9024	0.8937	0.1731
18	A	672.1390	1.6400	1.0582	0.3134
19	A	701.4811	3.3857	6.4331	1.4264
20	A	799.4725	2.6307	119.9635	1.5935
21	A	1015.0538	5.8866	50.2695	1.6766
22	A	1060.6741	6.2211	142.4903	0.7965
23	A	1083.1230	1.4122	97.0234	1.2658
24	A	1172.4891	4.6705	51.4508	4.5988
25	A	1331.6644	7.8955	53.9004	14.6487
26	A	1341.8088	11.6867	65.3304	8.0941
27	A	1399.2504	12.6007	357.5108	6.4744
28	A	1461.5761	7.7884	140.6799	1.3452
29	A	1544.6217	12.6641	18.2587	3.3180
30	A	1568.8616	4.0339	57.0257	5.2372
31	A	1607.3658	2.8082	345.7279	11.2702
32	A	3499.5753	7.5409	74.6633	140.4828
33	A	3614.1624	8.4976	62.3707	31.1697

py-04_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	93.2490	0.0901	0.0882	0.0567
2	A	132.8281	0.1184	0.4300	0.1728
3	A	198.3631	0.1872	1.1880	0.7350
4	A	210.9520	0.4416	0.6275	1.2362
5	A	274.7315	0.3389	4.0730	0.2329
6	A	293.6158	0.0633	217.2470	3.0082
7	A	299.2593	0.3034	2.5751	0.3700
8	A	306.7178	0.6289	8.1494	0.5263

9	A	321.9166	0.8626	2.0968	2.3610
10	A	379.8433	0.3571	4.3848	0.9406
11	A	392.3023	1.0782	3.2559	7.2309
12	A	456.7226	1.5864	2.5361	6.5083
13	A	468.7130	0.1616	4.0970	0.4902
14	A	587.4936	1.8935	4.6614	28.7377
15	A	605.4771	3.2901	7.4288	4.2188
16	A	614.7307	2.5564	4.6168	0.8983
17	A	641.2402	2.8915	0.6481	0.1834
18	A	674.5121	1.6344	0.9832	0.3672
19	A	694.6152	3.3363	6.7249	1.3174
20	A	814.4941	2.5514	110.1250	1.5313
21	A	1034.5935	5.1315	55.6026	1.4503
22	A	1077.1801	5.6941	118.7332	0.9417
23	A	1090.6067	1.4506	102.1165	0.9469
24	A	1191.7492	5.3093	46.6664	4.7857
25	A	1363.3186	9.7713	61.5345	11.2243
26	A	1368.2284	11.1730	78.1148	9.9652
27	A	1422.9363	13.0080	356.5002	6.8362
28	A	1483.5066	5.9347	135.5372	1.2946
29	A	1568.7196	5.2549	29.5090	5.2832
30	A	1572.4500	3.5139	5.2378	0.3282
31	A	1617.7917	6.1488	405.7598	13.1191
32	A	3502.8922	7.5583	72.0671	139.4693
33	A	3622.0397	8.5314	65.6512	31.6385

py-04_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	93.0312	0.0896	0.0868	0.0567
2	A	132.4854	0.1187	0.4064	0.1776
3	A	200.0321	0.1899	1.2442	0.7282
4	A	212.1688	0.4439	0.6360	1.2363
5	A	276.6853	0.3034	9.5756	0.2570
6	A	286.7629	0.0608	218.9330	3.1034
7	A	300.6727	0.3093	2.2476	0.4124
8	A	308.3196	0.7120	1.7448	0.3888
9	A	323.1960	0.8684	1.7867	2.3557
10	A	382.2948	0.3473	4.1749	0.9470
11	A	393.3151	1.0953	2.9612	7.0365
12	A	457.4948	1.5980	2.4042	6.4097
13	A	470.0274	0.1642	3.8865	0.4642
14	A	588.7794	1.9137	4.6605	28.1514
15	A	607.0679	3.3073	7.2035	4.4722
16	A	618.4132	2.5757	4.8699	0.7946
17	A	646.4052	2.9440	0.6532	0.1731
18	A	677.1731	1.6466	0.9785	0.3665
19	A	702.4345	3.4097	6.6977	1.1915

20	A	816.9612	2.5714	110.9289	1.5516
21	A	1037.2012	5.3266	55.7834	1.4148
22	A	1079.5501	5.9950	123.2172	0.8813
23	A	1093.3595	1.4309	100.6198	1.0327
24	A	1194.4117	5.3424	46.7760	4.6997
25	A	1367.6532	10.2734	55.6506	10.1151
26	A	1372.3561	10.6744	78.7498	11.1344
27	A	1426.8939	13.1222	360.8442	6.6945
28	A	1488.4060	6.1408	135.7689	1.2784
29	A	1574.8898	7.3926	28.8399	5.0326
30	A	1579.4073	3.0597	4.9678	0.7218
31	A	1623.4116	5.7588	406.1331	13.1255
32	A	3525.5311	7.6559	72.7134	136.4174
33	A	3644.8039	8.6398	65.0535	30.9050

py-04_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	46.1840	0.0021	181.2363	0.0532
2	A	102.8765	0.0583	9.4071	0.0292
3	A	149.6623	0.0448	35.2846	0.1210
4	A	211.3059	0.2911	0.7562	0.6728
5	A	223.4596	0.5025	0.7052	1.0265
6	A	290.4719	0.4443	2.7440	0.2443
7	A	315.8954	0.3220	1.8080	0.4811
8	A	324.3803	0.6948	0.1228	0.2523
9	A	340.3313	1.0308	1.8206	1.8045
10	A	404.2406	0.4373	2.5628	0.7566
11	A	413.2622	1.2730	1.3510	5.5503
12	A	481.8967	1.8467	1.0165	4.7669
13	A	505.3036	0.1788	0.0586	0.0423
14	A	619.7125	2.1710	2.6555	24.3286
15	A	644.4367	3.7608	4.9318	4.5847
16	A	674.2707	3.0417	5.6565	0.6892
17	A	703.4966	3.5184	0.4175	0.1353
18	A	708.2210	1.6868	1.2160	0.2036
19	A	780.1007	4.2607	13.5148	0.5555
20	A	863.4653	2.5901	90.6142	1.6712
21	A	1104.9551	3.4662	58.0234	1.6062
22	A	1129.5811	1.9840	106.2907	0.8492
23	A	1145.7068	5.6592	125.8142	0.3017
24	A	1270.4315	7.3897	46.0364	4.3610
25	A	1357.2578	8.8511	18.1268	27.3729
26	A	1459.0231	14.1338	73.4740	5.2977
27	A	1511.2570	12.5206	348.1237	2.9471
28	A	1556.0972	5.4956	234.1069	1.9565
29	A	1648.1659	2.5341	93.9188	3.1007
30	A	1673.2993	16.2996	43.0179	3.7263

31	A	1703.9095	12.4521	472.1280	21.7608
32	A	3639.4071	8.1539	118.6481	113.0748
33	A	3761.8974	9.2263	88.0562	25.4759

py-04_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	101.2523	0.1064	0.0579	0.0797
2	A	142.0156	0.1667	0.8136	0.2425
3	A	208.9668	0.0919	23.9176	0.9391
4	A	222.4102	0.3312	12.1317	1.7224
5	A	227.1127	0.0468	207.6200	2.3068
6	A	290.0537	0.4666	3.1403	0.2058
7	A	317.1693	0.3223	1.5130	0.4474
8	A	322.0101	0.7004	0.0712	0.2486
9	A	341.9514	1.0272	2.2283	1.8008
10	A	400.0091	0.3481	4.6481	1.1871
11	A	413.5763	1.2210	2.0640	5.4001
12	A	480.0022	1.6862	1.5887	4.8296
13	A	483.6198	0.1777	3.4113	0.1517
14	A	619.6256	2.1456	2.6550	23.8368
15	A	645.6824	3.7676	5.1295	4.3702
16	A	660.8990	2.8635	4.5041	1.0437
17	A	693.9462	3.4188	0.2471	0.2406
18	A	707.2016	1.7534	1.0227	0.2561
19	A	755.3988	4.0308	13.3671	1.0328
20	A	874.2089	2.6036	86.0545	1.9826
21	A	1113.3377	2.8792	67.9112	1.8064
22	A	1137.0640	2.2986	101.5912	0.4973
23	A	1158.8397	4.9933	94.5284	0.2156
24	A	1287.8169	7.4635	39.8668	4.1163
25	A	1353.9897	8.8447	13.3591	26.9395
26	A	1476.7932	14.3435	73.9659	5.7719
27	A	1520.7873	10.8055	287.0584	1.7992
28	A	1562.7362	5.6708	307.3716	2.8801
29	A	1645.6369	2.5421	110.2056	4.4543
30	A	1680.8006	16.3994	52.5273	4.7957
31	A	1708.7382	13.6518	423.8018	21.0165
32	A	3630.1278	8.1168	117.4115	123.2448
33	A	3754.3629	9.1811	87.6979	28.2898

py-04_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.7827	0.1007	7.5636	0.0638
2	A	118.5702	0.0224	104.4159	0.0236

3	A	154.8082	0.0238	103.2742	0.1550
4	A	208.7547	0.3200	2.4035	0.6700
5	A	220.1881	0.4961	0.7270	0.9743
6	A	283.0165	0.4311	2.8215	0.2149
7	A	310.5289	0.3045	1.7753	0.4557
8	A	319.1267	0.6714	0.0606	0.2343
9	A	336.6917	1.0257	1.8818	1.8922
10	A	399.4013	0.3838	3.2364	0.8658
11	A	406.9910	1.2062	1.4964	5.6197
12	A	468.9745	1.7113	1.3609	4.7722
13	A	492.5129	0.1755	0.0791	0.0163
14	A	613.4456	2.1571	2.2454	24.5924
15	A	634.4138	3.6625	3.6435	5.4988
16	A	663.9873	2.9895	4.7232	0.7125
17	A	691.1065	3.3978	0.3781	0.1024
18	A	696.5976	1.6152	1.0601	0.2745
19	A	762.7514	4.1047	13.9289	0.6310
20	A	864.1123	2.3608	81.7833	1.7251
21	A	1094.0554	1.7970	59.7765	2.0899
22	A	1122.7283	3.3304	130.5553	0.2552
23	A	1149.0375	6.5916	89.0037	0.3082
24	A	1273.7869	7.4395	43.1930	4.5355
25	A	1365.5571	10.1341	19.2607	24.9124
26	A	1469.3887	13.9214	78.3129	5.1683
27	A	1514.4739	8.7753	275.6522	2.3541
28	A	1551.7327	4.1202	285.5620	1.4914
29	A	1624.4191	3.0017	180.6441	4.4030
30	A	1671.6758	17.1731	54.2682	4.8602
31	A	1698.6930	15.9710	427.0744	19.6901
32	A	3641.4867	8.1658	113.3882	122.2194
33	A	3770.8252	9.2658	85.4889	28.6828

py-04_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	96.5539	0.0917	0.1711	0.0463
2	A	138.5674	0.1001	1.4920	0.1401
3	A	198.3483	0.2169	0.5843	0.5955
4	A	222.6551	0.5009	0.3483	0.9415
5	A	291.7154	0.4482	1.7957	0.2026
6	A	302.0643	0.5652	1.1142	0.3694
7	A	312.8620	0.3361	0.9573	0.3492
8	A	336.9870	0.9899	1.3836	1.5576
9	A	378.7996	0.1691	7.7937	1.0301
10	A	410.3903	1.1425	1.4820	5.3560
11	A	436.7925	0.2154	7.8617	1.4735
12	A	475.2238	1.7808	0.9801	4.9975
13	A	542.7763	0.2773	206.9916	4.2655

14	A	586.0438	1.6344	43.0053	7.3678
15	A	604.9388	1.8847	9.5365	16.5104
16	A	616.1298	1.2890	40.6369	8.7595
17	A	633.4458	2.7310	2.1535	0.6523
18	A	646.2715	2.6188	25.6484	3.1104
19	A	696.7627	1.9402	1.2177	0.4099
20	A	869.8139	2.8245	96.0899	2.4093
21	A	1091.4659	7.2087	112.4397	1.1585
22	A	1122.9248	6.8226	57.3516	0.8557
23	A	1167.7469	1.4297	68.8084	1.7036
24	A	1264.0468	5.7437	33.0038	3.6809
25	A	1438.1613	14.7449	63.2995	8.0392
26	A	1449.1245	10.5333	64.5992	21.7555
27	A	1495.6592	13.2294	299.3722	4.6576
28	A	1545.6703	8.5765	223.1698	6.9491
29	A	1640.6239	2.4400	16.4925	1.9512
30	A	1655.8709	14.9985	6.9594	2.1926
31	A	1695.0474	6.9759	330.9138	27.6880
32	A	3603.2417	8.0083	71.2912	150.2999
33	A	3723.6905	8.9987	57.0948	30.1952

py-04_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	96.1279	0.0935	0.1302	0.0553
2	A	136.4674	0.1205	0.4865	0.1621
3	A	208.9868	0.2137	1.0161	0.6890
4	A	220.7805	0.4804	0.6234	1.1758
5	A	289.5133	0.1756	56.3347	0.6554
6	A	294.9728	0.0788	182.7082	2.5967
7	A	311.8037	0.3373	1.9926	0.4578
8	A	319.6234	0.7536	1.0744	0.3545
9	A	335.1866	0.8727	2.2620	2.0588
10	A	396.3017	0.3232	5.1738	0.9852
11	A	404.5878	1.1481	2.9655	6.0823
12	A	469.7469	1.5976	2.3785	5.6657
13	A	476.0224	0.1773	4.2783	0.4363
14	A	603.7310	2.0055	3.7732	27.0246
15	A	626.8802	3.5567	6.9638	3.2491
16	A	645.1465	2.7809	5.6731	1.0242
17	A	680.1077	3.2835	0.6820	0.1808
18	A	699.2610	1.7680	0.8121	0.2906
19	A	742.1154	3.8173	7.9119	1.1451
20	A	846.2804	2.7232	106.2614	1.6325
21	A	1075.4430	5.3076	68.0757	1.1418
22	A	1112.4293	4.7078	98.2582	1.0630
23	A	1128.1280	1.6581	107.2507	0.8432
24	A	1237.3868	5.9542	46.2401	4.4655

25	A	1391.5394	9.3274	23.9632	19.2037
26	A	1423.1002	13.6537	71.2671	6.8531
27	A	1474.2717	12.9558	381.0532	4.0577
28	A	1529.5116	6.9024	200.1371	0.9485
29	A	1627.1088	3.2812	37.1832	5.3322
30	A	1632.0849	7.6799	10.9049	1.0194
31	A	1670.2741	5.9763	423.7707	15.8512
32	A	3625.8287	8.0993	84.9025	130.4289
33	A	3746.5628	9.1324	67.0008	28.8072

py-04_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	99.7696	0.1067	0.0534	0.0647
2	A	139.3818	0.1664	1.2417	0.2467
3	A	208.7916	0.0976	21.3300	0.8153
4	A	221.2788	0.4392	2.8487	1.3479
5	A	229.0241	0.0443	210.7589	3.7043
6	A	287.2762	0.3859	3.3592	0.2424
7	A	313.8237	0.3333	1.7282	0.3295
8	A	322.7672	0.7252	0.0194	0.2944
9	A	339.9341	1.0433	1.6546	1.8387
10	A	401.3132	0.3816	3.2970	0.9581
11	A	412.5592	1.2439	1.8870	5.5870
12	A	478.2286	1.7616	1.6778	5.0913
13	A	492.1123	0.1783	2.9759	0.3211
14	A	618.0634	2.1433	3.1229	25.4257
15	A	641.9413	3.7460	5.1713	3.8947
16	A	659.5390	2.8886	5.2970	1.1297
17	A	691.9971	3.3982	0.4345	0.2042
18	A	707.1283	1.7374	0.9654	0.3045
19	A	754.9128	3.9821	10.5900	1.2259
20	A	866.2313	2.6259	93.6144	1.6176
21	A	1103.7622	3.7158	65.6568	1.5099
22	A	1134.6491	2.1551	93.2925	0.9950
23	A	1148.0789	4.0150	112.7248	0.2305
24	A	1270.6631	6.9692	45.4901	4.6384
25	A	1403.6592	10.0891	23.1919	21.3834
26	A	1463.0949	14.3729	75.7458	5.8820
27	A	1511.0358	12.3791	359.5062	3.3465
28	A	1559.7367	4.9985	208.1653	1.0476
29	A	1642.3098	2.6749	77.9724	3.0813
30	A	1669.7233	16.1410	35.0939	3.6793
31	A	1701.9659	11.5217	446.1882	17.9235
32	A	3640.8735	8.1653	97.8249	121.2624
33	A	3765.8891	9.2341	79.6050	27.6100

py-04_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	93.6614	0.0917	0.0712	0.0551
2	A	133.1575	0.1239	0.3481	0.1799
3	A	198.9565	0.1828	1.4487	0.7343
4	A	212.2532	0.4468	0.6236	1.2201
5	A	275.4168	0.1956	35.0910	0.5109
6	A	280.5951	0.0649	191.9438	3.0900
7	A	300.7379	0.3001	2.3048	0.4017
8	A	307.9345	0.7100	0.7119	0.3651
9	A	323.6734	0.8902	1.6397	2.3430
10	A	382.5699	0.3721	3.7252	0.9226
11	A	394.0148	1.1052	2.7101	6.9758
12	A	457.5192	1.6117	2.2919	6.3912
13	A	474.2011	0.1635	3.8183	0.4790
14	A	590.3123	1.9361	4.5916	27.9524
15	A	608.0893	3.3151	6.5195	4.6364
16	A	618.4140	2.5725	4.9617	0.9616
17	A	647.3373	2.9576	0.7336	0.1775
18	A	676.6829	1.6384	0.9973	0.3640
19	A	703.8377	3.4194	6.3738	1.3498
20	A	819.9325	2.5316	107.5014	1.5211
21	A	1041.0248	5.0598	56.0926	1.3373
22	A	1083.4820	5.5980	116.5345	1.0404
23	A	1093.4769	1.4617	104.1712	0.8478
24	A	1198.2292	5.5094	45.3995	4.7768
25	A	1374.3184	12.0953	55.2229	6.8737
26	A	1378.9943	9.6306	89.8713	14.4354
27	A	1432.0751	13.1930	356.1918	7.1342
28	A	1493.0997	5.3460	129.1729	1.2871
29	A	1574.6681	2.5614	31.5920	3.6539
30	A	1581.7618	11.4184	13.5282	1.7776
31	A	1626.6793	7.4275	406.3334	13.3423
32	A	3519.5047	7.6294	76.5191	139.1987
33	A	3639.4714	8.6157	67.8879	30.8010

py-04_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	95.8060	0.0926	0.1842	0.0528
2	A	136.6450	0.1090	1.1677	0.1503
3	A	200.2021	0.2051	0.6824	0.6926
4	A	209.0544	0.4388	0.5938	1.1638
5	A	269.0928	0.3510	2.4106	0.2279
6	A	297.7705	0.2908	2.0073	0.3537
7	A	308.6312	0.5773	1.9814	0.3094

8	A	322.8018	0.9379	0.7658	2.4404
9	A	377.1205	0.2381	25.3672	0.7210
10	A	391.5647	0.4813	41.5839	3.5918
11	A	406.8578	0.1681	194.6805	5.5693
12	A	459.5748	1.2537	10.8528	7.0235
13	A	462.1816	0.1662	7.2876	0.5780
14	A	592.7798	1.8192	6.0714	29.4258
15	A	611.6462	3.1990	9.3987	2.7977
16	A	616.8384	2.7138	3.4975	0.6685
17	A	644.4094	2.9284	0.3691	0.1674
18	A	675.9521	1.7169	0.7999	0.4118
19	A	693.4469	3.3622	7.9267	0.8493
20	A	825.3404	2.7033	114.9837	1.5872
21	A	1046.0168	5.8457	59.9169	1.3677
22	A	1086.0934	6.1255	119.2961	0.7862
23	A	1118.4668	1.4833	86.4365	1.2796
24	A	1204.6429	4.8736	47.2580	4.4828
25	A	1377.6096	9.4831	67.2515	11.7461
26	A	1382.5454	11.6338	75.5119	9.0903
27	A	1442.9473	13.5209	354.9940	6.5221
28	A	1500.6406	7.7500	152.1303	1.1597
29	A	1592.1205	13.0311	14.7772	3.8837
30	A	1608.5019	2.9816	19.5719	3.0479
31	A	1648.3013	4.2473	369.3269	13.8863
32	A	3510.0916	7.5925	53.3150	143.6872
33	A	3625.4416	8.5380	49.9868	36.1704

py-04_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	97.7265	0.0975	0.1273	0.0516
2	A	138.3703	0.1243	0.5669	0.1535
3	A	206.1360	0.2073	0.8865	0.6749
4	A	213.0154	0.4449	0.6818	1.1506
5	A	276.1627	0.3432	3.1352	0.2245
6	A	303.9146	0.3167	1.9285	0.4080
7	A	310.9705	0.0800	196.7358	2.3130
8	A	317.9801	0.3547	42.7352	1.0420
9	A	329.6579	0.8474	5.6997	1.8456
10	A	392.5780	0.3588	6.2897	0.9671
11	A	402.8008	1.1134	3.9810	6.7338
12	A	468.1896	1.6431	2.8110	5.9114
13	A	478.7957	0.1718	4.8026	0.4517
14	A	602.6875	1.9719	4.0873	28.0221
15	A	624.6419	3.5186	7.6354	3.0523
16	A	638.2714	2.7316	5.0288	1.1444
17	A	667.4406	3.1425	0.4778	0.1666
18	A	690.2699	1.7266	0.8599	0.3644

19	A	724.3339	3.6468	8.7275	1.3658
20	A	840.3499	2.7085	107.8133	1.6134
21	A	1069.0866	5.3769	63.5894	1.3181
22	A	1107.3818	5.3397	110.6641	0.7958
23	A	1128.1262	1.6093	102.0008	0.9860
24	A	1230.2269	5.7776	46.5161	4.5463
25	A	1382.5410	9.0064	41.5688	17.9959
26	A	1412.5066	13.6705	68.1569	5.9961
27	A	1468.4184	13.2807	375.1764	4.6708
28	A	1523.8730	7.4487	187.2918	0.9674
29	A	1620.8353	11.9373	27.6576	4.5375
30	A	1630.1967	2.9944	10.0461	1.7362
31	A	1669.0549	5.0287	423.2679	15.8710
32	A	3577.7360	7.8860	74.8384	132.2859
33	A	3698.4007	8.8970	63.9686	32.1688

py-04_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	99.4733	0.1127	0.4260	0.0954
2	A	134.9927	0.1453	17.7334	0.8076
3	A	179.9013	0.0214	213.3280	4.2055
4	A	212.6355	0.3653	4.4042	0.8744
5	A	224.0570	0.5206	0.8794	0.9274
6	A	293.4476	0.4740	2.6109	0.2048
7	A	318.8776	0.3369	1.7412	0.4978
8	A	322.6163	0.6958	0.0969	0.2718
9	A	340.8370	0.9595	1.7633	1.8193
10	A	401.3009	0.3603	3.0273	0.8757
11	A	412.6277	1.2293	1.6548	5.5221
12	A	479.8251	1.7971	1.3029	4.8926
13	A	489.0200	0.1783	2.1069	0.2245
14	A	616.2928	2.1265	2.7984	24.9548
15	A	641.6767	3.7432	5.6625	3.8711
16	A	665.2117	2.9040	5.3376	1.3536
17	A	697.3082	3.4506	0.2986	0.2130
18	A	710.6044	1.7548	1.0163	0.2150
19	A	761.7013	4.0590	12.3941	1.3626
20	A	863.2297	2.6757	95.6227	1.7252
21	A	1103.1677	4.2613	65.9075	1.4700
22	A	1132.1656	2.1420	90.3169	0.9776
23	A	1145.5285	3.6244	124.7652	0.3944
24	A	1267.7079	7.0241	45.0644	4.1932
25	A	1366.4865	8.8475	14.1544	26.8271
26	A	1455.7358	14.2042	72.9448	5.3406
27	A	1508.3897	12.6032	359.4433	2.7754
28	A	1555.9416	6.0349	241.5075	1.9984
29	A	1651.7573	2.5379	60.7117	2.5742

30	A	1672.7339	16.2208	42.5805	3.5302
31	A	1702.7013	10.2708	473.5128	20.8335
32	A	3650.9017	8.2100	98.4626	114.8554
33	A	3775.5556	9.2848	76.9379	26.1156

py-04_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.5841	0.1062	0.1003	0.0774
2	A	136.9314	0.1779	3.5859	0.3655
3	A	203.5422	0.0369	115.0494	2.3461
4	A	213.1247	0.0882	108.7620	3.0715
5	A	220.1700	0.4223	3.8183	0.8886
6	A	288.7549	0.4373	2.9247	0.2398
7	A	312.0394	0.3242	1.8948	0.5293
8	A	319.8190	0.6940	0.0800	0.2993
9	A	335.1340	0.9316	1.6615	2.0935
10	A	397.1938	0.4064	3.0916	0.9311
11	A	406.4489	1.2096	1.7805	6.1611
12	A	475.5728	1.7855	1.4670	5.4356
13	A	490.6234	0.1722	2.4531	0.2911
14	A	608.2985	2.0468	3.2761	26.6305
15	A	632.0827	3.6259	7.0023	3.5323
16	A	654.7617	2.8501	5.8131	1.1946
17	A	684.9282	3.3267	0.6454	0.1964
18	A	700.8048	1.7131	1.0189	0.2559
19	A	751.7783	3.9315	10.1322	1.3983
20	A	846.0513	2.7018	102.7910	1.6730
21	A	1079.4560	4.8355	58.6177	1.3284
22	A	1116.1927	3.2141	100.5869	0.9292
23	A	1127.5386	2.1197	127.7413	0.6281
24	A	1242.2929	6.3959	47.4486	4.5301
25	A	1364.9182	8.6995	23.8447	21.4044
26	A	1425.1577	13.8183	70.4016	5.9641
27	A	1478.1149	12.8544	361.9134	3.6427
28	A	1530.1358	6.9697	214.9457	1.2353
29	A	1630.8981	6.0714	45.8951	5.9708
30	A	1635.5393	3.6635	5.6416	0.4240
31	A	1672.8964	6.1929	465.1220	18.3666
32	A	3611.9377	8.0335	98.4154	123.5843
33	A	3732.1844	9.0716	75.9694	27.9958

py-04_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	98.1304	0.1025	0.0516	0.0667

2	A	137.6133	0.1611	0.9953	0.2410
3	A	206.0066	0.1198	10.4963	0.7314
4	A	221.5453	0.4411	3.0724	1.4335
5	A	231.6341	0.0422	219.0592	3.7510
6	A	289.5173	0.4551	3.0650	0.2279
7	A	312.9588	0.3167	2.0169	0.5307
8	A	318.2923	0.7036	0.0183	0.3086
9	A	335.1389	0.9324	1.7220	1.9821
10	A	395.4143	0.4003	3.3715	0.9694
11	A	406.7245	1.2025	1.9430	6.2303
12	A	476.0406	1.7701	1.6070	5.5234
13	A	487.7927	0.1710	2.9451	0.3171
14	A	609.5810	2.0565	3.5335	26.6390
15	A	632.2165	3.6210	7.2324	3.7026
16	A	651.0256	2.8342	5.5163	1.1777
17	A	681.1573	3.2913	0.6166	0.1958
18	A	700.1902	1.7272	1.0575	0.2760
19	A	747.3593	3.8919	10.0429	1.4339
20	A	845.3684	2.7091	105.3060	1.6324
21	A	1077.8826	5.1532	58.9125	1.3028
22	A	1115.3781	3.8146	105.3197	0.8566
23	A	1126.7594	1.8688	122.4005	0.7531
24	A	1240.6846	6.3332	47.3252	4.5753
25	A	1364.7262	8.6138	25.4376	20.8828
26	A	1425.6367	13.9289	72.5923	5.9177
27	A	1474.8420	12.9610	370.3529	3.7498
28	A	1528.8933	6.9388	198.8702	1.2218
29	A	1627.0472	8.0582	41.5651	5.9316
30	A	1632.2165	3.2958	4.6957	0.7744
31	A	1669.6381	5.7076	459.0940	17.8075
32	A	3607.3534	8.0132	93.7929	124.1166
33	A	3727.2993	9.0461	74.0961	28.2603

py-04_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	101.2522	0.1064	0.0579	0.0797
2	A	142.0158	0.1667	0.8132	0.2425
3	A	208.9676	0.0920	23.8917	0.9388
4	A	222.4107	0.3316	12.0926	1.7211
5	A	227.1207	0.0468	207.6859	2.3081
6	A	290.0537	0.4666	3.1405	0.2058
7	A	317.1692	0.3223	1.5129	0.4474
8	A	322.0101	0.7004	0.0712	0.2486
9	A	341.9514	1.0272	2.2284	1.8008
10	A	400.0089	0.3481	4.6483	1.1872
11	A	413.5763	1.2210	2.0640	5.4001
12	A	480.0023	1.6862	1.5888	4.8297

13	A	483.6193	0.1777	3.4114	0.1517
14	A	619.6257	2.1456	2.6550	23.8369
15	A	645.6824	3.7676	5.1295	4.3701
16	A	660.8989	2.8635	4.5041	1.0437
17	A	693.9462	3.4188	0.2471	0.2406
18	A	707.2017	1.7534	1.0227	0.2561
19	A	755.3987	4.0308	13.3671	1.0328
20	A	874.2090	2.6036	86.0545	1.9827
21	A	1113.3380	2.8792	67.9108	1.8064
22	A	1137.0645	2.2986	101.5910	0.4972
23	A	1158.8400	4.9933	94.5282	0.2156
24	A	1287.8173	7.4635	39.8668	4.1163
25	A	1353.9894	8.8447	13.3591	26.9397
26	A	1476.7936	14.3435	73.9658	5.7718
27	A	1520.7873	10.8055	287.0607	1.7992
28	A	1562.7366	5.6707	307.3692	2.8800
29	A	1645.6375	2.5421	110.2046	4.4542
30	A	1680.8003	16.3993	52.5278	4.7958
31	A	1708.7385	13.6517	423.8022	21.0164
32	A	3630.1274	8.1168	117.4112	123.2460
33	A	3754.3620	9.1810	87.6975	28.2902

py-04_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	96.5539	0.0917	0.1711	0.0463
2	A	138.5654	0.1001	1.4920	0.1401
3	A	198.3443	0.2169	0.5843	0.5955
4	A	222.6546	0.5009	0.3483	0.9415
5	A	291.7154	0.4482	1.7956	0.2026
6	A	302.0596	0.5652	1.1140	0.3695
7	A	312.8619	0.3361	0.9573	0.3492
8	A	336.9871	0.9899	1.3836	1.5577
9	A	378.7980	0.1691	7.7916	1.0302
10	A	410.3904	1.1424	1.4823	5.3559
11	A	436.7905	0.2154	7.8634	1.4734
12	A	475.2228	1.7808	0.9802	4.9975
13	A	542.7661	0.2774	206.9237	4.2648
14	A	586.0239	1.6327	43.0852	7.3638
15	A	604.9374	1.8849	9.5306	16.5099
16	A	616.1244	1.2889	40.6383	8.7629
17	A	633.4407	2.7309	2.1542	0.6523
18	A	646.2687	2.6191	25.6398	3.1106
19	A	696.7620	1.9402	1.2176	0.4099
20	A	869.8126	2.8245	96.0909	2.4092
21	A	1091.4661	7.2088	112.4372	1.1585
22	A	1122.9223	6.8230	57.3584	0.8557
23	A	1167.7470	1.4297	68.8053	1.7037

24	A	1264.0428	5.7437	33.0063	3.6809
25	A	1438.1605	14.7449	63.3011	8.0391
26	A	1449.1271	10.5332	64.5953	21.7560
27	A	1495.6602	13.2296	299.3954	4.6576
28	A	1545.6684	8.5761	223.1445	6.9489
29	A	1640.6240	2.4400	16.4898	1.9511
30	A	1655.8712	14.9982	6.9643	2.1930
31	A	1695.0466	6.9756	330.9167	27.6877
32	A	3603.2399	8.0083	71.2921	150.3004
33	A	3723.6891	8.9986	57.0952	30.1940

py-06_A_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.1719	0.0861	1.3376	0.2765
2	A	122.1114	0.1263	0.5351	0.0831
3	A	200.2744	0.2065	0.6248	0.2982
4	A	203.1074	0.4697	0.4977	1.4209
5	A	281.7985	0.5094	3.7117	0.3101
6	A	303.5206	0.2509	4.9276	0.7315
7	A	322.4588	0.5389	1.5798	0.6083
8	A	323.6884	0.7252	1.6228	1.2276
9	A	388.4713	0.1148	211.2779	1.0994
10	A	390.9794	0.2141	62.6254	2.3666
11	A	428.5890	1.5565	1.9666	3.3933
12	A	451.9133	0.2283	30.5188	1.1890
13	A	466.5130	0.9416	10.2078	5.3674
14	A	551.0451	1.5953	13.5843	24.4677
15	A	588.6725	2.4990	10.4825	0.3451
16	A	678.3791	1.5474	1.1228	0.7726
17	A	691.1505	3.2405	1.3202	0.4327
18	A	700.6779	3.3509	8.8652	5.9092
19	A	739.2711	3.9043	6.0765	1.1929
20	A	911.2684	4.9188	128.9400	5.6297
21	A	956.6809	4.4401	114.8346	0.5208
22	A	1105.0323	1.3796	33.8647	1.5578
23	A	1165.0988	7.7045	8.5389	6.7969
24	A	1256.5972	6.6010	78.5614	1.2704
25	A	1333.6872	7.4763	24.8170	4.2018
26	A	1438.6957	9.9325	93.7799	8.2039
27	A	1477.1940	11.9602	71.0265	5.3617
28	A	1508.6384	8.7805	593.5428	1.3871
29	A	1615.0764	13.1265	45.9916	6.2639
30	A	1630.7327	2.3231	79.8147	1.3018
31	A	1672.6433	9.0088	263.8563	23.8835
32	A	3595.1777	7.9635	87.0444	184.7767
33	A	3713.7938	8.9676	56.2548	47.3320

py-06_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.4961	0.0856	1.3483	0.2785
2	A	123.3036	0.1314	0.4985	0.0727
3	A	200.9628	0.4612	0.4619	1.3855
4	A	202.4055	0.2099	0.7737	0.2982
5	A	278.4228	0.4398	4.2490	0.3329
6	A	301.1276	0.2547	4.6648	0.6829
7	A	324.5486	0.5837	0.8756	0.9932
8	A	326.0679	0.6616	2.0382	0.7349
9	A	383.8646	0.1085	257.7986	1.1910
10	A	393.6728	0.2119	21.4985	2.1688
11	A	430.7723	1.6547	1.5825	3.2458
12	A	453.8102	0.2491	24.4873	1.3204
13	A	466.1206	0.9040	9.4417	5.1537
14	A	553.7103	1.5964	12.8368	23.1724
15	A	590.5593	2.5175	9.8617	0.3487
16	A	680.6424	1.5307	0.7985	0.7033
17	A	693.0761	3.2623	1.1979	0.3976
18	A	703.6973	3.4832	7.8871	6.5921
19	A	737.3497	3.8816	5.8529	1.1449
20	A	924.4331	4.8019	125.6823	5.9854
21	A	969.3810	4.3093	104.2006	0.5642
22	A	1108.5609	1.3682	35.0208	1.3991
23	A	1186.1939	8.0497	9.2667	6.5540
24	A	1270.0433	6.6713	73.6405	1.1091
25	A	1363.8244	8.7602	38.5727	4.4376
26	A	1458.8322	9.0550	83.2930	7.4833
27	A	1496.3620	12.1652	64.3567	6.4021
28	A	1529.7851	7.8036	588.1197	1.1796
29	A	1629.6466	2.4452	129.5665	0.4537
30	A	1639.2603	10.1935	67.1377	7.3766
31	A	1693.5720	13.4484	233.2396	21.8715
32	A	3615.0447	8.0532	91.3639	180.6268
33	A	3737.2947	9.0813	59.8802	45.7537

py-06_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	114.8320	0.0841	1.3803	0.2800
2	A	122.7807	0.1315	0.4838	0.0712
3	A	201.6517	0.4622	0.4669	1.3880
4	A	202.8199	0.2112	0.7477	0.2984
5	A	279.1306	0.4492	4.1389	0.3213
6	A	301.8135	0.2537	4.6795	0.7021

7	A	324.4003	0.5956	0.9044	1.0482
8	A	325.9241	0.6410	2.2387	0.6850
9	A	386.0092	0.1115	222.1556	1.0829
10	A	394.4884	0.2042	53.8577	2.2544
11	A	429.7230	1.6336	1.8884	3.2259
12	A	453.6910	0.2613	26.4915	1.4028
13	A	465.2931	0.8239	12.0173	5.1442
14	A	552.3030	1.5849	13.1128	23.3759
15	A	591.3408	2.5246	9.9925	0.3384
16	A	680.0901	1.5502	0.9652	0.8255
17	A	693.6387	3.2618	1.3119	0.4043
18	A	702.2854	3.3949	7.6982	6.3986
19	A	738.6504	3.8946	5.6754	1.1404
20	A	921.3336	4.8329	126.2611	5.9513
21	A	966.2453	4.3287	106.0187	0.5476
22	A	1107.9959	1.3662	34.7315	1.4118
23	A	1181.0432	8.0024	9.0645	6.5405
24	A	1266.0600	6.5927	74.9405	1.1390
25	A	1358.7020	8.5469	37.6203	4.4931
26	A	1453.6397	9.3119	81.2955	7.7922
27	A	1491.7161	12.0461	66.6545	6.0183
28	A	1525.2933	8.1327	594.0389	1.2170
29	A	1629.0187	2.8546	100.3343	0.6062
30	A	1635.3666	6.1691	79.3902	7.0549
31	A	1688.8954	12.6466	235.4497	22.5549
32	A	3613.1316	8.0450	88.4338	181.1819
33	A	3734.8780	9.0686	57.8604	45.9890

py-06_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1713	0.0760	1.3778	0.3273
2	A	116.3602	0.1164	0.5574	0.1027
3	A	191.1382	0.1917	0.4906	0.3269
4	A	195.6613	0.4363	0.4955	1.6081
5	A	271.0760	0.4848	3.2881	0.3362
6	A	292.8058	0.2354	4.2465	0.8486
7	A	307.7171	0.4882	2.1581	0.3685
8	A	309.4561	0.6661	0.9114	1.7980
9	A	371.2474	0.2224	3.2053	2.1406
10	A	398.8390	0.1333	203.4469	1.1617
11	A	410.3241	0.8235	13.0810	3.3096
12	A	438.1902	0.2392	47.9611	1.7062
13	A	450.0345	0.4617	41.0512	5.3922
14	A	524.6026	1.4077	16.8021	29.1322
15	A	557.5257	2.2250	10.3427	0.4289
16	A	649.9746	1.5010	2.4849	1.2388
17	A	652.4834	2.9035	1.0680	0.5805

18	A	668.9565	2.7358	8.8706	4.8813
19	A	696.2313	3.4569	4.6372	1.1441
20	A	862.6463	4.6198	132.7280	5.6681
21	A	908.7408	4.2690	119.2558	0.5912
22	A	1063.1669	1.3765	25.7935	1.8022
23	A	1098.5435	5.9539	8.6630	7.9593
24	A	1190.3922	4.9618	77.4293	1.4918
25	A	1306.3422	7.3422	17.0155	3.3375
26	A	1359.2078	9.5405	126.7676	7.4006
27	A	1402.2030	10.6666	73.9618	4.2330
28	A	1436.2258	8.7481	513.7883	1.1710
29	A	1529.7857	13.2336	36.3822	7.9075
30	A	1572.9568	3.2955	28.8394	2.5225
31	A	1602.7661	3.2233	268.5253	16.7882
32	A	3488.1910	7.4950	70.2361	216.9524
33	A	3602.6049	8.4327	45.7277	54.3895

py-06_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1943	0.0746	1.4291	0.3264
2	A	117.2474	0.1200	0.5184	0.0896
3	A	192.2146	0.1925	0.7020	0.3196
4	A	194.5135	0.4349	0.4599	1.5704
5	A	268.0119	0.4081	3.8802	0.3880
6	A	290.4645	0.2365	3.8350	0.7494
7	A	309.6281	0.4749	2.2913	0.3409
8	A	311.8474	0.6716	0.8728	1.6193
9	A	372.1122	0.1978	3.5964	1.9965
10	A	403.8821	0.1451	177.7853	1.1270
11	A	413.7623	0.8306	10.6555	3.2925
12	A	439.7457	0.2992	53.2469	2.0880
13	A	451.2373	0.3629	64.8458	4.9604
14	A	530.4671	1.4226	16.0904	27.4940
15	A	557.2390	2.2055	10.6874	0.4566
16	A	651.4175	2.8994	0.9081	0.5502
17	A	653.0025	1.4565	1.5215	0.9580
18	A	672.8542	2.9710	7.8903	5.8432
19	A	690.7224	3.4125	4.8798	1.2185
20	A	879.9034	4.5314	130.4477	5.9651
21	A	924.4293	4.2122	106.6917	0.6707
22	A	1068.9386	1.3122	27.7235	1.5034
23	A	1122.6783	6.9095	8.5411	7.8299
24	A	1206.4621	5.2171	71.7944	1.2695
25	A	1338.5841	8.4608	29.3721	3.5365
26	A	1385.0482	9.2132	124.1326	6.6857
27	A	1424.1525	11.4768	64.0328	5.2855
28	A	1459.1340	7.6918	520.5289	1.1761

29	A	1553.9892	13.2390	39.4171	6.8775
30	A	1574.0015	2.1720	65.5199	1.2961
31	A	1617.4312	8.0973	251.5653	16.9311
32	A	3496.5673	7.5329	70.0849	214.9207
33	A	3614.4124	8.4861	47.8158	53.3659

py-06_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	107.9152	0.0739	1.4442	0.3244
2	A	117.2692	0.1213	0.5033	0.0867
3	A	193.6770	0.1950	0.6833	0.3159
4	A	196.0724	0.4407	0.4708	1.5593
5	A	269.7718	0.4192	3.8150	0.3771
6	A	292.3755	0.2386	3.9492	0.7617
7	A	311.1097	0.4799	2.2606	0.3437
8	A	313.1782	0.6872	0.8635	1.5770
9	A	375.2458	0.1936	3.6591	1.9372
10	A	402.1996	0.1402	198.2419	1.1398
11	A	414.7058	0.9714	8.9095	3.2539
12	A	441.0079	0.3057	42.6703	2.1654
13	A	451.7783	0.3721	56.8435	4.7881
14	A	532.0072	1.4358	15.8286	27.1783
15	A	561.5932	2.2518	10.4059	0.4201
16	A	655.2824	1.4880	1.4842	1.1123
17	A	656.6999	2.9432	1.0984	0.5091
18	A	674.7135	2.9312	7.7749	5.8021
19	A	697.3669	3.4727	4.5879	1.1408
20	A	882.5988	4.5720	131.2529	5.9850
21	A	926.8400	4.2565	107.9556	0.7043
22	A	1072.6654	1.3183	28.2845	1.4685
23	A	1124.5867	6.9497	8.2978	7.6710
24	A	1209.1684	5.2507	73.1502	1.2730
25	A	1343.0044	8.4921	30.9680	3.7027
26	A	1388.6687	9.4454	122.5131	6.7639
27	A	1428.4061	11.4808	66.5280	5.0577
28	A	1464.0764	7.8451	518.2941	1.0857
29	A	1559.1531	13.5587	40.6657	7.0485
30	A	1581.4835	2.2098	59.0037	1.1830
31	A	1623.1665	7.7126	255.0218	17.2887
32	A	3518.1128	7.6261	70.6234	209.1233
33	A	3636.3715	8.5899	47.5208	52.1835

py-06_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A	118.8497	0.0949	1.0493	0.2486
2	A	125.4085	0.1321	0.4987	0.0815
3	A	203.7769	0.4710	0.4942	1.2947
4	A	204.3977	0.2070	0.8431	0.2806
5	A	283.4188	0.4924	4.7198	0.3275
6	A	304.5335	0.2279	18.8244	0.7923
7	A	326.9097	0.4336	14.9683	0.8735
8	A	329.0990	0.5695	18.8836	1.0467
9	A	337.1783	0.0934	246.1578	1.5396
10	A	402.2074	0.2258	4.4197	2.0874
11	A	435.2359	1.8577	0.6695	3.2688
12	A	459.7981	0.2285	10.3788	1.1778
13	A	472.0900	1.1920	2.6909	5.0258
14	A	560.1403	1.6678	11.0180	22.0827
15	A	605.9882	2.6644	9.5347	0.2948
16	A	686.3946	1.5329	1.1435	0.6608
17	A	710.1130	3.4278	8.3990	4.4143
18	A	713.6242	3.6004	2.0692	2.4366
19	A	765.6532	4.1779	6.6176	1.2182
20	A	934.5590	4.8365	122.0920	5.4537
21	A	976.7676	4.4069	109.7960	0.6261
22	A	1112.6684	1.3831	45.1227	1.6407
23	A	1191.4678	8.3261	10.2511	6.6115
24	A	1282.6934	8.9705	91.9092	1.2274
25	A	1320.5680	6.5052	23.7943	5.3888
26	A	1472.2505	8.8708	74.8642	8.1458
27	A	1513.5375	12.6255	58.8403	6.0091
28	A	1541.7219	7.8599	608.3380	2.5401
29	A	1641.3296	2.3060	175.7318	1.3888
30	A	1662.7936	14.4179	66.5117	8.0365
31	A	1713.8675	15.7126	234.9553	27.5153
32	A	3627.2415	8.1050	107.9564	165.5428
33	A	3747.4238	9.1400	67.7922	42.0268

py-06_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.9171	0.0912	1.4576	0.2550
2	A	125.7624	0.1339	0.5092	0.0775
3	A	201.4091	0.4645	0.4448	1.3311
4	A	204.2974	0.2134	0.8096	0.3010
5	A	282.4703	0.5567	3.5550	0.2228
6	A	306.1642	0.2544	5.2008	0.6479
7	A	328.1751	0.5551	1.6152	1.1440
8	A	329.7942	0.5879	3.8886	0.6731
9	A	390.5394	0.1305	51.2915	1.4167
10	A	403.7503	0.1660	210.5991	2.4085
11	A	434.5211	1.5399	2.0807	3.4638

12	A	455.7011	0.2964	52.2507	1.3447
13	A	471.5000	0.8780	17.6054	5.6807
14	A	560.6634	1.6064	13.2701	20.9224
15	A	597.3953	2.5617	11.7250	0.4363
16	A	687.2756	1.5589	0.7221	0.5395
17	A	701.9439	3.3564	1.2013	0.3963
18	A	712.9666	3.6918	8.7267	7.1371
19	A	747.9941	4.0120	7.3253	1.4606
20	A	939.4389	4.9489	116.1557	5.7123
21	A	985.4659	4.1481	98.0612	0.3878
22	A	1120.0129	1.3810	41.1804	1.6467
23	A	1211.0671	8.6692	12.4804	5.9510
24	A	1293.6146	9.7970	88.1133	1.0301
25	A	1320.2121	5.8671	18.6783	4.4301
26	A	1484.5030	7.8987	32.3918	7.5147
27	A	1525.5383	12.6222	63.9708	6.7700
28	A	1550.4852	8.7855	653.7553	3.4158
29	A	1638.7197	2.2851	196.8184	2.7050
30	A	1672.1966	15.7437	60.9397	5.6373
31	A	1717.0806	16.5245	187.4729	28.2567
32	A	3618.3193	8.0698	104.0003	174.4457
33	A	3740.4365	9.0974	69.1678	44.2157

py-06_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	117.0483	0.0961	0.6001	0.2997
2	A	125.0502	0.1368	0.3836	0.0656
3	A	199.0339	0.4523	0.5051	1.2901
4	A	201.5952	0.1711	2.4225	0.3074
5	A	256.2010	0.0508	249.9572	2.4051
6	A	275.6804	0.4811	8.6681	0.2561
7	A	300.3315	0.2342	9.1343	0.7007
8	A	323.5010	0.6862	2.0888	1.3762
9	A	327.4725	0.4733	10.2375	0.3415
10	A	398.7674	0.2263	3.1520	2.0845
11	A	427.6336	1.8645	0.2464	3.5670
12	A	455.4062	0.2749	3.3858	2.1079
13	A	459.7579	0.5380	3.0068	4.0534
14	A	553.1176	1.6103	10.2442	21.3291
15	A	596.7175	2.5867	8.1692	0.3887
16	A	673.4409	1.4160	0.9844	0.4898
17	A	699.6356	3.4955	6.7167	5.1508
18	A	701.8927	3.5478	2.9284	3.4416
19	A	750.2586	4.0000	6.2843	1.3514
20	A	932.9493	4.2331	117.7475	5.4292
21	A	976.6709	3.6981	93.9563	0.4694
22	A	1088.1946	1.3724	51.9154	1.3491

23	A	1204.5826	8.2583	10.9756	6.4945
24	A	1280.1656	7.9608	75.8558	1.0042
25	A	1327.7394	8.4678	48.7926	5.1936
26	A	1477.3570	6.2110	48.0703	6.3144
27	A	1516.3112	12.6546	63.0217	8.4650
28	A	1545.0387	6.0759	554.2476	1.4090
29	A	1614.7910	2.6418	333.5648	3.1737
30	A	1660.6357	17.1213	69.2750	6.1823
31	A	1710.6445	17.9764	204.9536	26.1346
32	A	3640.0981	8.1620	112.5691	177.4745
33	A	3770.9344	9.2590	68.6374	45.7562

py-06_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.5478	0.0734	1.6229	0.2693
2	A	118.3291	0.1334	0.3018	0.0480
3	A	196.6670	0.2044	0.8435	0.2885
4	A	202.3486	0.4597	0.4936	1.3503
5	A	282.9909	0.4738	4.0625	0.2763
6	A	300.3807	0.5130	2.2298	0.1514
7	A	305.2815	0.2343	3.5933	0.6028
8	A	324.0841	0.6747	1.1779	0.9921
9	A	360.0092	0.1063	12.8154	1.2562
10	A	410.2088	0.8478	5.1732	2.0085
11	A	426.0628	0.5064	10.1772	2.6509
12	A	432.8446	1.9424	0.2571	3.3219
13	A	463.6340	1.5818	0.2202	5.0291
14	A	547.4136	1.7388	2.9580	17.9719
15	A	577.2548	0.7735	56.5358	4.5978
16	A	611.2124	0.5808	168.8855	7.1542
17	A	665.8388	1.1022	120.0089	3.7997
18	A	677.8251	1.4699	13.2560	0.6795
19	A	712.9892	2.1736	28.9516	7.7526
20	A	929.0689	4.8753	122.0124	5.7710
21	A	967.4011	4.7312	90.7535	0.8115
22	A	1133.9059	1.4630	16.3391	1.4912
23	A	1188.0883	6.5837	9.0685	2.7652
24	A	1276.1499	5.0719	58.6413	0.7460
25	A	1442.8121	10.8178	19.5369	2.6767
26	A	1451.9373	8.8250	68.0351	10.8268
27	A	1496.6927	13.4290	47.8936	7.5360
28	A	1524.3484	9.7887	629.2335	6.2274
29	A	1630.5282	3.5137	42.6346	3.1534
30	A	1644.3881	4.2214	51.2159	7.6143
31	A	1687.2921	10.0225	164.8648	29.4199
32	A	3595.8645	7.9788	64.7051	202.4133
33	A	3717.4170	8.9596	47.8066	44.6604

py-06_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.1517	0.0782	1.5098	0.2892
2	A	120.6587	0.1301	0.4237	0.0733
3	A	201.9528	0.2118	0.6408	0.3003
4	A	204.0977	0.4715	0.4850	1.4117
5	A	281.8198	0.5125	3.4373	0.2545
6	A	304.8959	0.2463	4.4349	0.7889
7	A	322.9771	0.4996	2.7312	0.5102
8	A	324.0478	0.7618	1.3985	1.2574
9	A	387.3291	0.1604	8.4835	1.7262
10	A	416.4158	0.1857	165.1246	1.6079
11	A	426.1142	0.8860	14.0777	2.9995
12	A	454.1164	0.4553	39.1976	2.5299
13	A	466.1079	0.3100	93.8649	4.3066
14	A	547.0271	1.5011	16.0437	24.8331
15	A	585.2476	2.4475	11.8495	0.3467
16	A	676.9237	1.6373	1.6829	1.2220
17	A	688.6955	3.2116	1.3366	0.4394
18	A	696.0697	3.0562	7.0802	5.3142
19	A	734.3261	3.8520	5.0222	1.2438
20	A	910.4049	4.8988	128.0362	5.8719
21	A	956.0585	4.3648	109.1685	0.5291
22	A	1107.0720	1.3631	30.3403	1.2982
23	A	1165.8563	7.7426	9.1797	6.9162
24	A	1251.3706	5.8965	74.7892	1.0342
25	A	1361.9129	8.4943	37.5001	4.3566
26	A	1436.7249	9.9098	80.4511	8.4378
27	A	1475.6186	11.7005	75.7076	5.1718
28	A	1509.9163	8.8710	601.1007	1.1844
29	A	1614.5846	12.5825	49.8944	5.0047
30	A	1627.6954	2.3109	76.2276	1.6346
31	A	1672.3300	9.4738	234.2988	22.0323
32	A	3610.7852	8.0371	77.1915	196.4881
33	A	3731.6759	9.0465	50.5654	48.4931

py-06_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.5418	0.0862	1.3964	0.2674
2	A	124.2463	0.1336	0.4815	0.0697
3	A	202.7169	0.4673	0.4484	1.3305
4	A	203.7718	0.2128	0.8461	0.2946
5	A	280.5114	0.4603	4.0819	0.3014

6	A	303.6088	0.2548	4.6643	0.6486
7	A	327.3443	0.5776	1.1551	0.9245
8	A	328.9184	0.6590	2.3864	0.7307
9	A	392.4055	0.1217	158.1521	1.1148
10	A	397.3954	0.1867	116.2597	2.2775
11	A	433.9803	1.6300	1.8850	3.1870
12	A	456.4793	0.2715	30.7602	1.4182
13	A	468.8029	0.8443	12.9347	5.1699
14	A	559.5248	1.6240	12.7427	22.5209
15	A	595.6463	2.5561	10.5859	0.3456
16	A	685.5642	1.5519	0.7608	0.6486
17	A	700.6844	3.3386	1.3421	0.4091
18	A	709.0836	3.5809	7.5879	6.6065
19	A	746.0287	3.9791	6.0221	1.1953
20	A	935.0766	4.8137	124.6455	5.8461
21	A	978.7484	4.3655	102.0461	0.6183
22	A	1117.3117	1.3765	35.4360	1.3527
23	A	1199.3738	8.2451	9.6837	6.2988
24	A	1282.5126	6.9286	72.6360	1.0012
25	A	1370.1746	8.8026	42.3423	4.6548
26	A	1475.2285	8.8080	76.0588	7.9292
27	A	1511.8069	12.1715	64.6872	6.7763
28	A	1544.0697	7.6500	592.7885	1.4676
29	A	1638.2092	2.3532	161.5234	1.0762
30	A	1656.7078	14.2631	61.5580	6.6056
31	A	1709.0993	14.8346	220.6372	23.1189
32	A	3631.5537	8.1281	91.1128	179.1504
33	A	3754.4796	9.1642	60.4778	45.0708

py-06_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.5631	0.0753	1.3956	0.3238
2	A	117.9648	0.1216	0.5072	0.0936
3	A	192.6720	0.1932	0.7071	0.3229
4	A	195.3146	0.4389	0.4615	1.5322
5	A	269.0587	0.4326	3.6415	0.3587
6	A	292.1190	0.2367	4.0767	0.7497
7	A	311.1195	0.4856	2.0291	0.3458
8	A	313.4096	0.6738	0.8717	1.5714
9	A	374.8907	0.2081	3.4744	2.0540
10	A	399.3758	0.1289	219.1331	1.0649
11	A	415.2668	1.0976	6.3745	3.2606
12	A	440.3349	0.2689	39.0581	1.9658
13	A	450.7802	0.4400	39.8347	4.9946
14	A	533.4240	1.4525	14.9630	27.2631
15	A	559.9182	2.2407	10.2759	0.4535
16	A	655.1385	1.4656	1.1618	0.9448

17	A	657.5881	2.9345	1.1733	0.5300
18	A	675.0391	3.0266	7.8817	5.7956
19	A	698.2052	3.4795	4.3032	1.1665
20	A	886.5500	4.5082	129.2736	5.8624
21	A	930.3566	4.2362	104.5025	0.7963
22	A	1071.7712	1.2998	29.1348	1.3378
23	A	1129.7759	7.1093	8.0478	7.7196
24	A	1211.7834	5.3688	70.8670	1.1507
25	A	1351.2018	8.8004	35.8942	3.6629
26	A	1394.3256	9.1856	127.3928	6.8911
27	A	1433.6641	11.6572	60.4554	5.4852
28	A	1468.8719	7.2290	509.8749	1.2050
29	A	1564.3556	12.3067	42.0078	6.1161
30	A	1576.6987	2.1732	86.1282	1.8877
31	A	1627.3612	9.8631	242.9811	16.9125
32	A	3512.9261	7.6033	73.9280	214.8572
33	A	3631.8481	8.5696	49.8257	52.5183

py-06_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	111.2758	0.0779	1.5538	0.3007
2	A	119.7986	0.1238	0.5180	0.0897
3	A	190.6959	0.4228	0.4009	1.4818
4	A	193.6423	0.1967	0.7744	0.3017
5	A	262.1530	0.3899	3.9032	0.3409
6	A	286.7041	0.2318	3.3673	0.5941
7	A	311.4698	0.4979	1.4228	1.3183
8	A	314.0089	0.5339	3.2427	0.5621
9	A	372.5326	0.1766	5.9175	1.9221
10	A	416.2612	1.7438	1.2691	3.6365
11	A	422.4622	0.2027	24.0828	1.2125
12	A	446.4403	1.3978	4.0992	4.7241
13	A	504.1421	0.2248	263.7828	2.6083
14	A	535.3402	1.0157	43.9056	26.8517
15	A	561.8552	1.7474	32.6910	0.8654
16	A	653.5140	2.9597	1.3433	0.5046
17	A	656.0358	1.4456	0.9356	0.4796
18	A	678.7838	3.0419	7.7257	5.8385
19	A	691.7927	3.3846	10.0184	1.7511
20	A	889.6817	4.6780	133.4704	5.7687
21	A	933.2071	4.4701	107.7182	0.6293
22	A	1092.8887	1.4237	19.3708	1.7115
23	A	1133.3317	6.4099	11.0920	7.2496
24	A	1220.7022	4.8232	72.8998	1.3706
25	A	1354.5804	8.5190	18.5070	3.1602
26	A	1401.1114	9.4334	108.3118	6.3875
27	A	1444.2048	11.8864	71.0862	5.4982

28	A	1475.8646	9.0315	568.1093	1.1460
29	A	1578.9520	13.4919	27.3605	7.8284
30	A	1612.6274	2.6237	37.5210	1.3154
31	A	1644.4509	5.0514	238.8436	18.1496
32	A	3503.4363	7.5657	48.4022	213.9015
33	A	3617.1106	8.4894	35.8682	58.4914

py-06_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	113.7294	0.0821	1.4802	0.2868
2	A	121.9485	0.1291	0.4944	0.0802
3	A	195.6229	0.4422	0.4198	1.4256
4	A	199.4720	0.2072	0.6866	0.2995
5	A	269.7932	0.4009	4.1848	0.3477
6	A	293.5062	0.2483	3.4229	0.6256
7	A	318.1102	0.5947	0.9501	1.3911
8	A	321.5778	0.5526	3.0982	0.4471
9	A	386.0844	0.1885	4.7829	1.9580
10	A	421.1016	0.2810	87.8786	2.2672
11	A	426.2870	0.3208	53.3966	2.3324
12	A	452.8632	0.5702	36.8948	2.9287
13	A	467.8872	0.2520	146.6202	4.0322
14	A	544.0447	1.4495	18.2552	25.3417
15	A	579.5986	2.3725	12.6536	0.3932
16	A	669.3442	1.4982	0.6960	0.5459
17	A	676.6419	3.1359	1.1482	0.4343
18	A	692.2766	3.3365	8.1032	6.4819
19	A	718.3461	3.6981	6.0937	1.1946
20	A	905.6741	4.8035	131.5742	5.7821
21	A	950.7037	4.4869	110.1439	0.5432
22	A	1104.6522	1.4031	26.6759	1.5439
23	A	1158.0857	7.3558	9.5010	7.0180
24	A	1246.1240	5.6760	75.2785	1.2600
25	A	1353.8166	8.2835	24.8074	3.7912
26	A	1428.8570	9.7586	90.9343	7.1596
27	A	1469.5299	12.1218	70.9291	5.6514
28	A	1502.1239	9.2247	607.3927	1.2319
29	A	1607.8581	13.7346	36.9793	7.0272
30	A	1632.6417	2.4367	54.9761	1.0685
31	A	1668.7274	6.9218	254.8320	20.8027
32	A	3569.7887	7.8541	69.2752	196.7906
33	A	3688.5077	8.8380	47.4781	52.2927

py-06_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A	117.1189	0.0873	1.3503	0.4950
2	A	123.9374	0.1334	0.4499	9.2049
3	A	203.7625	0.4716	0.4637	1.6444
4	A	205.4112	0.2147	0.7899	0.7210
5	A	284.7851	0.5151	3.9201	0.2945
6	A	307.3204	0.2516	6.3757	0.6753
7	A	327.9985	0.6030	0.9834	1.1125
8	A	329.3431	0.6332	2.7590	0.7335
9	A	377.1538	0.1059	253.1716	1.9632
10	A	398.7746	0.1857	34.1975	2.1383
11	A	433.6727	1.7396	1.4939	2.3644
12	A	456.3917	0.2839	25.0225	1.5964
13	A	470.4836	1.0541	7.6877	5.3681
14	A	557.2251	1.6260	12.5060	24.6172
15	A	600.4068	2.6067	10.0187	12.5571
16	A	687.5698	1.6068	1.3567	0.6091
17	A	705.1627	3.3192	2.1734	4.1380
18	A	710.4129	3.4334	7.3213	3.7296
19	A	752.5202	4.0453	6.5529	69.2025
20	A	929.6617	4.9929	123.3567	9.4149
21	A	974.4152	4.3565	109.2175	0.2930
22	A	1118.0195	1.3781	41.0198	4.7558
23	A	1191.0691	8.3522	11.4996	6.6031
24	A	1279.2638	8.0255	87.7914	13.1600
25	A	1330.2756	6.8466	31.4327	5.3003
26	A	1469.1803	9.2404	73.0484	41.5782
27	A	1509.3904	12.3243	65.8911	20.5907
28	A	1540.5910	8.2019	617.4017	3.4090
29	A	1643.8235	2.3231	148.0799	0.9795
30	A	1661.7664	13.1810	67.7803	11.2705
31	A	1711.5911	14.4606	226.8131	46.9967
32	A	3637.9338	8.1571	88.5280	179.2670
33	A	3760.3238	9.1944	58.0200	41.1187

py-06_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.9967	0.0881	1.2811	0.2731
2	A	122.8864	0.1278	0.5313	0.0809
3	A	201.5554	0.2106	0.5615	0.3198
4	A	201.8586	0.4572	0.5322	1.3863
5	A	281.1152	0.5063	3.7755	0.2974
6	A	303.0687	0.2508	5.2788	0.7543
7	A	323.0039	0.6154	0.6829	1.2564
8	A	324.7426	0.6410	2.0817	0.6223
9	A	380.1009	0.1064	270.2904	1.3193
10	A	392.4763	0.2227	11.5357	2.2691

11	A	428.4777	1.6237	1.7527	3.3425
12	A	452.7029	0.2281	23.1681	1.2355
13	A	466.4924	0.9867	7.8511	5.2889
14	A	549.4419	1.5857	13.2478	24.3367
15	A	591.2401	2.5276	9.9928	0.3100
16	A	678.9404	1.5520	1.1803	0.7970
17	A	694.5625	3.2471	1.7101	0.4953
18	A	701.2398	3.3572	8.4035	5.7961
19	A	742.6910	3.9343	5.8897	1.1737
20	A	911.4554	4.9320	126.5920	5.6194
21	A	957.9668	4.3831	114.3110	0.4642
22	A	1105.2920	1.3802	34.9858	1.5427
23	A	1167.3600	7.7918	8.7034	6.7932
24	A	1258.0296	6.7116	79.8488	1.2586
25	A	1333.1627	7.4513	26.3771	4.3075
26	A	1439.4389	9.8084	82.3652	8.4138
27	A	1479.6526	11.9534	68.9303	5.3448
28	A	1511.3094	8.9377	611.0049	1.4951
29	A	1619.4409	12.4904	48.3334	5.8632
30	A	1633.0328	2.3216	87.5499	1.5718
31	A	1676.3379	9.6163	260.0988	24.4947
32	A	3599.6095	7.9833	90.4607	184.0327
33	A	3718.5306	8.9918	57.8792	46.9753

py-06_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.1720	0.0861	1.3376	0.2765
2	A	122.1113	0.1263	0.5351	0.0831
3	A	200.2747	0.2065	0.6248	0.2982
4	A	203.1074	0.4697	0.4977	1.4209
5	A	281.7987	0.5094	3.7117	0.3101
6	A	303.5206	0.2509	4.9278	0.7315
7	A	322.4590	0.5389	1.5797	0.6083
8	A	323.6884	0.7252	1.6227	1.2277
9	A	388.4688	0.1148	211.3395	1.0994
10	A	390.9786	0.2141	62.5663	2.3666
11	A	428.5891	1.5565	1.9665	3.3933
12	A	451.9126	0.2283	30.5177	1.1889
13	A	466.5128	0.9417	10.2063	5.3674
14	A	551.0452	1.5953	13.5841	24.4678
15	A	588.6725	2.4990	10.4824	0.3451
16	A	678.3790	1.5474	1.1228	0.7726
17	A	691.1505	3.2405	1.3201	0.4327
18	A	700.6778	3.3509	8.8653	5.9092
19	A	739.2711	3.9043	6.0765	1.1929
20	A	911.2687	4.9188	128.9401	5.6297
21	A	956.6806	4.4402	114.8354	0.5208

22	A	1105.0317	1.3796	33.8644	1.5577
23	A	1165.0984	7.7044	8.5387	6.7969
24	A	1256.5966	6.6009	78.5611	1.2704
25	A	1333.6876	7.4763	24.8170	4.2018
26	A	1438.6956	9.9325	93.7783	8.2038
27	A	1477.1939	11.9602	71.0255	5.3617
28	A	1508.6383	8.7805	593.5449	1.3871
29	A	1615.0763	13.1264	45.9905	6.2640
30	A	1630.7327	2.3230	79.8162	1.3020
31	A	1672.6438	9.0091	263.8566	23.8834
32	A	3595.1791	7.9635	87.0446	184.7764
33	A	3713.7951	8.9676	56.2550	47.3320

py-06_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.9171	0.0912	1.4576	0.2550
2	A	125.7623	0.1339	0.5092	0.0775
3	A	201.4090	0.4645	0.4448	1.3311
4	A	204.2973	0.2134	0.8097	0.3010
5	A	282.4703	0.5567	3.5551	0.2228
6	A	306.1640	0.2544	5.2009	0.6479
7	A	328.1751	0.5551	1.6153	1.1439
8	A	329.7941	0.5879	3.8887	0.6731
9	A	390.5379	0.1305	51.3009	1.4166
10	A	403.7491	0.1660	210.5918	2.4085
11	A	434.5210	1.5399	2.0805	3.4638
12	A	455.7006	0.2964	52.2500	1.3447
13	A	471.4998	0.8781	17.6039	5.6807
14	A	560.6635	1.6064	13.2701	20.9224
15	A	597.3953	2.5617	11.7250	0.4363
16	A	687.2756	1.5589	0.7221	0.5395
17	A	701.9439	3.3564	1.2013	0.3963
18	A	712.9665	3.6918	8.7268	7.1370
19	A	747.9941	4.0120	7.3253	1.4606
20	A	939.4390	4.9489	116.1556	5.7123
21	A	985.4659	4.1481	98.0612	0.3878
22	A	1120.0126	1.3810	41.1804	1.6467
23	A	1211.0670	8.6692	12.4804	5.9510
24	A	1293.6146	9.7970	88.1133	1.0301
25	A	1320.2121	5.8671	18.6786	4.4301
26	A	1484.5032	7.8987	32.3917	7.5147
27	A	1525.5383	12.6221	63.9707	6.7699
28	A	1550.4852	8.7855	653.7547	3.4158
29	A	1638.7197	2.2851	196.8183	2.7050
30	A	1672.1966	15.7438	60.9395	5.6373
31	A	1717.0805	16.5244	187.4743	28.2568
32	A	3618.3205	8.0698	104.0004	174.4457

33 A 3740.4378 9.0974 69.1678 44.2156

py-06_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.5485	0.0735	1.6223	0.2692
2	A	118.3312	0.1334	0.3021	0.0481
3	A	196.6689	0.2044	0.8431	0.2885
4	A	202.3509	0.4597	0.4936	1.3503
5	A	282.9897	0.4738	4.0624	0.2763
6	A	300.3958	0.5131	2.2297	0.1516
7	A	305.2824	0.2343	3.5927	0.6027
8	A	324.0867	0.6748	1.1779	0.9924
9	A	360.0454	0.1064	12.8164	1.2562
10	A	410.2596	0.8485	5.1723	2.0096
11	A	426.0657	0.5062	10.1790	2.6502
12	A	432.8479	1.9423	0.2570	3.3220
13	A	463.6353	1.5818	0.2202	5.0291
14	A	547.4167	1.7388	2.9578	17.9723
15	A	577.2705	0.7735	56.5416	4.5991
16	A	611.2186	0.5808	168.8999	7.1546
17	A	665.8460	1.1025	119.9594	3.7975
18	A	677.8294	1.4698	13.2738	0.6801
19	A	712.9925	2.1735	28.9568	7.7529
20	A	929.0727	4.8755	122.0113	5.7711
21	A	967.4007	4.7311	90.7525	0.8112
22	A	1133.9103	1.4630	16.3400	1.4912
23	A	1188.0922	6.5840	9.0698	2.7649
24	A	1276.1536	5.0719	58.6418	0.7461
25	A	1442.8279	10.8150	19.6072	2.6808
26	A	1451.9402	8.8263	67.9641	10.8230
27	A	1496.7057	13.4287	47.9008	7.5348
28	A	1524.3502	9.7891	629.2249	6.2276
29	A	1630.5429	3.5109	42.6903	3.1474
30	A	1644.3957	4.2256	51.1724	7.6169
31	A	1687.2942	10.0224	164.8538	29.4244
32	A	3595.8387	7.9787	64.7078	202.4166
33	A	3717.3928	8.9595	47.8071	44.6606

py-06_C_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	97.0817	0.0575	0.9868	1.0249
2	A	109.5805	0.0993	0.0013	0.1640
3	A	161.8344	0.2015	0.6205	0.8858
4	A	205.6376	0.5355	0.0071	1.3288

5	A	281.5497	0.8377	0.4515	0.3260
6	A	285.0558	0.5861	3.4728	0.4997
7	A	313.6052	1.0592	1.7376	0.7785
8	A	331.9794	0.3910	2.9753	4.0625
9	A	341.4877	0.4640	0.9036	1.7257
10	A	416.9997	1.6214	4.0970	4.2149
11	A	446.5913	1.6392	1.7153	3.8219
12	A	504.8169	0.2198	58.2882	0.7822
13	A	543.5723	2.2661	7.6168	21.5820
14	A	583.5694	0.7766	61.1951	0.2827
15	A	646.5589	2.3818	0.3329	4.1414
16	A	670.5119	1.3266	7.5898	1.2750
17	A	699.9281	2.3988	1.4124	1.5906
18	A	720.9043	2.9208	30.2983	1.7799
19	A	774.8698	0.4076	50.7045	0.2889
20	A	908.5204	5.0782	108.8150	1.8002
21	A	946.6135	3.7568	102.7659	1.9211
22	A	1103.1911	1.3507	162.7849	11.4245
23	A	1201.3920	7.7773	26.2382	9.5606
24	A	1266.8304	3.2217	81.3158	11.8709
25	A	1297.2182	2.5339	54.4021	1.6997
26	A	1332.8123	4.0815	34.0583	41.6882
27	A	1427.3072	7.2343	116.6663	10.6739
28	A	1507.4608	6.4724	39.3236	76.2048
29	A	1612.9511	16.9645	1.0334	30.6160
30	A	1674.2014	9.2310	654.0702	173.0840
31	A	1733.7186	20.8217	222.0223	12.3610
32	A	3542.4772	7.9456	36.1500	85.1340
33	A	3596.3166	8.2103	119.1041	81.0752

py-06_C_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	97.1079	0.0563	0.7821	1.0590
2	A	112.4226	0.1049	0.0182	0.1043
3	A	162.7384	0.2073	0.3775	0.8687
4	A	205.0707	0.5350	0.0093	1.2198
5	A	281.0064	0.8376	0.7003	0.2339
6	A	291.4022	0.6077	3.9553	0.4740
7	A	318.0841	1.0727	2.2823	0.6048
8	A	338.3196	0.4096	2.9761	4.2714
9	A	355.3459	0.4707	1.7551	1.6347
10	A	420.1619	1.6149	3.9120	4.0886
11	A	449.2772	1.6541	1.6185	3.3003
12	A	503.1270	0.2119	65.5444	0.8028
13	A	553.9018	2.3671	7.2239	17.7764
14	A	588.3171	0.8864	59.0894	0.1781
15	A	649.7378	2.4702	0.0221	3.4349

16	A	676.7939	1.3567	6.4475	1.5270
17	A	698.4490	2.6540	1.6292	2.5117
18	A	729.5391	2.9651	30.4002	1.8954
19	A	799.4103	0.4282	54.8932	0.3693
20	A	935.6445	5.1430	97.8803	1.3879
21	A	971.3190	3.6155	95.0010	2.2021
22	A	1124.3033	1.2621	157.5183	11.2096
23	A	1245.1809	8.3246	52.7531	9.3931
24	A	1296.6319	2.2716	63.9303	7.3731
25	A	1320.4595	3.2329	36.2938	3.3191
26	A	1361.9614	5.8189	35.2101	63.5236
27	A	1466.1268	8.2882	127.1454	8.3217
28	A	1544.7227	8.1061	52.2308	79.2515
29	A	1676.6045	18.4563	4.4375	46.5499
30	A	1726.5525	11.7874	730.9545	183.5352
31	A	1794.4254	22.4006	223.4457	13.9035
32	A	3577.3828	8.1050	53.0690	76.9240
33	A	3618.3885	8.3142	142.1974	79.5123

py-06_C_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	95.7363	0.0561	1.3040	1.1207
2	A	110.1377	0.1038	0.0352	0.2739
3	A	162.6231	0.2011	0.9048	1.1187
4	A	206.9248	0.5406	0.0086	1.2116
5	A	281.4620	0.8073	0.4174	0.2667
6	A	291.1008	0.5496	2.2426	0.6878
7	A	316.0623	1.0947	2.1327	0.6086
8	A	329.6297	0.3966	3.1118	4.9683
9	A	347.7030	0.5684	1.2728	2.4124
10	A	420.8937	1.5930	3.1923	3.4533
11	A	446.9941	1.6254	1.5848	3.5901
12	A	506.3927	0.4375	12.8571	0.7924
13	A	545.9637	2.1139	6.2068	15.1398
14	A	579.8173	0.3451	116.4116	1.3395
15	A	619.8526	2.1231	2.9616	6.2235
16	A	667.8075	1.2944	6.4625	2.7257
17	A	704.5813	2.6783	7.2830	13.5696
18	A	723.9775	2.6326	33.0837	2.2281
19	A	750.5123	0.3753	32.7787	0.8076
20	A	932.2548	5.2121	113.2579	3.0904
21	A	953.1267	3.8112	70.6584	1.2178
22	A	1127.2915	1.2821	139.2980	8.8644
23	A	1216.5240	8.6643	28.3642	7.2856
24	A	1284.4325	2.7318	61.8754	8.9745
25	A	1311.4492	2.2975	53.3376	0.7181
26	A	1380.8514	7.5280	28.2960	86.9372

27	A	1464.3604	7.2212	83.0133	3.9367
28	A	1522.9849	8.7114	36.9804	146.2677
29	A	1606.6436	18.1500	23.6732	21.0587
30	A	1679.6060	9.1300	553.0584	236.9254
31	A	1750.2397	21.1387	160.5489	10.9628
32	A	3559.2957	8.0211	38.1021	71.6388
33	A	3605.8321	8.2536	124.6214	87.6761

py-08_A_b31yp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	114.9615	0.0765	1.6167	0.2738
2	A	197.1985	0.2161	0.4719	0.5957
3	A	280.5573	0.3439	5.3335	0.9569
4	A	296.1449	0.3596	6.4017	1.2998
5	A	298.8476	0.3181	3.6345	0.1338
6	A	348.2671	0.5396	1.3405	0.1032
7	A	397.2311	0.1298	23.7162	1.1037
8	A	408.8233	0.1502	232.2208	1.1151
9	A	450.1870	0.4655	14.8602	2.4474
10	A	456.9591	0.7722	11.9000	3.9808
11	A	479.5042	0.4058	40.6649	0.5623
12	A	515.6015	1.5909	7.8460	12.5380
13	A	634.9771	1.0601	2.5870	1.8531
14	A	690.8682	3.0805	14.5785	1.0806
15	A	695.2018	3.3311	2.6696	1.0268
16	A	734.3525	2.8887	13.4079	1.4152
17	A	760.3132	2.7029	13.4314	28.0692
18	A	886.6971	1.6204	87.5686	0.4624
19	A	890.3676	0.6480	27.9298	0.2156
20	A	1099.8237	1.3635	53.4524	1.1966
21	A	1133.5906	3.1035	49.8511	5.2076
22	A	1201.8168	1.8517	68.9170	0.8857
23	A	1250.7857	4.0756	140.8955	0.5102
24	A	1340.1518	6.2081	45.4072	1.3733
25	A	1419.4974	9.8765	44.7175	11.7237
26	A	1466.1377	8.9519	44.5509	2.9459
27	A	1520.0869	7.4338	649.6669	2.3121
28	A	1631.0665	2.7116	106.8378	1.0903
29	A	1634.2339	5.6462	30.2458	6.0661
30	A	1685.0887	10.7042	104.5291	26.1194
31	A	3216.6344	6.6665	1.5452	102.2118
32	A	3593.1856	7.9553	73.9049	171.9036
33	A	3710.6198	8.9492	53.3559	44.6502

py-08_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.0330	0.0767	1.5898	0.2684
2	A	199.1994	0.2195	0.4895	0.5851
3	A	277.7440	0.2996	5.9146	0.9706
4	A	297.1675	0.3447	2.6146	0.0849
5	A	298.3406	0.3542	6.9466	1.2702
6	A	350.5692	0.5437	1.3461	0.0898
7	A	397.3142	0.1191	69.1205	0.8769
8	A	406.5027	0.1536	198.6071	1.2339
9	A	452.5409	0.6804	4.8616	3.1070
10	A	456.9476	0.6100	13.2227	3.2822
11	A	479.8298	0.4165	35.6185	0.5065
12	A	514.8350	1.5806	7.2490	11.5639
13	A	636.8668	1.0564	2.6357	1.8681
14	A	694.5396	3.1145	11.2079	0.8641
15	A	697.6132	3.4085	3.8519	1.2770
16	A	734.0804	3.0135	12.2759	1.2839
17	A	762.9676	2.7117	11.7759	28.3835
18	A	886.3785	0.6325	29.2963	0.2164
19	A	894.9398	1.5476	78.9214	0.5025
20	A	1102.8175	1.3472	47.0383	1.1843
21	A	1149.3846	2.4177	59.7647	4.4573
22	A	1208.8349	2.1240	46.2998	1.3700
23	A	1261.4428	4.3824	149.2853	0.4994
24	A	1368.2229	7.6189	60.6079	1.0407
25	A	1439.6870	9.9145	46.3716	11.2540
26	A	1482.8152	8.6472	39.0945	3.0093
27	A	1540.2297	6.8061	623.2293	1.7680
28	A	1631.1632	2.2107	193.1217	1.3606
29	A	1654.8961	13.8402	8.6441	6.0124
30	A	1705.7706	13.5348	90.0521	24.8176
31	A	3229.5020	6.7220	2.0854	100.1071
32	A	3613.2374	8.0458	77.8904	167.9218
33	A	3734.3846	9.0640	56.9486	43.0742

py-08_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	114.3650	0.0757	1.6123	0.2682
2	A	199.1797	0.2200	0.4708	0.5870
3	A	278.1709	0.3023	5.8580	0.9696
4	A	297.6685	0.3782	1.5400	0.3115
5	A	297.8512	0.3227	8.0897	1.0564
6	A	350.1961	0.5443	1.3562	0.0919
7	A	396.2408	0.1191	52.1064	0.8953
8	A	409.3399	0.1553	211.0255	1.1926
9	A	452.1635	0.8136	3.2363	3.4325

10	A	456.7447	0.5412	17.2303	3.0127
11	A	480.2854	0.4127	39.3981	0.5293
12	A	513.9200	1.5728	7.4430	11.7111
13	A	636.8403	1.0604	2.5669	1.8540
14	A	693.0919	3.1367	13.1174	1.2131
15	A	697.5876	3.3636	2.1784	0.9653
16	A	734.5570	2.9829	12.2833	1.3707
17	A	760.6005	2.6939	11.9807	28.2283
18	A	886.9541	0.6353	29.0168	0.2188
19	A	893.0174	1.5649	80.5452	0.4889
20	A	1102.2107	1.3486	48.3062	1.1807
21	A	1146.1444	2.5581	57.1263	4.6007
22	A	1206.3219	2.0371	51.9274	1.2190
23	A	1257.8910	4.2425	147.3634	0.5184
24	A	1363.6285	7.4096	60.3847	1.0859
25	A	1434.0984	9.9439	44.3957	11.4124
26	A	1478.9105	8.7289	39.1788	2.8918
27	A	1536.2616	7.0329	632.0465	1.8843
28	A	1631.4012	2.1779	175.8019	1.2614
29	A	1650.6571	13.6578	8.6960	5.8248
30	A	1701.3207	13.0355	90.9611	25.6569
31	A	3225.3175	6.7043	1.7148	100.6618
32	A	3611.2388	8.0372	75.2709	168.4942
33	A	3731.8693	9.0509	54.9734	43.4208

py-08_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1289	0.0681	1.6435	0.3280
2	A	187.8660	0.1995	0.3709	0.6608
3	A	270.0650	0.3223	5.0374	1.2033
4	A	282.3049	0.3379	5.2398	1.3049
5	A	288.0296	0.2986	3.3354	0.1432
6	A	333.7542	0.4936	1.2802	0.1299
7	A	384.1908	0.1455	5.9843	1.3599
8	A	410.6800	0.1554	178.0762	0.7694
9	A	433.3480	0.4278	23.7043	2.4567
10	A	440.1809	0.5938	20.3987	3.6840
11	A	464.4741	0.3004	86.0297	0.9566
12	A	494.3115	1.4126	10.4922	15.7411
13	A	610.5233	0.9914	1.6295	2.1019
14	A	655.4836	2.7479	5.1064	0.4891
15	A	659.5391	2.9305	15.1417	1.6469
16	A	693.5481	2.6795	10.0069	1.1962
17	A	728.3146	2.4808	15.7652	29.1259
18	A	845.5442	0.6228	35.8158	0.2582
19	A	846.8458	1.3532	86.7942	0.5366
20	A	1058.9669	1.3095	58.4477	1.2082

21	A	1068.5633	3.4948	36.2148	7.1489
22	A	1150.8464	1.9255	135.0323	0.9630
23	A	1197.0132	2.3660	83.7984	1.0680
24	A	1313.2027	6.2036	30.8013	0.8396
25	A	1346.1394	8.4147	66.3855	9.5980
26	A	1395.9958	8.3832	36.2568	4.0978
27	A	1448.4742	7.0987	600.4867	1.2406
28	A	1550.9756	10.8141	6.0340	7.4334
29	A	1579.6378	2.3423	46.2966	0.6383
30	A	1612.0986	5.1204	136.5602	20.2679
31	A	3138.5254	6.3404	1.0698	110.7679
32	A	3486.4008	7.4876	59.1834	200.6927
33	A	3599.9407	8.4181	43.6189	50.9791

py-08_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	107.8743	0.0674	1.6412	0.3192
2	A	189.2273	0.2015	0.4184	0.6456
3	A	267.5400	0.2781	5.5812	1.2007
4	A	283.8936	0.3385	5.3914	1.2773
5	A	286.4962	0.3100	2.9426	0.0998
6	A	336.1769	0.4910	1.3471	0.1075
7	A	383.4603	0.1344	6.7793	1.2016
8	A	414.9215	0.1720	158.0102	0.8621
9	A	434.8204	0.6011	15.2608	2.9541
10	A	439.8043	0.5271	22.3048	2.8935
11	A	466.3251	0.2766	113.3317	1.0856
12	A	494.8407	1.4135	9.8079	14.2584
13	A	612.2167	0.9884	1.6475	2.1509
14	A	655.2460	2.8165	3.0284	0.4901
15	A	664.8828	2.9336	14.0339	1.6993
16	A	690.1292	2.8114	9.4365	1.1433
17	A	732.5129	2.4907	13.6834	29.7857
18	A	836.3218	0.5551	28.7854	0.2373
19	A	856.8470	1.5413	84.1855	0.5899
20	A	1063.6652	1.2874	48.4653	1.1852
21	A	1088.4480	2.7362	51.3221	6.4491
22	A	1157.5326	1.8867	92.0455	1.3430
23	A	1205.7984	2.9045	108.0002	0.9498
24	A	1342.7671	7.3922	41.8558	0.3832
25	A	1369.8586	8.9001	77.4209	9.5830
26	A	1414.9070	8.5930	34.4118	4.1161
27	A	1469.4451	6.6909	585.1650	1.0477
28	A	1572.0983	6.3330	33.3051	4.9905
29	A	1576.2576	2.3836	86.8162	2.8872
30	A	1629.6029	9.8532	101.3656	18.9339
31	A	3141.2311	6.3537	1.4065	110.2957

32	A	3495.0236	7.5264	59.2680	198.7682
33	A	3612.1282	8.4732	45.7924	49.8590

py-08_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	107.5819	0.0671	1.6514	0.3154
2	A	190.1545	0.2033	0.4009	0.6364
3	A	268.9983	0.2835	5.5429	1.1953
4	A	284.6922	0.3381	5.4773	1.2746
5	A	288.2240	0.3148	2.9239	0.0945
6	A	337.4401	0.5012	1.3317	0.1063
7	A	385.6945	0.1321	8.0897	1.1589
8	A	414.1005	0.1671	178.7134	0.8077
9	A	436.2370	0.6882	8.0845	3.3365
10	A	441.2288	0.4885	24.4339	2.6584
11	A	467.3434	0.2942	96.2913	0.9523
12	A	496.0470	1.4227	9.6505	14.1268
13	A	614.9106	0.9997	1.6397	2.1049
14	A	660.0706	2.8399	3.4967	0.4430
15	A	666.2208	2.9897	13.6763	1.7523
16	A	695.6302	2.7915	9.4642	1.1388
17	A	734.0992	2.5072	13.6957	29.4661
18	A	842.2348	0.5650	28.1847	0.2336
19	A	859.5978	1.5681	86.0381	0.5652
20	A	1067.2625	1.2942	50.0679	1.1772
21	A	1091.4295	2.8702	48.2811	6.3732
22	A	1161.1884	1.8935	100.0993	1.1974
23	A	1209.0794	2.8158	104.7514	0.9763
24	A	1347.5649	7.4302	45.3066	0.4069
25	A	1373.0701	8.9650	75.2008	9.4137
26	A	1419.9018	8.6802	33.7133	3.9386
27	A	1474.9971	6.8003	584.9351	0.9870
28	A	1578.2032	9.4122	16.7317	5.9645
29	A	1583.5820	2.1501	97.7993	1.6567
30	A	1635.4449	9.6263	103.7110	19.6382
31	A	3157.2270	6.4185	1.2555	108.2086
32	A	3516.5476	7.6195	59.8358	193.3606
33	A	3634.0365	8.5767	45.5114	48.8774

py-08_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	118.5744	0.0828	1.3980	0.2483
2	A	201.3078	0.2187	0.5556	0.5449
3	A	282.4849	0.3471	5.8578	0.8843

4	A	300.6954	0.3144	6.2000	0.1556
5	A	302.4917	0.3712	6.7964	1.2660
6	A	352.8794	0.5008	7.1826	0.1512
7	A	364.4153	0.1009	278.6517	1.1986
8	A	407.5231	0.1496	9.9607	1.3606
9	A	457.7795	0.5078	3.7396	2.6522
10	A	462.4318	0.8286	4.8185	3.7843
11	A	485.6383	0.4696	12.6967	0.2557
12	A	521.3628	1.6357	6.5868	11.0270
13	A	641.4497	1.0597	3.6731	1.7000
14	A	701.5423	3.3074	14.7666	1.3936
15	A	715.7194	3.4672	1.4349	0.6003
16	A	757.9563	2.8956	15.4936	1.6719
17	A	773.3752	2.8210	11.8160	27.5488
18	A	901.2835	1.5724	83.1577	0.4602
19	A	915.1397	0.6907	27.3769	0.2753
20	A	1107.3479	1.3640	56.2738	1.2599
21	A	1158.0259	2.5996	55.7400	4.0636
22	A	1215.1613	2.0143	25.5402	0.8766
23	A	1269.7970	6.6136	183.8148	0.2389
24	A	1328.0816	5.1478	52.3941	1.9981
25	A	1451.9089	9.7983	36.8765	12.7640
26	A	1496.9644	8.8808	40.2315	2.3807
27	A	1552.3524	6.7918	640.0292	3.5892
28	A	1642.2357	2.2308	227.6871	2.4077
29	A	1677.5949	14.4124	12.2663	6.3380
30	A	1725.7045	14.8114	91.4220	30.6707
31	A	3235.5069	6.7514	2.7040	97.2253
32	A	3625.2752	8.0972	92.4190	154.6350
33	A	3743.9820	9.1192	64.0974	39.8755

py-08_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.3146	0.0812	1.6830	0.2517
2	A	201.7105	0.2250	0.6009	0.5749
3	A	282.6641	0.3884	4.7526	0.7102
4	A	301.5253	0.2983	4.7237	0.2047
5	A	302.7930	0.3611	7.6611	1.2403
6	A	354.5040	0.5229	1.5838	0.0973
7	A	390.7435	0.1117	27.6594	0.9485
8	A	424.5487	0.1938	196.1349	1.6495
9	A	457.6638	0.9785	5.7837	3.2916
10	A	463.0351	0.5238	29.7498	3.0023
11	A	485.7624	0.3667	82.6722	1.1988
12	A	518.9641	1.6021	7.4270	10.3337
13	A	640.7312	1.0729	3.4653	1.7712
14	A	703.0218	3.0611	10.1068	0.5475

15	A	707.5308	3.4669	3.9361	1.1800
16	A	745.3396	3.1393	14.6785	1.3172
17	A	772.1194	2.7917	9.6833	28.3903
18	A	904.3142	0.6600	31.2611	0.2416
19	A	908.4297	1.5022	70.9496	0.5394
20	A	1113.6866	1.3497	46.5297	1.2417
21	A	1172.7522	1.8914	65.4698	2.7950
22	A	1219.1188	2.7717	6.3645	1.3370
23	A	1278.6880	7.3922	185.6394	0.1984
24	A	1325.5498	4.9583	47.5211	1.7929
25	A	1467.1909	9.7584	19.4584	13.5633
26	A	1506.6119	8.5638	33.7898	2.1791
27	A	1558.8156	7.3367	660.8276	4.2198
28	A	1639.0133	2.2467	237.1386	3.4356
29	A	1685.8328	14.8372	11.7936	4.7609
30	A	1728.5075	15.1894	68.5114	30.3905
31	A	3243.7287	6.7854	3.9728	94.8308
32	A	3616.4870	8.0627	88.7035	162.4250
33	A	3737.2240	9.0778	65.5445	41.6924

py-08_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.5163	0.0832	1.0310	0.2739
2	A	198.9632	0.1993	0.8544	0.5760
3	A	274.8967	0.2912	12.2732	0.9753
4	A	289.6144	0.1258	104.7581	0.8203
5	A	299.1433	0.3958	3.0100	1.2754
6	A	303.5097	0.0958	167.3430	0.9234
7	A	348.8749	0.5579	3.7920	0.0842
8	A	404.3996	0.1462	5.6896	1.3553
9	A	447.3138	1.1702	1.5415	4.2206
10	A	454.1929	0.4136	2.2134	2.0392
11	A	476.4841	0.4441	6.9290	0.1763
12	A	506.9549	1.5224	5.9287	10.0766
13	A	628.3464	1.0031	3.8578	1.8874
14	A	691.8251	3.3262	11.9871	1.4821
15	A	703.7730	3.3549	1.3410	0.5217
16	A	742.7969	2.9016	13.6143	1.1536
17	A	762.9341	2.7467	9.3624	29.9976
18	A	895.1251	1.3479	67.8774	0.6209
19	A	902.7358	0.6653	27.9285	0.3808
20	A	1082.1106	1.2898	47.2820	1.1413
21	A	1159.5730	1.8025	68.7615	3.1888
22	A	1211.7308	2.8731	12.6628	1.8467
23	A	1264.5737	5.8952	178.0975	0.2190
24	A	1330.9781	7.0951	73.4455	1.6543
25	A	1460.6797	8.5958	31.1148	12.4313

26	A	1493.7581	7.3729	30.6539	3.1076
27	A	1552.4830	5.2174	546.0395	1.8651
28	A	1615.2360	2.6478	395.6847	3.6974
29	A	1673.2750	15.4421	14.8932	5.6095
30	A	1720.6962	16.1211	78.8812	29.8375
31	A	3252.3136	6.8176	0.9167	107.2834
32	A	3637.7394	8.1524	95.6981	165.0560
33	A	3767.1263	9.2359	64.4318	43.1997

py-08_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.1722	0.0710	1.6632	0.2200
2	A	198.4409	0.2192	0.7092	0.4843
3	A	281.2790	0.3100	5.3283	0.7786
4	A	290.5024	0.3235	7.0950	1.1617
5	A	301.0686	0.3242	2.2231	0.0841
6	A	346.3688	0.2433	4.5081	0.1014
7	A	360.6021	0.1146	13.4757	0.7599
8	A	440.5713	0.7493	8.7789	2.9678
9	A	445.3745	0.6183	0.9273	0.3364
10	A	452.6729	1.2931	0.8494	4.1838
11	A	510.9462	1.6540	4.3681	10.8460
12	A	575.0547	1.0761	32.0073	2.1814
13	A	614.7592	0.5794	162.6738	4.1129
14	A	633.7609	1.1107	2.4022	2.3991
15	A	667.1911	0.9991	127.4244	2.5477
16	A	710.1377	1.6977	43.3833	3.4351
17	A	753.6652	2.2593	18.2924	28.4795
18	A	847.2518	0.5337	41.7441	0.0484
19	A	894.2702	1.6759	66.0572	0.6800
20	A	1124.8989	1.4394	34.4493	1.1593
21	A	1156.9553	2.7293	54.2312	3.2882
22	A	1212.9366	1.9643	66.7962	0.6149
23	A	1268.2112	3.1901	108.3914	0.5886
24	A	1429.6764	10.0288	0.5669	8.6625
25	A	1442.7424	9.2789	112.7583	8.2583
26	A	1475.4102	9.6320	28.7757	1.8493
27	A	1536.5272	8.1247	627.7012	7.9049
28	A	1636.2727	2.2094	115.6019	0.5516
29	A	1655.2742	10.4679	1.8671	7.4529
30	A	1696.6465	10.9552	53.8600	31.0216
31	A	3251.8839	6.8181	2.6095	98.4310
32	A	3595.0059	7.9757	55.0814	187.9388
33	A	3715.7953	8.9493	45.6004	42.5719

py-08_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	111.7086	0.0716	1.6846	0.2754
2	A	197.4765	0.2193	0.4192	0.6044
3	A	280.5270	0.3336	5.1887	0.9587
4	A	294.7566	0.3497	6.4370	1.3290
5	A	300.2780	0.3242	3.2213	0.1186
6	A	348.6138	0.5329	1.4567	0.1040
7	A	391.6799	0.1197	13.5603	0.9505
8	A	430.7332	0.2268	143.5105	1.2953
9	A	448.8256	1.1485	1.6768	4.0035
10	A	457.4297	0.4122	44.1350	1.8292
11	A	485.5863	0.3023	123.9439	1.0405
12	A	509.8908	1.4941	10.0751	12.7150
13	A	635.5432	1.0760	2.0342	1.8465
14	A	686.0997	3.0316	14.1502	1.2694
15	A	692.4614	3.2561	1.8106	0.8889
16	A	728.7693	2.7802	12.2337	1.6141
17	A	751.5913	2.6068	12.7873	27.6284
18	A	878.7002	0.6291	26.9474	0.2216
19	A	886.5127	1.6327	84.0130	0.4964
20	A	1100.7990	1.3529	48.7768	1.1058
21	A	1134.6096	2.8694	53.2224	5.3866
22	A	1196.6097	1.9047	74.1544	1.1473
23	A	1245.2666	3.5018	130.6145	0.6423
24	A	1367.8679	7.4833	62.8635	0.8208
25	A	1417.0809	9.9839	46.2166	11.6602
26	A	1465.2058	8.8740	37.9857	2.9233
27	A	1521.8779	7.5366	646.4450	1.7786
28	A	1628.6135	2.1604	124.6157	0.8615
29	A	1633.2952	12.1551	7.8890	5.1758
30	A	1685.0263	11.0239	90.6029	25.9967
31	A	3222.2672	6.6901	1.1184	104.9797
32	A	3608.7558	8.0286	65.1995	183.1863
33	A	3728.6639	9.0291	48.0676	46.0502

py-08_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.9857	0.0775	1.6169	0.2577
2	A	200.6284	0.2225	0.5321	0.5777
3	A	279.9531	0.3156	5.6360	0.8900
4	A	299.5044	0.3341	2.9995	0.0992
5	A	300.7591	0.3576	7.2372	1.2869
6	A	353.2037	0.5438	1.3928	0.0879
7	A	398.8548	0.1238	25.2510	0.9789
8	A	414.9308	0.1558	232.2209	1.1554

9	A	455.2393	0.8876	3.4964	3.4574
10	A	459.9018	0.5419	19.4884	2.9737
11	A	483.4758	0.4080	46.3574	0.6072
12	A	517.9874	1.6018	7.1259	11.1039
13	A	640.9730	1.0702	2.7307	1.8290
14	A	700.0516	3.1758	12.5696	1.1029
15	A	704.9431	3.4423	1.9800	0.9428
16	A	741.9165	3.0032	13.2742	1.3916
17	A	768.2907	2.7502	11.3235	28.0893
18	A	892.8288	0.6453	29.0916	0.2202
19	A	902.3042	1.5388	76.7272	0.5110
20	A	1111.1153	1.3541	45.9801	1.1668
21	A	1159.1396	2.1744	62.8377	3.9971
22	A	1216.5510	2.3316	34.2497	1.5691
23	A	1271.2306	4.7521	155.6904	0.4221
24	A	1374.1558	7.6684	66.4428	1.1031
25	A	1454.6486	10.1765	42.1626	12.4779
26	A	1496.8647	8.4149	40.3303	2.6097
27	A	1553.7898	6.6973	619.5746	2.0726
28	A	1639.0832	2.2743	215.3317	1.7961
29	A	1671.5695	14.5174	9.9266	5.3769
30	A	1720.7140	14.3943	84.7751	26.6436
31	A	3238.0050	6.7591	2.0489	100.2762
32	A	3629.7006	8.1205	77.6784	167.0422
33	A	3751.5071	9.1464	57.4680	42.5264

py-08_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1504	0.0680	1.6051	0.3201
2	A	189.7332	0.2023	0.4167	0.6501
3	A	268.9246	0.2990	5.1908	1.1556
4	A	285.1871	0.3441	5.1295	1.2717
5	A	288.0228	0.2992	3.3962	0.1340
6	A	337.7466	0.5017	1.2744	0.1088
7	A	386.8197	0.1398	6.5247	1.2279
8	A	411.1555	0.1503	200.4192	0.6840
9	A	435.5762	0.5670	9.3959	3.0083
10	A	440.2120	0.5688	16.6701	3.1600
11	A	465.2433	0.3044	80.1765	0.8825
12	A	495.8329	1.4299	8.9163	14.1200
13	A	614.1210	0.9898	1.7228	2.1035
14	A	661.2415	2.8384	3.5599	0.4695
15	A	666.9709	3.0119	13.2728	1.5534
16	A	696.5736	2.7325	9.4537	1.1037
17	A	735.5023	2.5218	13.0861	29.5145
18	A	838.8980	0.5636	28.1170	0.2409
19	A	861.2572	1.5191	82.7964	0.6150

20	A	1066.3040	1.2793	48.0974	1.1585
21	A	1093.6220	2.5377	52.5563	6.1764
22	A	1159.9879	1.9432	84.4004	1.5691
23	A	1209.5607	3.0497	111.6605	0.9342
24	A	1354.5429	7.7476	48.7447	0.2681
25	A	1378.6940	8.9739	84.4117	10.0197
26	A	1424.0657	8.6201	31.8758	4.1250
27	A	1478.8951	6.4394	570.6996	1.0160
28	A	1577.1931	2.1445	132.4825	0.7415
29	A	1582.9275	9.6805	8.1764	6.9299
30	A	1639.3295	11.0640	97.7571	19.5714
31	A	3151.0686	6.3940	1.6671	110.2562
32	A	3511.4633	7.5973	62.7824	199.2311
33	A	3629.6778	8.5572	47.8267	49.0437

py-08_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	110.8421	0.0702	1.7449	0.2989
2	A	191.2337	0.2063	0.5338	0.6116
3	A	262.7154	0.2764	5.4017	1.0501
4	A	282.4334	0.2994	2.1830	0.0824
5	A	288.9951	0.3299	6.8260	1.2933
6	A	336.3284	0.4473	1.5838	0.0899
7	A	380.6680	0.1276	8.9103	1.1252
8	A	428.3561	0.3438	18.6980	2.1463
9	A	436.3378	1.1613	0.9861	4.0061
10	A	446.8164	0.4610	12.8812	0.1931
11	A	495.6362	1.5405	3.6254	13.1406
12	A	522.9769	0.2254	312.7976	2.3102
13	A	612.2861	1.0114	1.5379	2.3778
14	A	657.2189	2.8897	2.5261	0.4725
15	A	673.1194	2.5974	13.9627	1.6539
16	A	692.1543	2.9568	15.6226	1.5400
17	A	739.1459	2.4659	15.6479	29.6723
18	A	860.9633	0.5822	28.3183	0.2004
19	A	865.5003	1.6335	84.9838	0.5776
20	A	1087.4075	1.3706	45.0390	1.2139
21	A	1099.5684	3.2509	51.7787	6.6895
22	A	1177.7603	1.9788	118.5460	0.8636
23	A	1223.9190	2.5242	86.9026	0.9967
24	A	1358.7222	7.2871	23.8956	0.3414
25	A	1385.9983	9.3213	66.6995	9.8979
26	A	1432.8131	8.8732	38.8052	3.7562
27	A	1486.3328	7.4528	623.0100	1.4289
28	A	1597.4327	9.9381	8.8862	7.5904
29	A	1616.4714	2.2577	65.5605	1.3024
30	A	1655.9119	7.5772	100.1484	19.0362

31	A	3182.0792	6.5213	0.2301	113.4297
32	A	3501.6465	7.5582	40.0437	197.9430
33	A	3614.5651	8.4753	33.8460	54.5765

py-08_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	113.2600	0.0738	1.6922	0.2817
2	A	196.2686	0.2161	0.4837	0.5988
3	A	269.6724	0.2771	5.8008	1.0223
4	A	289.5580	0.3334	2.0491	0.0665
5	A	294.8812	0.3471	6.7429	1.2956
6	A	343.6271	0.5058	1.4773	0.0891
7	A	392.6970	0.1320	8.1904	1.1695
8	A	433.0751	0.2391	99.2790	1.3635
9	A	445.4033	1.1692	2.9207	3.8466
10	A	455.0656	0.4133	43.4494	1.2472
11	A	487.3022	0.2601	181.4962	1.3482
12	A	506.5576	1.4162	12.6718	12.8218
13	A	625.6428	1.0491	1.8851	2.0876
14	A	679.7638	3.0276	3.8290	0.3819
15	A	685.8538	3.0806	12.0530	2.0602
16	A	716.2396	3.0269	11.8158	1.4020
17	A	751.2833	2.5883	14.1922	28.7588
18	A	880.6573	1.5479	83.4333	0.4901
19	A	882.5950	0.6342	30.2335	0.2083
20	A	1098.7447	1.3779	48.1623	1.2009
21	A	1125.9254	3.2541	50.7367	5.7986
22	A	1198.8474	1.9282	95.1515	0.8582
23	A	1244.3541	3.1365	113.6996	0.7281
24	A	1358.9629	7.0810	40.7032	0.8514
25	A	1411.0577	9.8011	49.0297	10.7559
26	A	1457.5342	9.0159	40.0747	3.2836
27	A	1513.3513	7.6524	656.3585	1.8621
28	A	1626.1416	8.9337	18.4957	5.8914
29	A	1635.2686	2.3302	86.4847	1.8803
30	A	1680.7550	9.2087	102.4578	22.5127
31	A	3219.0984	6.6766	0.9037	107.2860
32	A	3567.8384	7.8460	58.1550	182.7631
33	A	3685.5686	8.8211	44.8323	49.1000

py-08_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.7807	0.0786	1.5862	0.2366
2	A	201.7700	0.2240	0.5380	0.5326

3	A	283.2025	0.3136	6.0554	0.8946
4	A	301.1408	0.3467	8.3491	1.2718
5	A	302.4370	0.3562	2.7874	0.0935
6	A	354.2454	0.5491	1.3790	0.0919
7	A	392.0650	0.1112	83.4440	0.8122
8	A	409.3133	0.1535	192.1842	1.4828
9	A	457.9142	0.8927	3.4160	3.3304
10	A	462.3328	0.6047	17.6472	3.3072
11	A	483.9870	0.4505	33.1946	0.5185
12	A	519.7588	1.6249	7.0039	10.9509
13	A	644.2899	1.0898	3.0355	1.7008
14	A	700.2839	3.2050	14.3378	1.4703
15	A	709.4623	3.4622	1.2467	0.7361
16	A	747.5687	3.0166	14.2921	1.5994
17	A	768.0487	2.7525	11.8358	27.8379
18	A	901.9434	1.6069	82.9586	0.4603
19	A	906.8381	0.6692	29.2280	0.2288
20	A	1112.0344	1.3640	53.5367	1.2623
21	A	1158.6929	2.6661	57.4650	4.1662
22	A	1216.5715	1.9777	32.5603	0.8850
23	A	1267.6559	5.7033	175.7450	0.2930
24	A	1337.8336	5.5565	60.4863	1.8217
25	A	1448.3680	10.0571	36.7255	12.7922
26	A	1493.6226	8.8444	43.3815	2.1491
27	A	1551.5556	6.9617	644.5303	3.4778
28	A	1644.3535	2.2103	203.3163	1.8864
29	A	1676.5880	14.3801	12.2366	5.2184
30	A	1723.6876	14.0668	87.9004	30.1907
31	A	3235.1690	6.7499	1.4715	97.4931
32	A	3635.4649	8.1470	74.9912	154.4060
33	A	3756.4475	9.1715	54.6095	40.2749

py-08_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.7386	0.0779	1.5773	0.2716
2	A	198.2656	0.2184	0.4523	0.6006
3	A	280.0902	0.3384	5.4516	0.9492
4	A	297.5207	0.3730	5.5748	1.2769
5	A	298.5406	0.3158	4.2981	0.1558
6	A	348.8180	0.5440	1.3169	0.1054
7	A	396.5026	0.1172	101.9961	0.8462
8	A	404.3804	0.1583	168.3551	1.4052
9	A	451.0699	0.4791	10.2333	2.6085
10	A	457.2369	0.7618	10.8980	3.9709
11	A	480.3526	0.4297	30.1709	0.4467
12	A	514.9620	1.5865	7.6046	12.4698
13	A	635.6545	1.0585	2.7207	1.8307

14	A	691.8257	3.1427	15.1016	1.3079
15	A	698.2890	3.3240	1.9195	0.8316
16	A	737.5468	2.8950	13.2024	1.5179
17	A	759.8732	2.6981	13.0414	27.9679
18	A	887.8074	1.6285	87.0078	0.4586
19	A	894.2778	0.6513	27.5811	0.2123
20	A	1100.1648	1.3643	52.9466	1.1693
21	A	1136.6455	3.0930	50.6894	5.1610
22	A	1203.2056	1.8521	65.1928	0.8784
23	A	1252.1663	4.2074	145.0234	0.4711
24	A	1339.8225	6.1822	47.5900	1.3954
25	A	1420.7133	9.8225	41.3832	11.8789
26	A	1468.2998	9.0136	40.2094	2.9669
27	A	1523.2040	7.5112	661.6301	2.4947
28	A	1633.4723	2.3066	129.6212	0.6397
29	A	1638.2404	8.8629	15.1536	6.4782
30	A	1688.9673	11.1394	101.8756	26.7667
31	A	3218.2056	6.6734	1.6562	102.4293
32	A	3597.5678	7.9749	76.7993	171.3332
33	A	3715.2637	8.9727	54.8315	44.3830

py-08_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	114.9615	0.0765	1.6166	0.2738
2	A	197.1986	0.2161	0.4719	0.5957
3	A	280.5573	0.3439	5.3336	0.9569
4	A	296.1449	0.3596	6.4017	1.2998
5	A	298.8476	0.3181	3.6345	0.1338
6	A	348.2670	0.5396	1.3405	0.1032
7	A	397.2307	0.1298	23.7149	1.1037
8	A	408.8233	0.1502	232.2232	1.1151
9	A	450.1868	0.4655	14.8602	2.4474
10	A	456.9590	0.7722	11.8999	3.9808
11	A	479.5041	0.4058	40.6640	0.5623
12	A	515.6014	1.5909	7.8460	12.5380
13	A	634.9770	1.0601	2.5870	1.8531
14	A	690.8681	3.0805	14.5785	1.0806
15	A	695.2018	3.3311	2.6696	1.0267
16	A	734.3525	2.8887	13.4079	1.4152
17	A	760.3133	2.7029	13.4314	28.0692
18	A	886.6971	1.6204	87.5688	0.4624
19	A	890.3674	0.6480	27.9298	0.2156
20	A	1099.8234	1.3635	53.4526	1.1966
21	A	1133.5901	3.1034	49.8511	5.2076
22	A	1201.8170	1.8517	68.9163	0.8857
23	A	1250.7854	4.0756	140.8953	0.5102
24	A	1340.1516	6.2081	45.4066	1.3733

25	A	1419.4972	9.8765	44.7168	11.7238
26	A	1466.1374	8.9519	44.5502	2.9459
27	A	1520.0866	7.4338	649.6697	2.3121
28	A	1631.0665	2.7116	106.8367	1.0903
29	A	1634.2339	5.6461	30.2456	6.0662
30	A	1685.0885	10.7042	104.5302	26.1193
31	A	3216.6347	6.6665	1.5452	102.2118
32	A	3593.1860	7.9553	73.9050	171.9036
33	A	3710.6201	8.9492	53.3559	44.6502

py-08_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.3146	0.0812	1.6830	0.2517
2	A	201.7105	0.2250	0.6009	0.5749
3	A	282.6642	0.3884	4.7526	0.7102
4	A	301.5254	0.2983	4.7235	0.2047
5	A	302.7932	0.3611	7.6612	1.2403
6	A	354.5039	0.5229	1.5838	0.0973
7	A	390.7445	0.1117	27.6551	0.9485
8	A	424.5507	0.1938	196.1300	1.6494
9	A	457.6639	0.9785	5.7831	3.2916
10	A	463.0355	0.5238	29.7524	3.0021
11	A	485.7633	0.3666	82.6798	1.1989
12	A	518.9641	1.6021	7.4272	10.3337
13	A	640.7313	1.0729	3.4652	1.7712
14	A	703.0218	3.0611	10.1068	0.5475
15	A	707.5309	3.4669	3.9361	1.1800
16	A	745.3397	3.1393	14.6787	1.3173
17	A	772.1194	2.7917	9.6833	28.3903
18	A	904.3143	0.6600	31.2611	0.2416
19	A	908.4298	1.5022	70.9496	0.5394
20	A	1113.6869	1.3497	46.5297	1.2417
21	A	1172.7526	1.8914	65.4697	2.7950
22	A	1219.1188	2.7717	6.3644	1.3370
23	A	1278.6881	7.3922	185.6394	0.1985
24	A	1325.5497	4.9583	47.5203	1.7928
25	A	1467.1906	9.7585	19.4579	13.5633
26	A	1506.6117	8.5638	33.7900	2.1791
27	A	1558.8155	7.3367	660.8300	4.2199
28	A	1639.0130	2.2467	237.1372	3.4356
29	A	1685.8329	14.8371	11.7935	4.7610
30	A	1728.5071	15.1894	68.5105	30.3904
31	A	3243.7283	6.7854	3.9728	94.8308
32	A	3616.4860	8.0627	88.7029	162.4251
33	A	3737.2229	9.0778	65.5443	41.6924

py-08_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.1722	0.0710	1.6632	0.2200
2	A	198.4409	0.2192	0.7092	0.4843
3	A	281.2794	0.3100	5.3282	0.7786
4	A	290.5026	0.3235	7.0949	1.1617
5	A	301.0689	0.3242	2.2231	0.0841
6	A	346.3693	0.2433	4.5074	0.1014
7	A	360.6037	0.1146	13.4762	0.7599
8	A	440.5713	0.7493	8.7787	2.9681
9	A	445.3752	0.6183	0.9278	0.3362
10	A	452.6730	1.2931	0.8493	4.1837
11	A	510.9461	1.6540	4.3681	10.8460
12	A	575.0581	1.0761	32.0148	2.1817
13	A	614.7581	0.5794	162.6849	4.1129
14	A	633.7610	1.1107	2.4024	2.3992
15	A	667.1905	0.9992	127.4087	2.5473
16	A	710.1376	1.6978	43.3798	3.4353
17	A	753.6653	2.2593	18.2917	28.4794
18	A	847.2519	0.5337	41.7437	0.0485
19	A	894.2702	1.6759	66.0574	0.6800
20	A	1124.8987	1.4394	34.4494	1.1593
21	A	1156.9555	2.7293	54.2314	3.2882
22	A	1212.9371	1.9643	66.7945	0.6149
23	A	1268.2111	3.1901	108.3924	0.5886
24	A	1429.6772	10.0288	0.5672	8.6628
25	A	1442.7425	9.2790	112.7591	8.2582
26	A	1475.4108	9.6319	28.7759	1.8491
27	A	1536.5270	8.1248	627.7032	7.9048
28	A	1636.2728	2.2094	115.6005	0.5516
29	A	1655.2749	10.4683	1.8662	7.4528
30	A	1696.6461	10.9552	53.8609	31.0218
31	A	3251.8849	6.8181	2.6095	98.4310
32	A	3595.0055	7.9757	55.0818	187.9389
33	A	3715.7951	8.9493	45.6006	42.5718

py-08_C_b31yp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	101.4827	0.0605	1.0681	1.1209
2	A	159.1761	0.1805	1.2656	1.5305
3	A	256.5575	0.3153	4.4133	1.1649
4	A	279.4274	0.7441	0.2741	0.8054
5	A	318.9508	0.4583	3.5388	0.9479
6	A	344.4651	0.7027	3.1741	1.5343
7	A	360.1763	0.4021	2.2970	1.9144

8	A	427.1021	0.4015	1.8842	0.1375
9	A	435.3837	1.3274	1.6592	3.5896
10	A	504.5430	1.8194	0.8142	10.8145
11	A	546.0789	0.2138	100.2328	0.4318
12	A	638.2596	1.0202	2.1000	3.6485
13	A	639.1756	2.4312	5.2764	2.8601
14	A	705.3587	2.7239	26.5019	3.8315
15	A	712.3016	1.9170	1.9766	1.4123
16	A	741.3467	2.5796	38.9921	16.8771
17	A	778.5235	0.4261	49.2874	0.3500
18	A	878.9430	1.5617	105.5196	0.4972
19	A	881.7554	0.6281	37.1131	0.9336
20	A	1098.1827	1.3481	131.1804	8.5130
21	A	1155.9236	2.0521	63.8303	3.4850
22	A	1217.0700	2.9209	56.9793	4.6410
23	A	1270.4516	2.5406	114.9712	13.8961
24	A	1291.8980	2.3272	81.4524	1.6308
25	A	1334.9900	3.6582	36.7750	28.3304
26	A	1443.8142	5.6780	48.9615	16.3168
27	A	1499.8049	5.9217	33.0140	71.5191
28	A	1624.1224	13.7439	16.5627	38.8623
29	A	1674.0496	9.1400	675.7327	152.9517
30	A	1745.2486	17.9390	106.3470	8.2246
31	A	3208.0359	6.6262	2.1998	114.9216
32	A	3540.1977	7.9344	32.6635	89.0527
33	A	3596.6229	8.2107	102.2660	74.1748

py-08_C_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	101.6522	0.0596	0.8806	1.1681
2	A	160.4358	0.1856	0.9131	1.5196
3	A	262.6534	0.3257	5.2015	1.0960
4	A	279.3614	0.7535	0.4884	0.6332
5	A	324.8974	0.4686	3.7574	1.1824
6	A	350.0495	0.7411	3.4609	1.5999
7	A	368.3430	0.3670	3.2023	1.6629
8	A	431.8551	0.4454	1.3857	0.1602
9	A	436.4635	1.3072	1.9228	3.1705
10	A	507.5214	1.8161	0.5493	9.1996
11	A	543.4724	0.2143	105.5250	0.4869
12	A	643.3257	1.0237	1.6913	4.0910
13	A	648.2880	2.5444	5.6329	2.8586
14	A	712.3257	2.2127	1.6297	2.1037
15	A	714.5379	2.7837	24.5761	3.6982
16	A	749.0389	2.6371	37.0752	13.6140
17	A	795.0733	0.4372	50.7241	0.4150
18	A	893.2779	0.6370	42.4655	1.1255

19	A	896.8014	1.4553	95.1104	0.6866
20	A	1117.1887	1.2358	120.7278	8.4804
21	A	1182.3277	1.5360	58.0366	2.5506
22	A	1244.2071	4.7495	59.8471	6.8247
23	A	1291.5835	2.0814	98.6904	7.6704
24	A	1314.7991	2.9784	89.6509	4.9478
25	A	1362.0678	5.2556	39.7961	48.0999
26	A	1476.8121	6.2895	63.4074	8.9938
27	A	1535.1905	7.5819	42.1504	77.7588
28	A	1681.3345	15.3714	11.5718	53.9191
29	A	1725.7055	11.6368	753.4419	166.2757
30	A	1803.3414	19.7137	113.8253	10.0283
31	A	3236.6859	6.7510	5.3142	103.1550
32	A	3575.3214	8.0946	49.1842	79.9802
33	A	3619.5013	8.3182	123.6718	72.4779

py-08_C_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	92.1903	0.0489	1.2129	1.4989
2	A	154.4658	0.1779	0.8723	1.4654
3	A	253.4874	0.3072	4.4471	1.3778
4	A	278.2920	0.7209	0.3596	0.7685
5	A	319.5201	0.4362	3.8927	2.2360
6	A	341.2094	0.6430	2.9930	1.6030
7	A	361.7120	0.4591	2.1013	1.8815
8	A	409.3058	0.4524	0.5294	0.4082
9	A	432.8737	1.2764	1.8368	3.1973
10	A	502.1347	1.5106	3.0854	9.6582
11	A	545.9121	0.2630	72.6725	0.6654
12	A	555.4978	0.8158	42.0645	4.4634
13	A	627.2967	1.7489	4.3414	3.7652
14	A	639.3654	1.1904	3.8887	3.9174
15	A	708.2488	2.4662	26.4759	3.7789
16	A	737.2374	0.4328	30.2945	2.6705
17	A	740.1198	1.1507	30.4769	11.4156
18	A	853.6248	0.5522	44.0077	0.8788
19	A	881.3081	1.5430	92.4462	0.3446
20	A	1121.7670	1.2652	110.8747	7.5131
21	A	1172.1090	1.9620	56.9922	4.1987
22	A	1228.0007	2.9862	51.2519	3.3618
23	A	1281.4595	2.3681	91.5572	8.4417
24	A	1306.5930	2.0729	84.2260	0.6170
25	A	1373.3120	6.9260	31.4752	65.5538
26	A	1469.8347	5.8457	41.1531	9.3117
27	A	1514.3405	7.8245	25.6554	141.3295
28	A	1621.8937	13.7801	59.0385	24.1936
29	A	1681.2764	9.1666	557.3731	227.8329

30	A	1757.5599	18.8698	88.0234	5.2739
31	A	3244.8574	6.7823	3.6751	109.3137
32	A	3559.1980	8.0200	35.9428	75.3534
33	A	3607.3583	8.2598	109.5791	80.0823

py-10_A_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	93.4857	0.1098	0.0000	0.0226
2	A'	98.6693	0.0871	16.5584	0.8619
3	A'	147.5197	0.0147	183.0340	4.7914
4	A'	204.1916	0.5566	0.2964	1.7412
5	A'	209.0240	0.2433	0.0048	0.7439
6	A''	247.9885	0.5889	0.7532	0.7140
7	A'	306.7919	0.6513	0.6520	0.2595
8	A'	321.3928	1.3630	0.2695	4.5234
9	A''	327.9412	0.2999	3.3148	0.0053
10	A''	363.7722	0.4547	0.1240	0.0319
11	A'	407.3376	1.4512	2.0982	6.1548
12	A''	410.3759	1.0057	1.6097	4.6646
13	A''	509.5307	0.1708	0.9762	0.1171
14	A'	598.3072	2.0928	0.0116	20.8120
15	A'	617.6277	3.0252	5.2984	10.9316
16	A'	660.7588	2.8927	4.1016	1.2975
17	A''	677.5488	1.4220	0.2059	0.1901
18	A''	688.0299	3.3750	0.0005	1.0289
19	A''	746.7836	3.1388	85.8776	0.0463
20	A'	760.6064	4.0581	16.6517	1.5379
21	A''	1071.5840	2.8660	0.0982	0.6062
22	A'	1088.1736	8.0092	176.8121	1.7912
23	A''	1118.7401	1.6726	108.0801	0.2109
24	A'	1136.2175	6.6608	0.0109	3.5248
25	A''	1353.4151	7.8306	29.2422	27.2424
26	A'	1422.5888	14.3209	98.8970	7.5448
27	A''	1455.7431	13.0731	354.6163	1.3547
28	A'	1501.6098	5.5704	22.1787	1.3569
29	A''	1605.5824	14.6894	92.5609	3.6240
30	A'	1619.2920	3.9426	32.4732	5.9492
31	A'	1657.4325	3.6825	514.1018	13.1323
32	A'	3608.0522	8.0141	85.7969	106.0652
33	A''	3729.7630	9.0619	77.4429	17.9646

py-10_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	87.0598	0.0188	76.4295	2.0655

2	A''	94.1633	0.1114	0.0000	0.0240
3	A'	127.4568	0.0137	120.9502	2.2987
4	A'	201.5851	0.5396	0.2997	1.6831
5	A'	210.7103	0.2361	0.1062	0.7243
6	A''	245.4156	0.5369	0.8879	0.6835
7	A'	308.5099	0.6565	0.7747	0.2426
8	A'	322.2807	1.3659	0.2588	4.2628
9	A''	323.5640	0.2847	3.3545	0.0018
10	A''	366.6931	0.4523	0.0708	0.0206
11	A'	411.0265	1.4600	1.9992	5.5190
12	A''	411.7931	1.0421	1.7495	4.4544
13	A''	515.2876	0.1752	0.5592	0.0989
14	A'	599.6313	2.1424	0.0513	20.5326
15	A'	620.2590	3.0177	4.1329	10.7826
16	A'	664.3840	2.9116	3.7541	1.0410
17	A''	678.3823	1.4070	0.3395	0.2412
18	A''	692.5709	3.4210	0.0003	0.9888
19	A''	759.5111	3.1004	78.5710	0.0110
20	A'	761.6707	4.0750	17.2781	1.1441
21	A''	1082.4782	1.9358	4.5280	0.4287
22	A'	1099.7918	8.2316	171.7074	1.7880
23	A''	1126.3821	2.3016	95.4954	0.1536
24	A'	1150.8357	6.6007	0.0104	3.6883
25	A''	1384.0365	8.9873	36.3107	26.7779
26	A'	1440.8287	14.4030	99.3364	6.8833
27	A''	1476.5885	13.9152	358.2205	1.4750
28	A'	1516.0858	4.2622	13.5744	1.2695
29	A'	1624.1653	2.9883	4.4822	2.8839
30	A''	1629.9183	15.8568	101.9830	3.5457
31	A'	1671.3957	7.2885	562.7055	15.1768
32	A'	3620.7494	8.0714	87.9177	104.1050
33	A''	3746.6190	9.1451	82.4996	17.1865

py-10_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	86.3185	0.0180	78.6842	2.1986
2	A''	93.5182	0.1098	0.0000	0.0208
3	A'	125.9796	0.0135	119.1120	2.3987
4	A'	201.7720	0.5407	0.3046	1.7087
5	A'	211.3525	0.2384	0.1142	0.7312
6	A''	245.7904	0.5379	0.8810	0.6886
7	A'	308.6283	0.6523	0.8006	0.2349
8	A'	321.7124	1.3634	0.2460	4.3181
9	A''	323.2690	0.2857	3.3817	0.0017
10	A''	367.8109	0.4409	0.0811	0.0210
11	A'	410.0641	1.4520	1.9916	5.4589
12	A''	410.8396	1.0339	1.7386	4.4691

13	A''	512.9530	0.1748	0.5900	0.1351
14	A'	597.8914	2.1214	0.0514	20.6973
15	A'	618.5889	3.0200	4.2566	10.6586
16	A'	665.0331	2.9197	4.0248	1.0327
17	A''	677.8557	1.4042	0.2716	0.2291
18	A''	693.3921	3.4308	0.0003	1.0017
19	A''	757.2094	3.1127	79.4756	0.0139
20	A'	763.7821	4.0909	16.8982	1.2181
21	A''	1080.0675	2.0511	2.8031	0.4469
22	A'	1096.3787	8.1739	172.3809	1.7446
23	A''	1123.3715	2.1501	98.7130	0.1646
24	A'	1146.9570	6.6093	0.0064	3.7620
25	A''	1378.6841	8.8066	33.6451	27.0801
26	A'	1435.8032	14.3058	98.4747	7.0162
27	A''	1471.6871	13.7294	357.6646	1.3985
28	A'	1512.9873	4.5163	16.5648	1.2492
29	A'	1623.3642	3.0410	0.8557	3.3165
30	A''	1625.7062	15.7511	102.1970	3.4141
31	A'	1667.6652	6.4127	561.2357	15.0154
32	A'	3621.5926	8.0752	86.6990	105.0392
33	A''	3747.0678	9.1470	80.6265	17.6288

py-10_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	87.8219	0.0970	0.0000	0.0202
2	A'	99.9739	0.0735	0.2569	0.1674
3	A'	195.1032	0.4846	0.5432	2.1685
4	A'	199.9851	0.1654	1.9399	0.7473
5	A'	224.2238	0.0364	195.3413	5.0765
6	A''	237.0208	0.5352	0.5448	0.8279
7	A'	294.6029	0.5957	0.7304	0.2902
8	A'	304.8972	1.2270	0.1220	6.4643
9	A''	313.5731	0.2758	3.9005	0.0245
10	A''	349.9161	0.4375	0.2658	0.0537
11	A'	387.3901	1.2875	3.3922	8.1904
12	A''	392.1218	0.9007	1.1410	5.3716
13	A''	488.9918	0.1576	2.2914	0.2716
14	A'	570.8202	1.9916	0.0397	18.4982
15	A'	585.8634	2.5146	7.0448	16.3261
16	A'	624.3196	2.5912	4.2359	1.1705
17	A''	646.8984	2.9397	0.0008	1.0553
18	A''	650.3614	1.3208	0.0099	0.2659
19	A''	702.0652	3.0107	100.2843	0.1987
20	A'	713.2340	3.5330	11.5412	1.8156
21	A''	1010.4165	4.2702	8.1391	1.7217
22	A'	1030.5571	7.4774	176.3201	1.7332
23	A'	1076.5362	5.9388	2.2113	2.9786

24	A''	1077.3441	1.2823	113.9333	0.0426
25	A''	1319.2732	6.6077	59.0757	22.3388
26	A'	1336.8880	12.6071	85.7620	9.0023
27	A''	1382.1892	12.3367	314.2293	3.5707
28	A'	1439.2078	6.2666	16.2402	2.8529
29	A''	1524.5898	12.6807	59.7149	2.8072
30	A'	1551.5616	5.4747	107.0077	7.9726
31	A'	1599.7705	2.4290	358.4767	7.8460
32	A'	3498.0147	7.5319	66.4093	121.0703
33	A''	3614.1372	8.5015	65.7382	18.9669

py-10_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	88.4129	0.0983	0.0000	0.0200
2	A'	101.6377	0.0744	0.2428	0.1510
3	A'	194.2442	0.4928	0.3672	1.9793
4	A'	200.5271	0.1637	2.5870	0.7432
5	A'	233.9097	0.0396	196.4851	4.8978
6	A''	235.7809	0.4996	0.6594	0.7556
7	A'	295.3148	0.6195	0.5475	0.2882
8	A'	307.7134	1.2345	0.1159	5.5941
9	A''	310.8233	0.2611	3.8482	0.0176
10	A''	351.0878	0.4339	0.2986	0.0526
11	A'	393.4870	1.3014	3.3546	7.5421
12	A''	394.9402	0.9424	1.3991	4.9909
13	A''	491.0845	0.1599	2.6631	0.3322
14	A'	574.4748	2.0670	0.0010	18.5783
15	A'	592.1306	2.5351	5.8324	16.0363
16	A'	624.8982	2.6015	3.5118	1.1120
17	A''	648.8284	2.9516	0.0001	1.0008
18	A''	652.2179	1.3394	0.0884	0.3759
19	A'	709.5865	3.5137	12.0091	1.7181
20	A''	720.1788	2.9147	91.7966	0.0703
21	A''	1030.1797	3.1274	1.0479	1.4369
22	A'	1044.4678	7.6859	170.6720	1.4717
23	A''	1083.1581	1.4198	107.6243	0.0171
24	A'	1096.1450	5.9374	0.7465	3.0960
25	A''	1350.2933	7.6994	85.7627	20.9207
26	A'	1363.2324	13.0662	89.6867	8.2289
27	A''	1406.2318	13.3752	308.4187	4.3023
28	A'	1458.7666	4.6006	7.7432	2.9245
29	A''	1550.3204	13.8444	65.3042	2.9806
30	A'	1558.9065	3.0449	4.8775	3.9139
31	A'	1605.1323	4.6442	474.0171	10.7695
32	A'	3498.4608	7.5349	64.2555	121.2535
33	A''	3618.7397	8.5225	69.1977	18.4100

py-10_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	88.1098	0.0976	0.0000	0.0223
2	A'	101.3032	0.0758	0.2870	0.1536
3	A'	195.2334	0.4920	0.4649	1.9927
4	A'	202.1577	0.1503	4.2661	0.7540
5	A'	223.5654	0.0368	194.3307	4.5434
6	A''	237.1563	0.5005	0.6759	0.7574
7	A'	297.0297	0.6170	0.6285	0.2801
8	A'	308.7510	1.2448	0.1088	5.4029
9	A''	311.5729	0.2628	3.8572	0.0149
10	A''	354.5111	0.4258	0.3037	0.0571
11	A'	394.6662	1.3142	3.1610	7.2353
12	A''	395.8548	0.9501	1.4267	4.8766
13	A''	491.9171	0.1614	2.4538	0.3034
14	A'	576.0051	2.0782	0.0006	18.4189
15	A'	593.2076	2.5576	5.8159	15.7599
16	A'	628.8843	2.6325	3.7844	1.0810
17	A''	653.9867	2.5204	0.0074	0.8448
18	A''	654.6668	1.4740	0.0734	0.5375
19	A'	717.5028	3.5877	12.0067	1.7816
20	A''	723.0850	2.9413	91.6113	0.0659
21	A''	1032.5921	3.2381	1.6166	1.4175
22	A'	1047.6119	7.7023	172.2784	1.3797
23	A''	1085.3398	1.4100	108.4652	0.0179
24	A'	1099.4121	6.0130	0.5536	3.2978
25	A''	1354.8814	7.7556	81.3103	21.0117
26	A'	1366.9118	13.0934	89.0652	8.1482
27	A''	1409.7660	13.3918	310.8773	4.0903
28	A'	1464.0523	4.7465	8.9972	2.9540
29	A''	1556.5036	14.0647	67.2661	2.9857
30	A'	1565.6667	3.1734	8.1359	4.5376
31	A'	1611.0882	4.3884	470.0747	10.5168
32	A'	3521.5598	7.6346	64.8022	118.4589
33	A''	3642.2315	8.6340	68.5333	18.1607

py-10_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	96.4144	0.1168	0.0000	0.0174
2	A'	103.7189	0.1109	9.8575	0.0634
3	A'	152.0720	0.0154	194.4549	0.0272
4	A'	206.1618	0.5679	0.2466	1.6057
5	A'	213.1508	0.2489	0.0008	0.6595
6	A''	250.9297	0.5937	0.9132	0.6504

7	A'	312.7169	0.6790	0.5099	0.2229
8	A'	327.0323	1.4031	0.4619	3.7662
9	A''	331.7632	0.3041	3.0118	0.0000
10	A''	371.1727	0.4449	0.0000	0.0085
11	A'	414.5760	1.4996	1.5817	5.2418
12	A''	417.0936	1.0671	1.9969	4.3942
13	A''	517.8674	0.1780	0.0000	0.0461
14	A'	609.1531	2.1372	0.0378	21.4714
15	A'	627.8312	3.2228	3.9945	8.1660
16	A'	681.7369	3.1025	3.5978	0.3374
17	A''	686.8553	1.4450	0.6236	0.0908
18	A''	712.7308	3.6411	0.0000	0.9949
19	A''	768.8568	3.1001	73.8365	0.0267
20	A'	791.3608	4.4213	21.1208	0.1107
21	A''	1096.1815	1.9930	3.1913	0.1458
22	A'	1115.1010	7.9440	172.4001	1.7274
23	A''	1134.1438	2.3809	100.4274	0.4338
24	A'	1166.4598	7.1582	1.8258	4.3086
25	A''	1347.5852	8.0744	19.7122	34.4975
26	A'	1455.9621	14.5202	97.9227	6.5093
27	A''	1491.5105	13.7979	366.3658	1.0204
28	A'	1523.2771	4.8786	34.3727	0.6543
29	A'	1644.6079	2.7718	13.6851	2.2860
30	A''	1652.1621	16.0851	120.0630	3.6650
31	A'	1686.3454	8.0755	594.3894	19.8012
32	A'	3634.5586	8.1328	101.7399	98.7584
33	A''	3755.8315	9.1934	86.2051	17.6635

py-10_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	92.4082	0.0174	95.7878	2.5152
2	A''	97.0175	0.1181	0.0000	0.0255
3	A'	119.6974	0.0132	111.0946	2.0745
4	A'	206.6227	0.5724	0.1982	1.5751
5	A'	212.2671	0.2284	0.1246	0.7202
6	A''	251.4977	0.6323	0.7871	0.6721
7	A'	309.8318	0.6691	0.7976	0.2272
8	A'	327.9869	1.4179	0.5081	3.9891
9	A''	335.9098	0.3251	2.4362	0.0039
10	A''	365.4956	0.4055	0.1169	0.0219
11	A'	415.3096	1.4737	1.8511	5.0616
12	A''	417.5522	1.0182	2.0536	4.5240
13	A''	505.4949	0.1721	0.6675	0.1257
14	A'	607.2618	2.1537	0.0277	22.1304
15	A'	628.8734	3.2055	3.2238	7.3290
16	A'	669.7529	2.8973	2.5892	1.2908
17	A''	685.0506	1.4633	0.7787	0.0929

18	A''	703.5714	3.5410	0.0002	0.9615
19	A'	769.8859	4.2084	21.6266	1.0644
20	A''	774.8548	3.0343	69.8967	0.0090
21	A''	1101.6774	1.5281	15.7494	0.0832
22	A'	1119.4238	8.2431	164.5428	2.1681
23	A''	1146.7674	3.5207	75.4704	0.2833
24	A'	1169.6818	6.9051	0.2833	4.1258
25	A''	1344.4851	8.3399	20.0680	33.4767
26	A'	1473.1633	14.6808	98.6977	6.8865
27	A''	1502.4730	14.0771	363.6582	0.7800
28	A'	1525.7796	4.5413	35.6754	0.7021
29	A'	1642.6655	2.7210	28.6606	2.2805
30	A''	1655.2394	16.4312	125.2248	3.2807
31	A'	1688.7187	9.6435	580.7016	20.4033
32	A'	3635.1808	8.1370	113.2818	101.9978
33	A''	3761.3593	9.2198	90.9942	19.0235

py-10_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	95.5546	0.1147	0.0000	0.0188
2	A'	106.0863	0.0981	0.5495	0.0891
3	A'	173.5948	0.0201	196.4969	0.0020
4	A'	203.2939	0.5515	0.2711	1.5540
5	A'	209.5805	0.2628	0.2281	0.7724
6	A''	247.5125	0.5889	0.9052	0.6316
7	A'	306.9910	0.6671	0.3978	0.2006
8	A'	322.0953	1.3565	0.4087	3.9192
9	A''	326.5160	0.2964	3.0284	0.0000
10	A''	362.6747	0.3864	0.0000	0.0016
11	A''	409.4900	0.9988	1.8000	4.7189
12	A'	410.2015	1.4205	2.1584	5.0746
13	A''	499.3342	0.1689	0.0000	0.0860
14	A'	597.8191	2.2471	0.0079	20.3869
15	A'	618.9026	2.8654	2.6382	10.5091
16	A'	666.8868	2.9790	2.3845	0.4984
17	A''	674.1043	1.3928	0.7533	0.1349
18	A''	699.5131	3.5086	0.0000	0.8972
19	A''	769.6546	2.9078	70.6000	0.0102
20	A'	770.6965	4.2255	21.6874	0.0318
21	A''	1081.1993	1.3339	23.0498	0.1611
22	A'	1108.8377	8.0748	170.9282	2.1202
23	A''	1135.8251	4.3937	68.6034	0.1723
24	A'	1161.7124	6.6135	0.5683	3.9945
25	A''	1355.3112	9.3125	23.6031	32.1573
26	A'	1466.2860	14.1377	99.6204	5.9411
27	A''	1497.1939	14.3479	382.1230	0.9701
28	A'	1512.7245	3.6249	21.0716	0.3105

29	A'	1619.9493	2.7998	67.9885	2.0376
30	A''	1649.7711	16.8927	128.3177	4.0041
31	A'	1679.3561	12.8976	550.2209	19.9773
32	A'	3633.4692	8.1303	97.3651	105.8734
33	A''	3761.1513	9.2152	83.0787	19.5190

py-10_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	90.4716	0.1029	0.0007	0.0077
2	A'	104.6117	0.0558	0.9903	0.1165
3	A'	194.1916	0.1976	0.7254	0.7315
4	A'	205.9809	0.4805	0.1924	1.4022
5	A''	248.9657	0.5914	0.3792	0.5971
6	A'	292.9267	0.6499	0.9766	0.4178
7	A'	323.7124	1.3268	0.3357	3.2765
8	A''	325.2936	0.3114	1.2330	0.0057
9	A''	332.6709	0.3206	1.8694	0.2312
10	A'	412.3961	1.5123	0.8188	5.5162
11	A''	413.8137	0.8341	3.2384	4.1988
12	A''	441.8911	0.1402	12.2732	1.1321
13	A'	530.3115	0.2254	234.2797	3.8594
14	A'	596.7698	1.6961	3.2324	31.1558
15	A'	612.2674	3.1840	3.8176	5.7913
16	A'	631.0145	2.4725	7.0525	0.7192
17	A''	631.6882	2.8185	0.0174	0.8663
18	A'	643.6592	1.9233	52.9448	1.3148
19	A''	674.9675	1.6741	0.4629	0.1227
20	A''	779.8832	2.9863	69.1987	0.0654
21	A'	1090.0692	6.8594	146.1809	1.5565
22	A''	1095.3347	5.5707	9.5732	0.1615
23	A''	1161.0485	1.3176	72.2321	0.0613
24	A'	1165.8833	7.4951	6.3460	6.9602
25	A''	1433.0543	9.2816	69.4242	26.1084
26	A'	1434.9262	14.7807	86.9361	11.1463
27	A''	1479.8633	14.3295	329.4887	3.9616
28	A'	1510.5683	6.6558	22.3934	6.3945
29	A'	1630.7362	2.9436	9.3107	3.0887
30	A''	1636.6646	14.9766	42.6979	1.9131
31	A'	1680.2956	4.8208	389.6411	20.9353
32	A'	3602.8719	8.0050	64.2394	132.1479
33	A''	3724.5117	9.0039	56.6569	22.1517

py-10_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A''	90.8836	0.1037	0.0000	0.0170
2	A'	103.3493	0.0789	0.3096	0.1743
3	A'	202.6867	0.3682	4.9340	2.4368
4	A'	209.7293	0.0471	82.5342	1.6510
5	A'	213.1100	0.0691	119.7392	3.3680
6	A''	247.4041	0.5518	0.7502	0.7215
7	A'	307.0148	0.6506	0.5719	0.2567
8	A'	319.3882	1.3418	0.1455	4.8468
9	A''	322.6638	0.2906	3.4964	0.0100
10	A''	367.9297	0.4256	0.3767	0.0575
11	A'	406.3852	1.3846	2.8326	5.8567
12	A''	407.0428	0.9955	1.6523	4.4659
13	A''	498.5198	0.1677	2.5323	0.2494
14	A'	590.5352	2.0662	0.0452	20.0668
15	A'	611.9133	2.9232	5.0643	11.5423
16	A'	656.4297	2.8407	4.9399	1.1916
17	A''	675.6312	1.4401	0.0570	0.2499
18	A''	686.5414	3.3525	0.0010	0.9793
19	A''	748.6356	3.1126	85.6506	0.0204
20	A'	755.7165	3.9695	13.2498	1.5722
21	A''	1072.1393	2.8146	0.0934	0.7451
22	A'	1081.0841	8.0388	169.7637	1.4178
23	A''	1119.0184	1.6425	102.8271	0.1398
24	A'	1132.0146	6.5105	0.1001	3.7184
25	A''	1378.0875	8.2707	32.0446	26.1720
26	A'	1419.2861	14.0755	96.1871	8.1986
27	A''	1454.9880	13.2899	359.9856	1.4310
28	A'	1502.1585	5.3736	20.8646	1.7823
29	A''	1610.3435	15.3771	94.0859	2.9032
30	A'	1616.1590	3.5930	19.6211	5.1939
31	A'	1657.4826	4.1037	492.3249	12.4482
32	A'	3628.6142	8.1088	79.6803	110.6500
33	A''	3752.0747	9.1651	71.8213	18.4714

py-10_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	91.4476	0.0258	63.9304	2.0504
2	A''	95.0481	0.1135	0.0000	0.0205
3	A'	130.4472	0.0134	136.1915	2.9160
4	A'	203.9433	0.5526	0.2915	1.6274
5	A'	212.1331	0.2432	0.0735	0.7257
6	A''	248.1079	0.5517	0.9095	0.6706
7	A'	310.6060	0.6715	0.7012	0.2419
8	A'	325.7359	1.3879	0.2983	3.9188
9	A''	326.4928	0.2903	3.2412	0.0011
10	A''	369.5308	0.4524	0.0935	0.0254
11	A''	414.9608	1.0572	1.9197	4.3359

12	A'	415.1406	1.4780	1.9115	5.2329
13	A''	517.8392	0.1776	0.7102	0.1002
14	A'	604.9286	2.1905	0.0634	20.2837
15	A'	626.4556	3.0849	3.9123	10.3867
16	A'	670.7462	2.9680	3.9274	0.9868
17	A''	683.1885	1.4403	0.4745	0.2191
18	A''	700.7031	3.5066	0.0003	0.9807
19	A''	770.3076	3.0891	74.9913	0.0026
20	A'	771.0428	4.1755	17.5747	1.0148
21	A''	1093.3555	1.7972	7.3638	0.2983
22	A'	1110.6209	8.2898	168.4234	1.7322
23	A''	1137.0733	2.6109	89.0251	0.1571
24	A'	1164.1016	6.7599	0.2426	3.9884
25	A''	1392.0730	9.2930	31.3576	27.9980
26	A'	1459.9979	14.7525	102.1491	7.0846
27	A''	1491.6618	14.1470	365.6059	1.1558
28	A'	1528.3093	4.0505	13.4694	1.0966
29	A'	1635.0651	3.0098	11.1182	2.7470
30	A''	1647.1363	16.3132	110.2151	3.6053
31	A'	1684.8473	8.3828	569.5179	16.2239
32	A'	3640.3116	8.1593	91.0811	103.7276
33	A''	3767.4459	9.2477	83.8592	17.3721

py-10_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	-163.3223	0.0214	169.3620	0.0791
2	A''	88.8700	0.0993	0.0000	0.0197
3	A'	107.3012	0.0366	9.4187	0.1304
4	A'	195.5865	0.5068	0.3380	1.8447
5	A'	201.0841	0.1983	0.5840	0.7787
6	A''	237.3159	0.5045	0.6814	0.7918
7	A'	296.3812	0.5887	1.1644	0.2273
8	A'	309.2353	1.2563	0.1122	5.2969
9	A''	312.4135	0.2629	3.9007	0.0003
10	A''	353.0695	0.4460	0.0000	0.0203
11	A'	395.3095	1.3688	2.0363	6.7104
12	A''	396.5694	0.9617	1.5217	5.0765
13	A''	506.9562	0.1674	0.0000	0.0369
14	A'	577.3105	2.1364	0.0003	17.2562
15	A'	594.3534	2.5591	4.9361	17.2973
16	A'	629.5251	2.5462	4.7622	0.2815
17	A''	652.8371	1.3063	0.2656	0.3427
18	A''	653.8003	3.0253	0.0000	1.1558
19	A'	717.3129	3.5402	11.2111	0.1255
20	A''	725.8268	2.9301	86.1755	0.0696
21	A''	1033.6415	2.5068	0.0144	1.2265
22	A'	1051.0436	7.8203	170.9061	1.2777

23	A''	1079.8467	1.5967	110.6765	0.0548
24	A'	1105.0119	5.9654	0.6081	3.4526
25	A''	1361.6028	8.2641	101.1032	20.1284
26	A'	1371.8216	13.1097	90.1625	8.5614
27	A''	1415.6774	13.8028	295.9327	4.9951
28	A'	1469.3723	3.9357	4.7784	3.2210
29	A''	1561.5557	14.5238	71.4698	2.5840
30	A'	1563.6726	2.9907	0.0406	3.8915
31	A'	1613.8029	5.8960	499.7099	10.8470
32	A'	3524.3006	7.6439	76.5144	116.4706
33	A''	3648.3207	8.6704	76.8690	17.2853

py-10_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	90.9980	0.1041	0.0000	0.0151
2	A'	105.4492	0.0638	0.7821	0.1063
3	A'	193.1621	0.4954	0.2351	1.7999
4	A'	202.7404	0.1978	0.8279	0.6967
5	A''	234.3638	0.5030	0.6430	0.7207
6	A'	298.0240	0.5706	2.0587	0.2947
7	A'	308.4005	1.2372	0.4109	4.8161
8	A''	310.8255	0.2669	3.3470	0.0296
9	A'	341.4379	0.0893	219.9682	2.2107
10	A''	353.2084	0.4064	0.8095	0.0841
11	A''	397.9515	0.9348	1.4671	4.8750
12	A'	398.4341	0.9243	14.6671	8.6307
13	A''	482.5549	0.1586	5.7431	0.6054
14	A'	578.0395	2.0787	0.0104	19.4937
15	A'	599.0549	2.4871	7.4385	14.2333
16	A'	626.9766	2.6484	2.9896	0.6307
17	A''	653.3785	2.4147	0.0132	0.7433
18	A''	654.1262	1.6242	0.1116	0.4691
19	A'	710.6084	3.5333	12.6109	1.1215
20	A''	729.5088	2.8823	92.8422	0.0546
21	A''	1042.8260	3.9506	4.2819	1.2334
22	A'	1054.9368	7.6692	169.6311	1.5295
23	A'	1108.3092	6.1512	0.3518	3.2538
24	A''	1111.8118	1.3652	97.3516	0.0075
25	A''	1365.8983	7.6203	91.1171	20.5413
26	A'	1377.9984	13.4291	86.6918	7.5830
27	A''	1425.9228	13.6894	315.7242	4.2807
28	A'	1476.5864	6.0344	17.3276	2.1355
29	A''	1570.6684	13.3784	53.2686	3.4531
30	A'	1594.1626	3.9124	45.7346	5.4612
31	A'	1637.2660	3.2924	411.5427	10.7481
32	A'	3508.9480	7.5844	48.9948	124.2447
33	A''	3626.1170	8.5470	53.5007	22.9403

py-10_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A''	92.9404	0.1085	0.0000	0.0169
2	A'	105.6609	0.0800	0.2839	0.1434
3	A'	196.2479	0.5036	0.3924	1.8521
4	A'	208.3941	0.1821	2.0377	0.6878
5	A'	234.2583	0.0397	211.6173	4.4768
6	A''	238.6535	0.4976	0.8713	0.7057
7	A'	305.2388	0.6522	0.6565	0.2846
8	A'	314.8899	1.2902	0.1725	4.7246
9	A''	315.1226	0.2712	3.4144	0.0142
10	A''	363.8370	0.4430	0.3975	0.0574
11	A'	404.2363	1.3621	3.4149	6.7976
12	A''	405.2564	1.0032	1.4487	4.6649
13	A''	502.6329	0.1690	3.0324	0.3407
14	A'	588.9385	2.0886	0.0196	20.5346
15	A'	610.6790	2.8172	5.4868	11.8556
16	A'	649.6585	2.7788	4.2415	1.1830
17	A''	666.9288	1.4229	0.1612	0.2946
18	A''	676.7629	3.2485	0.0019	0.8747
19	A'	742.4723	3.8408	14.2480	1.7079
20	A''	742.6033	3.0144	87.4523	0.0387
21	A''	1064.4158	3.0881	0.4628	0.8551
22	A'	1076.9914	7.9629	174.5992	1.7060
23	A''	1119.3267	1.5770	102.3928	0.0734
24	A'	1127.9867	6.4396	0.1584	3.4492
25	A''	1370.6842	8.1066	51.1987	24.3025
26	A'	1408.4628	14.0020	93.4672	7.3403
27	A''	1450.1524	13.5202	351.8264	2.2855
28	A'	1497.4512	5.7317	21.0541	1.5906
29	A''	1598.9426	14.3986	75.6250	3.3958
30	A'	1615.9799	3.8379	32.8778	5.3260
31	A'	1656.7780	3.6779	480.8725	12.1027
32	A'	3576.8857	7.8790	69.5334	114.0964
33	A''	3699.7928	8.9100	67.8246	20.3411

py-10_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	70.3152	0.0063	139.5768	0.0052
2	A''	95.0204	0.1133	0.0000	0.0196
3	A'	117.4818	0.0175	66.1984	0.0818
4	A'	204.1921	0.5546	0.3073	1.6305
5	A'	213.3939	0.2280	0.2878	0.6695

6	A''	249.4560	0.5564	0.9935	0.6781
7	A'	310.3686	0.6584	0.7725	0.2249
8	A'	326.1798	1.4091	0.3577	3.9942
9	A''	327.1038	0.2931	3.0610	0.0001
10	A''	368.7549	0.4201	0.0000	0.0102
11	A'	414.0626	1.4882	1.6433	4.9509
12	A''	415.2506	1.0587	1.9162	4.3650
13	A''	511.3845	0.1752	0.0000	0.0654
14	A'	604.2947	2.1081	0.0350	21.6063
15	A'	625.9633	3.1967	4.0612	8.1436
16	A'	675.8464	2.9848	3.2743	0.2638
17	A''	685.0476	1.4108	0.2854	0.1107
18	A''	707.9449	3.5865	0.0000	1.0352
19	A''	765.2554	3.1716	74.9152	0.0191
20	A'	777.8255	4.2609	21.0946	0.1637
21	A''	1091.6653	1.7895	6.3166	0.1561
22	A'	1110.4689	8.1298	171.4313	1.9658
23	A''	1131.6936	2.6750	94.6239	0.3891
24	A'	1160.3863	6.8994	0.3792	4.1816
25	A''	1355.9186	8.4470	20.6970	33.6992
26	A'	1452.2734	14.4068	100.3149	6.4942
27	A''	1488.5620	13.8499	368.5849	1.0751
28	A'	1522.5404	4.5559	28.9898	0.5536
29	A'	1639.5982	2.8248	14.0448	2.4105
30	A''	1650.8114	16.2827	122.4565	3.3328
31	A'	1684.9020	8.2794	595.0225	18.2769
32	A'	3650.0352	8.2048	91.8812	97.7479
33	A''	3775.9572	9.2901	80.7954	17.4219

py-10_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A'	81.5820	0.0130	93.6380	2.1017
2	A''	94.0745	0.1112	0.0000	0.0241
3	A'	123.1140	0.0142	103.4307	1.6434
4	A'	202.6202	0.5477	0.2709	1.7570
5	A'	210.3017	0.2298	0.0849	0.7241
6	A''	246.8243	0.5707	0.7998	0.7308
7	A'	308.0823	0.6468	0.7845	0.2420
8	A'	320.5847	1.3661	0.2691	4.7279
9	A''	326.3064	0.2971	3.3129	0.0031
10	A''	365.3514	0.4538	0.0560	0.0245
11	A'	406.7947	1.4515	1.9782	5.8798
12	A''	410.1959	1.0114	1.5901	4.6734
13	A''	512.0141	0.1725	0.4291	0.0684
14	A'	596.7573	2.0584	0.0205	21.3921
15	A'	616.5913	3.0613	4.8739	10.2002
16	A'	664.5302	2.9038	4.3224	0.9535

17	A''	677.5081	1.4022	0.1392	0.1668
18	A''	691.8913	3.4155	0.0002	1.0839
19	A''	746.1697	3.1748	84.1090	0.0559
20	A'	764.5499	4.0931	16.9036	0.9931
21	A''	1073.0241	2.6442	0.0091	0.5405
22	A'	1089.4003	8.0608	176.8277	1.8526
23	A''	1118.9392	1.7621	107.9551	0.2611
24	A'	1135.6333	6.6437	0.0696	3.5052
25	A''	1353.3061	7.8691	27.5140	27.8220
26	A'	1420.9606	14.1528	96.4270	7.5623
27	A''	1458.5766	13.0954	353.1911	1.2906
28	A'	1501.1126	5.6105	26.9377	1.1990
29	A''	1609.7954	14.9369	98.8211	3.3683
30	A'	1622.7036	3.7705	24.5836	5.6558
31	A'	1659.7638	3.8602	530.9038	13.8407
32	A'	3612.2561	8.0330	89.8323	105.4938
33	A''	3734.1655	9.0845	79.1740	18.0415

py-10_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	93.4857	0.1098	0.0000	0.0226
2	A	98.6700	0.0871	16.5556	0.8618
3	A	147.5220	0.0147	183.0371	4.7916
4	A	204.1916	0.5566	0.2964	1.7412
5	A	209.0240	0.2433	0.0048	0.7439
6	A	247.9885	0.5889	0.7532	0.7140
7	A	306.7918	0.6513	0.6520	0.2595
8	A	321.3928	1.3630	0.2695	4.5234
9	A	327.9412	0.2999	3.3148	0.0053
10	A	363.7721	0.4547	0.1240	0.0319
11	A	407.3376	1.4512	2.0982	6.1548
12	A	410.3759	1.0057	1.6097	4.6646
13	A	509.5304	0.1708	0.9763	0.1171
14	A	598.3072	2.0928	0.0116	20.8120
15	A	617.6277	3.0252	5.2984	10.9316
16	A	660.7587	2.8927	4.1016	1.2975
17	A	677.5488	1.4220	0.2059	0.1901
18	A	688.0299	3.3750	0.0005	1.0289
19	A	746.7837	3.1388	85.8776	0.0463
20	A	760.6064	4.0581	16.6518	1.5379
21	A	1071.5842	2.8660	0.0982	0.6062
22	A	1088.1737	8.0092	176.8119	1.7912
23	A	1118.7402	1.6726	108.0801	0.2109
24	A	1136.2175	6.6608	0.0109	3.5248
25	A	1353.4151	7.8306	29.2421	27.2424
26	A	1422.5889	14.3209	98.8971	7.5448
27	A	1455.7431	13.0731	354.6165	1.3547

28	A	1501.6098	5.5704	22.1786	1.3569
29	A	1605.5824	14.6894	92.5609	3.6240
30	A	1619.2919	3.9426	32.4732	5.9492
31	A	1657.4325	3.6825	514.1016	13.1323
32	A	3608.0523	8.0141	85.7967	106.0652
33	A	3729.7631	9.0619	77.4429	17.9646

py-10_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	92.4077	0.0174	95.7915	2.5153
2	A	97.0175	0.1181	0.0000	0.0255
3	A	119.6970	0.0132	111.0909	2.0744
4	A	206.6227	0.5724	0.1982	1.5751
5	A	212.2671	0.2284	0.1246	0.7202
6	A	251.4977	0.6323	0.7871	0.6721
7	A	309.8318	0.6691	0.7976	0.2272
8	A	327.9869	1.4179	0.5081	3.9891
9	A	335.9098	0.3251	2.4362	0.0039
10	A	365.4956	0.4055	0.1169	0.0219
11	A	415.3096	1.4737	1.8511	5.0616
12	A	417.5522	1.0182	2.0536	4.5240
13	A	505.4950	0.1721	0.6675	0.1257
14	A	607.2619	2.1537	0.0277	22.1304
15	A	628.8734	3.2055	3.2238	7.3290
16	A	669.7529	2.8973	2.5892	1.2908
17	A	685.0506	1.4633	0.7787	0.0929
18	A	703.5714	3.5410	0.0002	0.9615
19	A	769.8860	4.2084	21.6266	1.0644
20	A	774.8547	3.0343	69.8967	0.0090
21	A	1101.6773	1.5281	15.7494	0.0832
22	A	1119.4238	8.2431	164.5428	2.1681
23	A	1146.7674	3.5207	75.4705	0.2833
24	A	1169.6817	6.9051	0.2833	4.1258
25	A	1344.4850	8.3399	20.0681	33.4767
26	A	1473.1632	14.6808	98.6978	6.8865
27	A	1502.4730	14.0771	363.6581	0.7800
28	A	1525.7796	4.5413	35.6753	0.7021
29	A	1642.6655	2.7210	28.6610	2.2805
30	A	1655.2392	16.4311	125.2248	3.2807
31	A	1688.7187	9.6435	580.7014	20.4033
32	A	3635.1808	8.1370	113.2818	101.9978
33	A	3761.3593	9.2198	90.9942	19.0235

py-10_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A	90.4723	0.1029	0.0007	0.0077
2	A	104.5981	0.0558	0.9904	0.1165
3	A	194.1998	0.1976	0.7247	0.7317
4	A	205.9848	0.4804	0.1925	1.4019
5	A	248.9661	0.5913	0.3791	0.5971
6	A	292.9306	0.6499	0.9762	0.4178
7	A	323.7103	1.3267	0.3356	3.2766
8	A	325.2912	0.3115	1.2323	0.0057
9	A	332.5585	0.3207	1.8656	0.2309
10	A	412.3913	1.5122	0.8189	5.5147
11	A	413.8096	0.8339	3.2392	4.1987
12	A	441.8901	0.1402	12.2775	1.1325
13	A	530.3189	0.2254	234.2727	3.8594
14	A	596.7649	1.6962	3.2315	31.1574
15	A	612.2636	3.1837	3.8158	5.7943
16	A	631.0102	2.4694	7.1014	0.7189
17	A	631.6762	2.8183	0.0175	0.8663
18	A	643.6741	1.9250	52.9016	1.3169
19	A	674.9506	1.6740	0.4634	0.1228
20	A	779.8823	2.9863	69.1988	0.0653
21	A	1090.0725	6.8599	146.1807	1.5570
22	A	1095.3175	5.5713	9.5714	0.1615
23	A	1161.0510	1.3176	72.2298	0.0613
24	A	1165.8544	7.4942	6.3381	6.9585
25	A	1433.0583	9.2811	69.4634	26.1040
26	A	1434.9313	14.7807	86.9278	11.1474
27	A	1479.8481	14.3295	329.4322	3.9644
28	A	1510.5743	6.6555	22.3965	6.3931
29	A	1630.7412	2.9434	9.3035	3.0877
30	A	1636.6633	14.9767	42.7075	1.9134
31	A	1680.2993	4.8215	389.6503	20.9371
32	A	3602.8636	8.0050	64.2412	132.1477
33	A	3724.5032	9.0038	56.6581	22.1520

py-14_A_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.8740	0.1546	0.0708	0.0004
2	A	157.9994	0.1886	0.3204	0.0230
3	A	210.2776	0.3123	1.3666	0.1352
4	A	277.2948	0.7462	2.5513	0.2970
5	A	279.3700	0.4337	3.5099	0.3083
6	A	318.4389	0.6264	2.8748	0.1725
7	A	344.0979	0.7242	0.0001	0.7020
8	A	347.2793	1.1552	2.0846	0.3342
9	A	419.9512	0.2144	61.8404	2.8227
10	A	446.0693	0.2381	66.4548	0.7232

11	A	463.0497	1.9826	0.2393	4.8595
12	A	486.2226	1.9819	0.5526	6.1067
13	A	604.9591	2.9581	0.7009	18.5167
14	A	637.2332	2.8558	4.5729	0.3703
15	A	677.7551	3.2543	0.0315	0.0184
16	A	697.1424	4.3952	5.0383	11.4094
17	A	725.0670	3.7559	6.4416	0.3259
18	A	736.4757	3.1153	6.0428	0.1937
19	A	952.9017	3.7321	211.1496	0.2551
20	A	1101.9707	9.5440	283.8020	0.0711
21	A	1144.7852	6.7650	20.2286	1.8474
22	A	1271.2148	1.9532	87.9964	0.5473
23	A	1290.9080	7.6166	67.1977	3.2523
24	A	1373.2118	4.5336	35.5618	8.7457
25	A	1437.4584	15.0832	26.0988	3.8888
26	A	1503.5846	15.8528	640.6636	1.8508
27	A	1541.6953	14.4141	155.3435	1.8406
28	A	1663.3605	17.4090	123.9842	8.1941
29	A	1670.0679	15.1917	60.5198	3.5055
30	A	3790.5341	9.0248	139.7154	69.9129

py-14_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	120.1705	0.1552	0.0730	0.0002
2	A	158.8948	0.1900	0.2854	0.0236
3	A	212.1551	0.3183	1.0380	0.1360
4	A	274.4295	0.5268	5.2218	0.1909
5	A	275.5202	0.5247	1.1822	0.3729
6	A	319.1114	0.6384	2.8433	0.1632
7	A	346.5461	0.7327	0.0032	0.6749
8	A	349.8269	1.1715	2.0508	0.3346
9	A	425.3858	0.2446	53.8705	2.8372
10	A	452.0266	0.2226	73.5918	0.5972
11	A	463.1293	1.9715	0.2314	4.7541
12	A	485.0791	1.9645	0.6679	5.8573
13	A	609.0520	2.9926	0.6308	17.6464
14	A	638.3960	2.8606	3.8889	0.2976
15	A	677.9963	3.2523	0.0500	0.0216
16	A	701.3511	4.4400	3.8645	11.8440
17	A	719.0313	3.7055	6.7124	0.3393
18	A	740.8781	3.1247	6.0757	0.2026
19	A	966.6779	3.6528	201.0802	0.2447
20	A	1117.8339	9.8351	278.3135	0.0728
21	A	1165.5105	6.2542	24.8821	1.5750
22	A	1281.7069	1.7363	106.7863	0.7917
23	A	1308.3177	9.6016	52.0755	2.8698
24	A	1401.1171	6.2499	21.1814	8.7067

25	A	1457.9415	15.5879	27.0573	3.7806
26	A	1527.9868	16.5795	663.3862	1.7648
27	A	1566.4765	15.2571	164.6047	1.8778
28	A	1686.5963	18.7107	135.3834	8.0048
29	A	1692.6674	15.9780	51.0033	3.2248
30	A	3815.6677	9.1447	143.4644	67.3934

py-14_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.6042	0.1538	0.0705	0.0003
2	A	158.1224	0.1877	0.2930	0.0236
3	A	212.5524	0.3203	1.0413	0.1368
4	A	275.4632	0.6415	3.7989	0.2276
5	A	276.9713	0.4555	2.4873	0.3342
6	A	319.3808	0.6388	2.8128	0.1654
7	A	346.5892	0.7284	0.0044	0.6774
8	A	349.5277	1.1699	2.0127	0.3403
9	A	424.2083	0.2151	62.6597	2.7697
10	A	450.6355	0.2477	64.3390	0.7018
11	A	462.1343	1.9636	0.2338	4.7595
12	A	483.9037	1.9551	0.6464	5.8885
13	A	607.2263	2.9768	0.6428	17.8006
14	A	638.9001	2.8678	4.0693	0.3222
15	A	679.1406	3.2642	0.0349	0.0191
16	A	699.3664	4.4172	4.0171	11.7596
17	A	721.4223	3.7271	6.5040	0.3245
18	A	740.2752	3.1247	6.0246	0.2025
19	A	963.5162	3.6690	203.0715	0.2473
20	A	1113.7056	9.7619	279.0808	0.0699
21	A	1160.3888	6.3887	23.4848	1.6325
22	A	1279.4397	1.7582	102.7438	0.7303
23	A	1303.4244	8.9886	56.0654	2.9293
24	A	1396.2846	5.9849	23.4211	8.8571
25	A	1452.8794	15.4621	25.9022	3.8892
26	A	1522.7973	16.4096	657.8684	1.7359
27	A	1560.8990	14.9989	164.4997	1.8539
28	A	1681.6535	18.6837	138.1751	8.0818
29	A	1687.9522	15.7446	47.6829	3.1854
30	A	3816.6556	9.1497	141.2704	67.7349

py-14_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.5253	0.1364	0.0639	0.0007
2	A	150.3806	0.1725	0.3405	0.0266

3	A	199.8397	0.2855	1.2066	0.1556
4	A	267.0406	0.6806	2.7230	0.3891
5	A	270.4627	0.4138	3.2370	0.3719
6	A	305.9839	0.5754	2.8287	0.2108
7	A	328.9355	0.7131	0.0341	0.7123
8	A	331.8711	1.0562	1.7132	0.4322
9	A	405.5544	0.3696	24.9291	3.0124
10	A	440.2334	0.1581	93.3296	0.5931
11	A	444.3800	1.8352	0.2588	5.3628
12	A	466.0643	1.8429	0.5962	7.7227
13	A	576.4081	2.6871	1.0440	20.8151
14	A	603.5724	2.5437	5.0315	0.3571
15	A	638.7960	2.8731	0.0211	0.0329
16	A	662.8889	3.9850	5.7353	11.9925
17	A	681.6833	3.2980	4.0679	0.2890
18	A	705.4173	2.9034	6.1138	0.2528
19	A	901.6790	3.5736	222.4393	0.2420
20	A	1044.7707	8.5814	277.6316	0.0613
21	A	1073.9802	6.9828	14.8799	2.5398
22	A	1212.7284	7.4969	9.2536	1.5119
23	A	1235.0789	1.6726	166.3908	3.0590
24	A	1344.1765	5.2365	20.3366	8.2957
25	A	1353.7582	11.8435	30.9960	3.2891
26	A	1419.9946	13.9016	597.7215	2.1787
27	A	1461.8744	11.8865	116.7789	0.8006
28	A	1580.7479	13.3859	73.5573	7.0228
29	A	1588.4956	14.0397	90.9914	3.7287
30	A	3640.3001	8.3222	115.6463	79.9030

py-14_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.5384	0.1362	0.0656	0.0004
2	A	151.0981	0.1736	0.2858	0.0274
3	A	200.8641	0.2879	0.7713	0.1543
4	A	264.4946	0.5774	4.0604	0.3020
5	A	266.1986	0.4283	2.2783	0.4080
6	A	306.7444	0.5884	2.7931	0.1932
7	A	330.4620	0.7142	0.0029	0.6886
8	A	334.6786	1.0731	1.6693	0.4175
9	A	409.3669	0.4276	20.2650	2.9547
10	A	444.6326	1.8234	0.2464	5.2553
11	A	447.0025	0.1565	96.5468	0.5634
12	A	465.8860	1.8275	0.7251	7.2130
13	A	582.6907	2.7516	0.9343	19.9612
14	A	603.3100	2.5419	4.2117	0.2866
15	A	636.0327	2.8373	0.0553	0.0398
16	A	668.2151	4.0415	4.2763	12.6011

17	A	670.8959	3.2111	4.2521	0.3008
18	A	709.4153	2.9065	5.9731	0.2641
19	A	917.4882	3.5108	209.6092	0.2276
20	A	1062.5948	8.8967	271.7819	0.0440
21	A	1098.4926	6.7395	17.7686	2.2341
22	A	1231.6987	4.3868	10.8345	0.6566
23	A	1245.6455	1.8498	161.2955	3.8966
24	A	1373.9776	7.1871	7.7044	7.9626
25	A	1379.5075	12.1028	36.6098	3.2856
26	A	1445.6289	14.7138	628.6037	2.1538
27	A	1489.0847	12.9455	124.2769	0.8469
28	A	1604.6504	14.5454	72.4058	6.5666
29	A	1611.1643	15.0448	93.9190	3.4942
30	A	3655.6054	8.3915	117.2289	77.2680

py-14_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.3632	0.1358	0.0644	0.0005
2	A	150.9449	0.1725	0.2987	0.0271
3	A	202.3357	0.2928	0.8112	0.1552
4	A	266.4351	0.6408	3.2699	0.3308
5	A	268.7313	0.4127	2.9643	0.3699
6	A	308.4288	0.5939	2.7845	0.1959
7	A	332.2435	0.7160	0.0035	0.6778
8	A	335.9876	1.0818	1.6722	0.4166
9	A	411.6155	0.3843	24.3956	2.9417
10	A	445.5016	1.8302	0.2483	5.1894
11	A	447.1093	0.1629	92.5635	0.5395
12	A	466.5983	1.8318	0.7193	7.1442
13	A	583.9559	2.7652	0.9604	19.6874
14	A	607.0756	2.5829	4.3194	0.2987
15	A	641.6672	2.8930	0.0322	0.0335
16	A	669.8120	4.0603	4.2994	12.5642
17	A	678.9224	3.2865	4.2175	0.2823
18	A	712.2533	2.9303	5.9578	0.2623
19	A	919.6613	3.5447	211.9757	0.2263
20	A	1065.0403	8.9373	273.5474	0.0423
21	A	1099.9057	6.8055	17.3699	2.2168
22	A	1234.4488	4.5852	10.0128	0.6727
23	A	1248.7932	1.8220	162.6916	3.7914
24	A	1378.4747	7.4965	5.8495	8.0669
25	A	1383.5848	11.5829	36.7250	3.3112
26	A	1449.7861	14.7249	627.1552	2.0640
27	A	1493.3854	12.9053	125.3491	0.7943
28	A	1609.7584	14.9206	78.0779	6.6904
29	A	1616.2832	14.9890	88.8655	3.4182
30	A	3679.9221	8.5039	117.2750	75.9180

py-14_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	123.5438	0.1640	0.0787	0.0004
2	A	161.6320	0.1966	0.3234	0.0216
3	A	214.1248	0.3224	1.5608	0.1233
4	A	278.2316	0.6588	3.7495	0.2223
5	A	279.3414	0.4660	2.5390	0.3242
6	A	321.5170	0.6388	2.9788	0.1533
7	A	350.2568	0.7240	0.0030	0.6773
8	A	352.1616	1.1870	2.2861	0.2956
9	A	426.5040	0.1916	77.5890	2.5090
10	A	452.2665	0.2910	57.0595	0.8237
11	A	469.0847	2.0302	0.2363	4.6016
12	A	491.6691	2.0181	0.5347	5.4964
13	A	615.0959	3.0488	0.5692	16.8275
14	A	653.3736	3.0163	4.1340	0.3528
15	A	698.2349	3.4673	0.0323	0.0110
16	A	710.0079	4.5421	4.4877	11.6995
17	A	746.6407	3.1573	6.2854	0.1466
18	A	750.6829	4.0366	8.2104	0.3202
19	A	973.6323	3.6788	203.0504	0.2566
20	A	1127.1301	9.9816	283.8387	0.1479
21	A	1173.4128	5.9200	28.0230	1.6852
22	A	1276.6920	2.1101	90.0428	1.1852
23	A	1322.3682	11.5412	40.9606	2.2796
24	A	1364.0114	3.6879	47.0004	10.3547
25	A	1472.4929	15.9110	24.3033	4.1001
26	A	1543.4088	16.9142	655.3387	1.9222
27	A	1579.1990	15.8115	182.1256	3.0180
28	A	1707.2923	19.5969	154.6175	9.0687
29	A	1713.9319	16.5141	44.3930	3.5557
30	A	3825.6762	9.1935	157.5236	64.0603

py-14_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	124.7201	0.1673	0.0691	0.0001
2	A	161.9139	0.1968	0.2741	0.0243
3	A	214.7698	0.3203	1.3725	0.1220
4	A	276.8038	0.7176	0.2245	0.3104
5	A	279.2435	0.4496	5.3516	0.1536
6	A	321.8896	0.6372	2.9030	0.1518
7	A	349.2522	0.6627	0.1762	0.6181
8	A	354.3395	1.1974	2.6949	0.2935

9	A	413.3964	0.1291	116.2632	2.1215
10	A	445.8899	0.6412	18.5605	1.5731
11	A	467.8547	2.0096	0.1919	4.6851
12	A	489.1109	1.9858	0.4988	5.2579
13	A	616.6188	3.0802	0.3632	15.5696
14	A	645.8844	2.9141	3.5780	0.2710
15	A	688.4992	3.3628	0.0352	0.0137
16	A	713.1795	4.5627	3.9387	12.1647
17	A	731.7589	3.8526	8.3925	0.3397
18	A	745.1014	3.1526	5.9563	0.1549
19	A	987.0325	3.6892	186.9554	0.3011
20	A	1136.2955	10.1493	275.8664	0.2492
21	A	1195.9911	4.9173	34.8073	1.5870
22	A	1285.1397	2.4211	74.5058	1.2131
23	A	1340.8788	11.5291	36.0135	2.0638
24	A	1361.7633	3.4457	50.9594	9.5036
25	A	1491.1646	16.4169	27.6409	4.3872
26	A	1560.9755	17.6185	665.6172	1.8255
27	A	1593.6511	16.3832	198.4049	4.4495
28	A	1715.2302	20.4022	162.2799	8.6346
29	A	1723.1446	16.5698	24.1485	2.9038
30	A	3851.2256	9.3181	164.1865	67.1790

py-14_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	121.9345	0.1594	0.0844	0.0001
2	A	159.9173	0.1908	0.3303	0.0245
3	A	211.9391	0.3143	1.5076	0.1424
4	A	268.6110	0.6507	0.2331	0.3199
5	A	272.1048	0.4284	5.7657	0.1409
6	A	316.2320	0.6067	3.1425	0.1592
7	A	346.9029	0.6953	0.0106	0.6346
8	A	349.3853	1.1601	2.8725	0.2902
9	A	425.4867	0.2079	69.9862	2.7100
10	A	450.1894	0.2609	64.5746	0.6831
11	A	457.3247	1.9059	0.2030	4.7538
12	A	477.7811	1.8866	0.7915	5.4727
13	A	610.2350	2.9927	0.4401	15.7052
14	A	643.3721	2.9331	3.4373	0.2637
15	A	685.7461	3.3483	0.1027	0.0204
16	A	702.6663	4.4272	2.8114	13.5987
17	A	732.2584	3.8523	8.2121	0.3539
18	A	736.7612	3.0124	6.4484	0.1699
19	A	977.4908	3.2635	188.1537	0.2792
20	A	1130.7300	10.0490	282.2912	0.1518
21	A	1183.2875	3.7928	52.3726	1.3205
22	A	1261.7482	1.9350	92.9913	0.9403

23	A	1328.3725	12.0426	33.7579	2.3650
24	A	1362.4172	6.1230	17.3401	9.6302
25	A	1483.7250	16.2686	31.2957	4.1591
26	A	1555.9751	17.6370	695.8026	1.8121
27	A	1589.9018	16.7398	207.9068	3.6090
28	A	1705.0886	20.2794	161.7450	9.0174
29	A	1711.2381	17.3153	31.6139	3.6515
30	A	3859.6055	9.3563	161.4373	66.9876

py-14_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	117.3267	0.1497	0.0008	0.0008
2	A	146.6091	0.1632	0.0385	0.0164
3	A	208.8140	0.2947	0.3869	0.1177
4	A	278.8105	0.7432	2.3898	0.2288
5	A	280.6583	0.4349	3.3042	0.2837
6	A	315.3313	0.0736	103.2091	0.3253
7	A	319.4930	0.6609	2.6496	0.1618
8	A	342.7136	0.4787	22.7420	1.2453
9	A	348.0005	1.1580	2.0628	0.2682
10	A	415.7658	0.8930	0.3171	1.0327
11	A	439.7543	1.2080	0.2295	1.6091
12	A	462.4676	1.9603	0.1776	5.0327
13	A	483.9483	1.9655	0.6506	6.0012
14	A	597.9912	2.5314	8.1193	0.5642
15	A	602.2982	2.9242	0.3712	17.1684
16	A	613.7539	2.5361	0.8935	0.0015
17	A	703.2042	4.4950	3.6901	12.9524
18	A	731.5025	3.0950	5.7172	0.1378
19	A	963.1364	3.8306	182.0483	0.2051
20	A	1103.2121	9.5884	272.9223	0.2442
21	A	1166.7742	6.8697	17.0032	0.8116
22	A	1294.9535	2.6651	38.8226	0.1491
23	A	1306.9709	2.7001	114.3050	3.1252
24	A	1448.6226	15.3652	33.3552	5.2438
25	A	1460.7880	9.9516	14.1380	9.2841
26	A	1527.7065	16.6702	624.4132	2.6185
27	A	1566.3934	15.2954	127.9034	3.8587
28	A	1683.3044	15.5345	36.4941	5.5537
29	A	1690.9665	18.3463	119.9424	7.3265
30	A	3833.6760	9.2323	146.3487	71.0244

py-14_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A	117.1800	0.1479	0.0604	0.0005
2	A	155.3440	0.1802	0.3068	0.0233
3	A	211.5995	0.3211	0.9642	0.1367
4	A	278.0690	0.7571	2.3470	0.2809
5	A	281.9603	0.4392	3.5079	0.2911
6	A	319.7947	0.6381	2.6903	0.1766
7	A	345.2202	0.7383	0.0002	0.7089
8	A	347.9062	1.1604	1.7780	0.3845
9	A	418.4320	0.1759	74.7102	2.6310
10	A	446.8671	0.3004	48.1640	1.0084
11	A	457.6426	1.9257	0.2377	4.8278
12	A	478.8299	1.9152	0.6345	6.2377
13	A	600.6220	2.9185	0.7275	18.8275
14	A	634.6772	2.8273	5.1151	0.4504
15	A	677.6159	3.2466	0.0084	0.0193
16	A	690.7068	4.3149	4.2839	11.1929
17	A	724.0482	3.7312	4.9350	0.2802
18	A	735.2945	3.1090	5.7170	0.2148
19	A	952.9956	3.7236	207.5010	0.2530
20	A	1099.6750	9.5228	275.6653	0.0480
21	A	1144.6290	6.7820	18.9566	1.9041
22	A	1273.9537	2.0260	68.0671	0.3062
23	A	1287.4600	4.6760	96.0115	3.6030
24	A	1399.6091	6.3176	22.7771	8.7082
25	A	1435.6525	15.0277	24.9925	4.2823
26	A	1504.4996	15.8411	660.9475	1.6083
27	A	1544.2519	14.1759	156.7012	1.2980
28	A	1663.3659	18.2333	133.9561	7.5179
29	A	1670.0619	15.1036	44.9346	2.8029
30	A	3819.5397	9.1640	131.7291	70.9338

py-14_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	121.3423	0.1582	0.0725	0.0002
2	A	160.0344	0.1920	0.2829	0.0226
3	A	213.8525	0.3225	0.9715	0.1272
4	A	276.4840	0.7386	2.5939	0.2457
5	A	277.1889	0.4215	3.5978	0.2798
6	A	321.5176	0.6448	2.8558	0.1543
7	A	349.4551	0.7319	0.0165	0.6880
8	A	352.8069	1.1909	2.0872	0.3216
9	A	426.8400	0.2096	66.2585	2.7409
10	A	453.3127	0.2617	61.7629	0.7700
11	A	465.5621	1.9882	0.2305	4.6811
12	A	487.7348	1.9793	0.6608	5.6329
13	A	614.4297	3.0535	0.5910	17.2674
14	A	645.0912	2.9312	3.9769	0.3487

15	A	687.0516	3.3440	0.0397	0.0181
16	A	706.8218	4.5051	3.7435	11.7321
17	A	730.3013	3.8218	6.8527	0.3351
18	A	745.7629	3.1617	6.0174	0.1914
19	A	976.0641	3.6950	198.3491	0.2505
20	A	1128.1440	10.0184	276.6393	0.0906
21	A	1178.7490	6.1550	25.8299	1.5041
22	A	1290.8682	1.7566	108.3972	0.8937
23	A	1321.6165	10.5634	45.9529	2.5929
24	A	1407.7581	6.2089	22.4623	8.9887
25	A	1475.5380	15.9992	27.8867	4.0989
26	A	1544.6458	16.9625	672.0473	1.7171
27	A	1582.5445	15.7102	172.8774	2.3412
28	A	1702.9732	19.6377	151.7674	8.1742
29	A	1709.6124	16.1736	37.7583	3.0413
30	A	3842.9271	9.2761	145.9382	66.2119

py-14_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.9211	0.1371	0.0665	0.0005
2	A	151.7347	0.1750	0.2918	0.0265
3	A	201.3992	0.2890	0.7523	0.1491
4	A	265.2469	0.6984	2.3297	0.3653
5	A	267.1378	0.3887	3.7928	0.3221
6	A	308.0252	0.5873	2.8434	0.1929
7	A	332.3884	0.7219	0.0026	0.6956
8	A	336.2036	1.0817	1.6925	0.4220
9	A	411.5234	0.4215	21.1176	2.9774
10	A	445.4531	1.8272	0.2438	5.1666
11	A	449.7907	0.1596	95.5343	0.5707
12	A	466.5013	1.8295	0.7451	7.1818
13	A	585.3431	2.7801	0.9608	19.5934
14	A	607.5476	2.5919	4.4303	0.3377
15	A	643.4237	2.9115	0.0359	0.0356
16	A	670.8514	4.0686	4.0248	12.4970
17	A	682.4169	3.3167	3.9997	0.2837
18	A	711.8566	2.9220	5.9267	0.2607
19	A	922.7861	3.5303	208.7464	0.2304
20	A	1068.9454	9.0078	270.7438	0.0551
21	A	1104.8323	6.7294	18.1557	2.1281
22	A	1238.0242	3.6376	16.0306	0.4193
23	A	1250.6353	1.9961	155.2761	4.0799
24	A	1385.9458	9.6443	0.2198	7.4589
25	A	1389.4606	9.5336	40.7401	4.1644
26	A	1455.0712	14.8863	636.2852	2.0577
27	A	1499.5296	13.1812	126.9135	0.8115
28	A	1615.1675	15.1728	77.4175	6.5536

29	A	1621.5299	15.2595	89.8878	3.3391
30	A	3669.3500	8.4548	118.9391	77.1615

py-14_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.4160	0.1431	0.0666	0.0003
2	A	154.3218	0.1817	0.2943	0.0253
3	A	202.4148	0.2901	0.8740	0.1382
4	A	257.9783	0.5324	0.4447	0.4474
5	A	259.4398	0.4222	5.6379	0.1967
6	A	304.9455	0.5760	2.8535	0.1696
7	A	333.2928	0.7387	0.0109	0.6830
8	A	336.0016	1.0775	1.8762	0.3902
9	A	412.9348	0.5230	14.6116	2.9241
10	A	446.4642	1.8248	0.2664	5.2126
11	A	456.4122	0.1550	100.7574	0.6436
12	A	467.9101	1.8421	0.7605	6.9630
13	A	588.6295	2.8036	0.7986	19.9459
14	A	606.3923	2.5597	4.1711	0.2852
15	A	638.0963	2.8370	0.0654	0.0453
16	A	669.6709	3.2042	4.5340	0.2812
17	A	674.8217	4.1277	4.2089	12.4137
18	A	710.1917	2.9058	5.8710	0.2842
19	A	925.5176	3.5988	208.6008	0.2437
20	A	1071.7229	9.0700	274.0727	0.0346
21	A	1110.0465	7.3313	16.9787	2.1826
22	A	1242.6901	7.2218	6.7550	1.2234
23	A	1261.6556	1.6375	168.8471	3.3744
24	A	1387.6714	6.9973	11.1665	7.5802
25	A	1393.6925	12.4958	36.5784	3.1659
26	A	1465.2214	15.2717	628.3145	2.5191
27	A	1507.9515	13.6531	124.6318	0.8926
28	A	1629.6496	13.3125	33.1347	5.5413
29	A	1637.7165	17.1728	135.1817	4.9798
30	A	3661.8686	8.4201	105.1868	76.8759

py-14_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	118.1288	0.1500	0.0685	0.0003
2	A	156.9667	0.1866	0.2975	0.0244
3	A	208.8883	0.3096	1.0592	0.1367
4	A	266.5800	0.4507	5.7466	0.1912
5	A	267.2046	0.5504	0.5992	0.4149
6	A	312.1653	0.6106	2.8101	0.1665

7	A	341.6943	0.7471	0.0056	0.6845
8	A	342.9786	1.1259	1.9819	0.3634
9	A	422.5128	0.3608	30.1058	3.0100
10	A	453.8057	0.1760	92.2697	0.5180
11	A	455.8289	1.9063	0.2503	4.9761
12	A	477.7903	1.9150	0.6739	6.3840
13	A	599.1763	2.8974	0.6710	19.1679
14	A	626.0609	2.7403	4.3275	0.3190
15	A	662.1072	3.0814	0.0338	0.0273
16	A	688.8348	4.2993	4.2594	11.7634
17	A	699.9272	3.5012	5.5618	0.2939
18	A	726.4351	3.0277	5.9550	0.2414
19	A	945.6808	3.6684	206.7089	0.2475
20	A	1093.0198	9.4129	279.3940	0.0421
21	A	1137.2018	7.0782	19.4631	1.9268
22	A	1268.5355	2.6737	38.2112	0.0895
23	A	1280.0864	3.0537	129.3935	4.0255
24	A	1390.3309	5.8911	21.1832	8.1758
25	A	1424.5879	14.7627	26.5587	3.7226
26	A	1495.5389	15.8396	648.8121	2.0322
27	A	1534.8540	14.2340	145.8014	1.2889
28	A	1658.3473	15.6420	77.3646	6.9741
29	A	1664.1877	16.2612	100.6321	4.0424
30	A	3748.9833	8.8274	123.8237	72.1579

py-14_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	122.0401	0.1602	0.0685	0.0003
2	A	159.8492	0.1908	0.2907	0.0217
3	A	215.5056	0.3286	1.1473	0.1269
4	A	280.2412	0.6050	4.5149	0.2002
5	A	281.8791	0.5031	1.8659	0.3359
6	A	323.4741	0.6610	2.7677	0.1480
7	A	349.5584	0.7109	0.0247	0.6652
8	A	353.5307	1.1982	2.0851	0.3052
9	A	422.7227	0.1579	93.5121	2.2383
10	A	450.3608	0.3924	37.8906	1.1117
11	A	467.3776	2.0108	0.2391	4.6450
12	A	489.5597	1.9998	0.5360	5.4583
13	A	612.9653	3.0278	0.6167	17.1917
14	A	648.9215	2.9506	3.9634	0.3273
15	A	691.1119	3.3880	0.0234	0.0111
16	A	706.9520	4.5090	4.5336	11.6816
17	A	736.0268	3.8812	7.7699	0.3188
18	A	747.9404	3.1844	6.1082	0.1518
19	A	973.0639	3.7318	204.6460	0.2497
20	A	1126.8316	9.9776	281.0345	0.1363

21	A	1173.1914	6.2418	24.0606	1.6845
22	A	1283.0544	2.0469	92.3266	1.0677
23	A	1319.9260	11.1735	43.1095	2.3771
24	A	1374.2941	3.9254	47.7191	10.3314
25	A	1469.0919	15.8485	25.6334	4.0601
26	A	1541.0563	16.7245	667.6141	1.8235
27	A	1579.8601	15.6321	176.2531	2.8983
28	A	1704.5339	19.7916	163.6690	8.7359
29	A	1712.2475	16.1286	36.0873	3.2755
30	A	3871.9321	9.4180	146.1085	63.3161

py-14_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	120.7254	0.1568	0.0717	0.0004
2	A	158.7612	0.1905	0.3181	0.0228
3	A	211.4386	0.3162	1.3927	0.1332
4	A	276.6803	0.7014	3.1054	0.2632
5	A	278.7206	0.4444	3.0232	0.3252
6	A	318.5456	0.6282	2.8594	0.1698
7	A	345.7235	0.7305	0.0002	0.7077
8	A	347.8429	1.1589	2.1025	0.3417
9	A	420.7805	0.2019	67.3803	2.7792
10	A	446.7791	0.2555	61.8804	0.7984
11	A	463.4171	1.9844	0.2349	4.8295
12	A	485.7949	1.9795	0.5552	6.0843
13	A	604.6319	2.9443	0.6525	18.4678
14	A	640.4333	2.8795	4.6886	0.3859
15	A	681.4636	3.2919	0.0335	0.0180
16	A	698.0456	4.4065	4.9223	11.2754
17	A	729.3147	3.7984	6.5276	0.3284
18	A	737.9480	3.1195	6.0508	0.1899
19	A	955.5006	3.7133	209.2076	0.2616
20	A	1104.4604	9.5866	283.1909	0.0748
21	A	1148.2045	6.6829	21.1451	1.8313
22	A	1272.0642	1.9216	92.3948	0.6447
23	A	1293.5641	8.2836	62.1712	3.0886
24	A	1373.3625	4.5526	35.7609	8.8707
25	A	1438.5167	15.1149	24.5323	4.0222
26	A	1508.2207	15.9930	642.7082	1.8048
27	A	1545.0025	14.5157	161.9520	1.9385
28	A	1668.3169	17.6887	127.2133	8.2459
29	A	1674.8035	15.3915	59.0990	3.4734
30	A	3796.7271	9.0548	142.6221	69.9475

py-14_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.8738	0.1546	0.0708	0.0004
2	A	157.9993	0.1886	0.3204	0.0230
3	A	210.2774	0.3123	1.3665	0.1352
4	A	277.2946	0.7462	2.5512	0.2970
5	A	279.3699	0.4337	3.5100	0.3083
6	A	318.4388	0.6264	2.8748	0.1725
7	A	344.0976	0.7242	0.0001	0.7020
8	A	347.2792	1.1552	2.0846	0.3342
9	A	419.9497	0.2144	61.8487	2.8226
10	A	446.0679	0.2381	66.4465	0.7233
11	A	463.0497	1.9826	0.2393	4.8595
12	A	486.2226	1.9819	0.5526	6.1067
13	A	604.9592	2.9581	0.7009	18.5167
14	A	637.2330	2.8558	4.5729	0.3703
15	A	677.7549	3.2543	0.0315	0.0184
16	A	697.1423	4.3952	5.0383	11.4094
17	A	725.0667	3.7559	6.4416	0.3258
18	A	736.4757	3.1153	6.0429	0.1937
19	A	952.9016	3.7321	211.1496	0.2551
20	A	1101.9710	9.5440	283.8028	0.0711
21	A	1144.7854	6.7650	20.2283	1.8474
22	A	1271.2143	1.9531	87.9986	0.5474
23	A	1290.9082	7.6169	67.1957	3.2522
24	A	1373.2123	4.5336	35.5623	8.7458
25	A	1437.4589	15.0833	26.0982	3.8889
26	A	1503.5853	15.8529	640.6602	1.8508
27	A	1541.6959	14.4140	155.3472	1.8406
28	A	1663.3610	17.4091	123.9865	8.1941
29	A	1670.0679	15.1917	60.5178	3.5055
30	A	3790.5368	9.0249	139.7155	69.9129

py-14_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	124.7201	0.1673	0.0691	0.0001
2	A	161.9141	0.1968	0.2741	0.0243
3	A	214.7699	0.3203	1.3725	0.1220
4	A	276.8037	0.7176	0.2245	0.3104
5	A	279.2442	0.4496	5.3516	0.1536
6	A	321.8895	0.6372	2.9030	0.1518
7	A	349.2521	0.6627	0.1762	0.6181
8	A	354.3395	1.1974	2.6949	0.2935
9	A	413.3953	0.1291	116.2653	2.1214
10	A	445.8903	0.6412	18.5584	1.5731
11	A	467.8545	2.0096	0.1919	4.6851
12	A	489.1111	1.9858	0.4988	5.2579

13	A	616.6191	3.0803	0.3632	15.5697
14	A	645.8843	2.9141	3.5781	0.2710
15	A	688.4989	3.3628	0.0352	0.0137
16	A	713.1791	4.5627	3.9387	12.1646
17	A	731.7584	3.8525	8.3925	0.3397
18	A	745.1015	3.1526	5.9564	0.1549
19	A	987.0318	3.6892	186.9559	0.3011
20	A	1136.2964	10.1493	275.8661	0.2492
21	A	1195.9912	4.9174	34.8081	1.5870
22	A	1285.1389	2.4210	74.5085	1.2130
23	A	1340.8773	11.5289	36.0145	2.0639
24	A	1361.7641	3.4458	50.9557	9.5036
25	A	1491.1652	16.4169	27.6415	4.3872
26	A	1560.9764	17.6185	665.6127	1.8255
27	A	1593.6512	16.3832	198.4055	4.4495
28	A	1715.2316	20.4022	162.2789	8.6347
29	A	1723.1444	16.5699	24.1529	2.9038
30	A	3851.2269	9.3181	164.1873	67.1789

py-14_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	117.3270	0.1497	0.0008	0.0008
2	A	146.6091	0.1632	0.0385	0.0164
3	A	208.8144	0.2947	0.3870	0.1177
4	A	278.8105	0.7432	2.3905	0.2288
5	A	280.6583	0.4349	3.3036	0.2837
6	A	315.3371	0.0736	103.2032	0.3253
7	A	319.4932	0.6610	2.6495	0.1618
8	A	342.7140	0.4786	22.7477	1.2454
9	A	348.0007	1.1580	2.0628	0.2682
10	A	415.7664	0.8931	0.3171	1.0328
11	A	439.7546	1.2080	0.2295	1.6090
12	A	462.4677	1.9603	0.1776	5.0327
13	A	483.9484	1.9655	0.6506	6.0012
14	A	597.9915	2.5314	8.1194	0.5642
15	A	602.2979	2.9242	0.3712	17.1683
16	A	613.7540	2.5361	0.8934	0.0015
17	A	703.2045	4.4950	3.6902	12.9524
18	A	731.5024	3.0950	5.7171	0.1378
19	A	963.1367	3.8306	182.0480	0.2051
20	A	1103.2118	9.5884	272.9240	0.2442
21	A	1166.7737	6.8697	17.0017	0.8116
22	A	1294.9552	2.6650	38.8231	0.1491
23	A	1306.9713	2.7001	114.3044	3.1252
24	A	1448.6215	15.3648	33.3610	5.2431
25	A	1460.7884	9.9518	14.1295	9.2849
26	A	1527.7051	16.6702	624.4150	2.6184

27	A	1566.3950	15.2953	127.9030	3.8586
28	A	1683.3039	15.5350	36.5094	5.5544
29	A	1690.9664	18.3458	119.9277	7.3259
30	A	3833.6723	9.2323	146.3485	71.0246

py-15_A_b31yp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.0345	0.1060	0.3232	0.0685
2	A	200.1315	0.2588	0.7117	0.3141
3	A	282.5106	0.6525	2.0207	0.7061
4	A	297.2886	0.4403	0.9153	1.4708
5	A	304.7713	0.6159	1.7324	0.1131
6	A	353.9965	0.6898	8.0522	0.0559
7	A	426.1038	0.2170	55.5106	1.4537
8	A	454.9058	1.4201	1.2821	4.3596
9	A	462.1737	0.3802	26.4623	2.0024
10	A	495.4903	0.3565	45.2279	0.7712
11	A	517.4863	1.8410	6.1749	12.0407
12	A	650.7409	1.3234	18.9484	1.4290
13	A	695.1743	4.2332	18.2298	1.2479
14	A	697.0692	3.3215	0.9715	0.2275
15	A	731.6278	2.8171	12.4584	0.8353
16	A	759.3582	3.0354	12.1155	25.2609
17	A	894.8676	0.6548	27.4324	0.1785
18	A	900.9700	1.9729	75.6400	0.3150
19	A	1150.0803	3.6806	26.0515	3.9674
20	A	1175.7937	1.9189	344.4830	1.4269
21	A	1205.3350	1.7774	65.3333	0.2825
22	A	1274.1338	4.0337	170.1281	1.6508
23	A	1357.1571	3.7706	3.5089	0.9119
24	A	1417.4205	13.1283	9.2132	13.4129
25	A	1467.5325	10.0513	87.4477	0.2159
26	A	1525.2169	9.8662	688.0519	2.1160
27	A	1652.4222	11.9779	0.4088	8.9321
28	A	1677.4455	15.4750	32.4214	6.1341
29	A	3216.9214	6.6674	2.5548	97.0314
30	A	3788.9331	9.0082	121.4257	99.5880

py-15_A_b3p86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.0977	0.1061	0.3144	0.0662
2	A	202.0446	0.2637	0.5073	0.3060
3	A	280.8154	0.6311	2.1051	0.6802
4	A	299.4473	0.4443	0.9474	1.4336

5	A	304.0427	0.6157	1.7503	0.0946
6	A	356.5795	0.7001	8.1466	0.0525
7	A	430.4272	0.2199	55.5651	1.4256
8	A	454.2822	1.3933	1.4461	4.2450
9	A	465.9403	0.4347	19.8839	1.8051
10	A	499.1520	0.3359	51.7106	0.9146
11	A	517.1449	1.8121	6.3840	11.1573
12	A	653.3435	1.3164	19.3844	1.4434
13	A	699.0316	3.3460	1.0019	0.2212
14	A	699.2267	4.2594	15.8079	1.3204
15	A	731.8930	2.9614	11.6640	0.7270
16	A	762.1920	3.0534	10.8474	25.4908
17	A	891.0226	0.6430	29.0709	0.1821
18	A	910.6233	1.8501	64.6859	0.3555
19	A	1166.0815	2.4181	51.4493	3.6078
20	A	1183.3114	1.9488	323.5503	0.9243
21	A	1211.9596	2.1948	49.8807	0.6862
22	A	1288.4547	3.5547	180.1072	1.5905
23	A	1380.9015	5.1103	1.2027	0.7988
24	A	1439.9455	13.6326	8.4627	12.9460
25	A	1486.0011	11.0312	82.6923	0.1758
26	A	1548.5412	10.9031	725.4858	1.8662
27	A	1674.7572	13.0674	0.2488	8.3046
28	A	1698.5300	16.4053	32.7171	6.6691
29	A	3229.6213	6.7221	3.2204	94.9931
30	A	3815.4371	9.1339	125.7077	97.0409

py-15_A_b3pw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	114.5429	0.1051	0.3150	0.0666
2	A	201.9706	0.2633	0.5189	0.3088
3	A	281.2907	0.6347	2.0766	0.6796
4	A	298.9888	0.4427	0.9346	1.4436
5	A	304.6240	0.6181	1.7596	0.0955
6	A	356.1690	0.7003	8.0287	0.0539
7	A	430.5127	0.2157	56.7836	1.4084
8	A	453.3368	1.3934	1.4090	4.2614
9	A	465.8668	0.4394	19.5659	1.8585
10	A	498.5006	0.3402	50.3307	0.8959
11	A	516.1539	1.8067	6.3511	11.2786
12	A	653.2229	1.3212	19.2773	1.4342
13	A	697.2970	4.2353	16.0168	1.3306
14	A	699.4678	3.3508	0.9778	0.2185
15	A	732.4929	2.9339	11.6561	0.7554
16	A	759.8396	3.0358	10.9492	25.4421
17	A	891.5560	0.6449	28.6504	0.1855
18	A	908.4245	1.8761	66.9757	0.3431

19	A	1162.6956	2.6475	44.1684	3.6814
20	A	1181.3509	1.9510	328.7808	1.0139
21	A	1209.4474	2.0575	54.1961	0.5538
22	A	1284.8365	3.5129	179.3956	1.6341
23	A	1376.8227	4.9028	0.9305	0.8091
24	A	1434.2050	13.5132	8.4008	13.1030
25	A	1481.7944	10.8221	82.6946	0.1756
26	A	1543.9313	10.7057	718.8700	1.8711
27	A	1670.6789	12.8858	0.2771	8.2194
28	A	1693.8307	16.2712	32.3702	6.8662
29	A	3225.5409	6.7048	2.7587	95.5138
30	A	3814.4836	9.1296	123.2563	96.8505

py-15_A_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1832	0.0942	0.3220	0.0888
2	A	190.4932	0.2365	0.6408	0.3538
3	A	272.4254	0.6144	1.8274	0.9061
4	A	283.0544	0.4046	0.7750	1.4960
5	A	293.9705	0.5765	1.8111	0.1467
6	A	339.1127	0.6326	7.2805	0.0690
7	A	412.7026	0.2871	33.3314	1.6540
8	A	437.6891	1.3368	1.1587	4.7508
9	A	445.5094	0.3150	25.3790	1.4347
10	A	480.8045	0.2691	59.3443	1.2371
11	A	495.8757	1.7034	6.3762	15.1590
12	A	624.9322	1.2428	16.8234	1.6349
13	A	658.3507	2.8987	1.4467	0.3140
14	A	662.7581	3.8742	19.0865	1.2593
15	A	689.3475	2.5887	9.0997	0.7169
16	A	727.0302	2.8008	12.9739	26.0707
17	A	851.2018	0.5861	26.3600	0.2006
18	A	858.2860	1.9829	87.6616	0.3537
19	A	1083.6739	4.8037	11.4561	5.0871
20	A	1125.6542	1.9069	329.3099	1.8260
21	A	1158.0659	1.6039	123.0771	0.2756
22	A	1227.5306	2.4659	126.3180	2.1704
23	A	1326.4575	4.6707	6.2192	0.3008
24	A	1338.7329	11.1498	13.6373	11.9409
25	A	1395.7257	7.6854	99.2445	0.3989
26	A	1446.5204	7.8384	594.0327	1.6912
27	A	1569.3104	9.9660	2.0995	9.5658
28	A	1598.3302	13.3242	24.4467	4.1038
29	A	3138.7589	6.3411	1.9022	105.2696
30	A	3636.1987	8.2947	95.0136	120.5599

py-15_A_bp86

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	107.9057	0.0937	0.3078	0.0856
2	A	191.7568	0.2395	0.3587	0.3463
3	A	270.7749	0.5901	1.9193	0.8769
4	A	284.6809	0.4063	0.8385	1.4656
5	A	293.1126	0.5751	1.8609	0.1190
6	A	341.7878	0.6442	7.3586	0.0606
7	A	415.7487	0.2853	33.8201	1.6350
8	A	437.0705	1.3045	1.3619	4.6120
9	A	446.8530	0.3716	17.3276	1.2349
10	A	484.7204	0.2513	66.1750	1.4050
11	A	496.8194	1.6829	6.5818	13.8200
12	A	627.0865	1.2334	17.3467	1.6795
13	A	657.4020	2.8953	1.5256	0.3168
14	A	668.1360	3.9188	16.1881	1.3969
15	A	686.3539	2.7350	8.2252	0.6038
16	A	731.2319	2.8321	11.6298	26.6367
17	A	841.7799	0.5666	28.2961	0.2151
18	A	869.8220	1.8306	72.9631	0.3961
19	A	1105.0865	3.3293	24.5869	4.9043
20	A	1133.3007	1.8482	322.6757	1.2760
21	A	1161.7224	1.7431	86.9820	0.4512
22	A	1239.1727	2.4351	151.4755	2.0782
23	A	1354.2309	6.2546	1.3798	0.2339
24	A	1366.1797	11.4733	14.4888	11.5466
25	A	1414.9649	8.8591	82.8437	0.3232
26	A	1469.7495	9.0184	651.9922	1.4311
27	A	1591.5896	11.1734	1.2467	8.9262
28	A	1619.3775	14.2938	25.3361	4.4033
29	A	3141.2590	6.3534	2.3335	104.6982
30	A	3653.0747	8.3703	97.0766	118.4515

py-15_A_bpw91

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	107.7451	0.0934	0.3122	0.0843
2	A	192.6246	0.2413	0.3926	0.3410
3	A	272.2827	0.5976	1.9006	0.8704
4	A	285.5238	0.4083	0.8363	1.4540
5	A	294.9465	0.5821	1.8715	0.1177
6	A	343.0162	0.6502	7.3250	0.0610
7	A	418.2691	0.2802	35.1626	1.5950
8	A	437.9145	1.3140	1.3439	4.5696
9	A	449.2054	0.3801	16.8418	1.2458
10	A	486.6787	0.2566	65.4612	1.3539

11	A	497.9978	1.6893	6.6086	13.6641
12	A	629.9301	1.2488	17.2799	1.6461
13	A	662.5459	2.9446	1.3993	0.2901
14	A	669.4273	3.9292	16.2152	1.3781
15	A	692.1113	2.7194	8.5295	0.6183
16	A	732.8534	2.8470	11.5470	26.3978
17	A	847.6781	0.5766	27.7301	0.2131
18	A	872.5985	1.8650	75.1001	0.3760
19	A	1107.7207	3.5579	22.0433	4.8052
20	A	1136.9473	1.8709	325.7474	1.2958
21	A	1165.7643	1.7121	92.8384	0.3715
22	A	1242.4369	2.4034	148.7292	2.0801
23	A	1359.2970	6.3049	1.1135	0.2393
24	A	1369.3499	11.4520	14.8090	11.3201
25	A	1419.5594	8.9152	81.0545	0.2942
26	A	1474.8653	9.0397	650.5740	1.4121
27	A	1597.7496	11.2332	1.0257	8.8732
28	A	1624.5388	14.4430	25.5981	4.6503
29	A	3157.3326	6.4185	2.1404	102.7706
30	A	3675.7133	8.4748	97.1482	115.2799

py-15_A_camb3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	118.6078	0.1124	0.3247	0.0591
2	A	204.3257	0.2690	0.8366	0.2879
3	A	284.2212	0.6591	2.1061	0.6259
4	A	303.4397	0.4534	1.0198	1.4304
5	A	306.9100	0.6214	1.8363	0.0990
6	A	358.9957	0.7057	8.5930	0.0512
7	A	431.3754	0.1955	67.7172	1.2809
8	A	460.6063	1.4391	1.3595	4.2159
9	A	470.6241	0.4511	23.0371	2.1062
10	A	503.5394	0.3899	42.1490	0.6582
11	A	523.3989	1.8693	6.0753	10.5922
12	A	658.2928	1.3268	20.9913	1.3228
13	A	705.9755	4.3302	17.8481	1.0987
14	A	717.8796	3.5562	0.6616	0.1725
15	A	756.2715	2.8482	15.3762	0.8689
16	A	772.4984	3.1318	10.8599	25.0824
17	A	917.3037	1.8941	68.1179	0.3009
18	A	918.9133	0.7014	27.7046	0.2332
19	A	1174.7527	2.5866	57.1341	3.5801
20	A	1191.5804	1.9193	337.9007	1.2667
21	A	1217.5306	2.0990	26.6408	0.5746
22	A	1282.7078	7.7777	189.6994	1.5187
23	A	1351.7136	3.0028	8.0847	1.0093
24	A	1452.2046	13.8829	7.3048	14.3125

25	A	1500.6726	11.4384	82.2444	0.1887
26	A	1562.9896	11.0090	732.6396	2.5789
27	A	1696.7999	13.5902	0.3524	8.8117
28	A	1720.1543	16.9492	37.3550	7.9213
29	A	3235.5579	6.7512	3.9944	92.3896
30	A	3828.8557	9.1999	141.0667	88.2407

py-15_A_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.2852	0.1139	0.3064	0.0586
2	A	204.5545	0.2657	0.6181	0.3084
3	A	283.1900	0.6575	2.0823	0.5248
4	A	304.2852	0.4595	0.8234	1.4194
5	A	306.2581	0.6208	1.5497	0.0936
6	A	361.0723	0.7214	8.5979	0.0546
7	A	420.1362	0.1463	91.1469	1.0834
8	A	458.8011	1.4188	1.4114	4.2822
9	A	465.9717	0.6420	13.3071	2.7186
10	A	493.5897	0.4521	29.2539	0.5364
11	A	521.2925	1.8440	5.6293	9.8076
12	A	657.3408	1.3239	20.2388	1.2877
13	A	707.1049	4.2806	16.7683	1.0107
14	A	708.4481	3.5091	0.5907	0.1612
15	A	745.0150	3.0998	12.7877	0.8094
16	A	771.9521	3.1318	9.3143	25.3853
17	A	907.8960	0.6669	30.8239	0.1977
18	A	925.4005	1.8126	58.3046	0.3761
19	A	1186.6216	1.6846	68.2036	2.2508
20	A	1197.2091	1.9363	320.5896	1.8472
21	A	1224.5109	3.7594	8.5651	1.0319
22	A	1288.0534	8.9312	183.0102	1.3184
23	A	1353.3523	2.8384	14.0009	0.7776
24	A	1471.5377	14.5017	3.3900	15.3513
25	A	1512.6779	12.3800	92.0398	0.2453
26	A	1574.4216	11.9033	750.9304	2.7170
27	A	1704.9400	14.0076	0.4441	7.2778
28	A	1725.1663	17.2243	34.5323	7.9504
29	A	3243.7241	6.7850	5.4585	90.0469
30	A	3855.4491	9.3299	149.3127	90.2659

py-15_A_mn15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.7294	0.1083	0.3320	0.0628
2	A	202.1152	0.2626	0.7867	0.2909

3	A	275.4899	0.6018	2.3170	0.5777
4	A	299.2408	0.5822	1.6894	0.0873
5	A	300.5863	0.4402	1.1054	1.4454
6	A	354.6167	0.6884	9.3920	0.0461
7	A	425.9579	0.1874	67.5855	1.2851
8	A	447.1203	1.3121	1.7131	4.2440
9	A	465.6109	0.5055	15.5236	1.9610
10	A	498.0648	0.3596	48.9370	0.9053
11	A	509.7616	1.7234	6.5513	9.7187
12	A	646.5293	1.2569	20.4653	1.4363
13	A	696.7429	4.1714	14.3932	1.1512
14	A	707.1678	3.4551	0.6434	0.1664
15	A	743.2371	2.8891	14.3101	0.7224
16	A	762.5760	3.0605	9.1422	26.7767
17	A	907.2955	0.6765	28.4423	0.3258
18	A	914.5689	1.6344	50.7092	0.4747
19	A	1169.9454	1.6064	384.4841	2.4157
20	A	1174.8368	1.6146	20.3786	1.3302
21	A	1217.6715	3.9966	14.6521	1.3053
22	A	1282.2291	5.8880	193.3028	1.1979
23	A	1344.1685	4.3061	1.0436	0.9530
24	A	1465.6131	14.2735	4.8433	14.7143
25	A	1501.8198	13.0194	85.1511	0.1177
26	A	1572.3626	12.3149	790.0202	2.2333
27	A	1694.0927	14.5535	1.4761	8.1410
28	A	1715.2425	17.5171	36.4439	9.4659
29	A	3252.8421	6.8193	1.8108	101.4713
30	A	3862.2133	9.3604	140.0074	95.9173

py-15_A_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	110.5282	0.1063	0.0548	0.0455
2	A	199.9722	0.2306	0.0868	0.3172
3	A	282.8431	0.6338	2.0513	0.6140
4	A	288.5157	0.4021	0.0366	1.3296
5	A	306.0500	0.6454	1.3654	0.0635
6	A	354.0374	0.7002	8.1678	0.0533
7	A	365.6881	0.0874	124.2516	0.6334
8	A	440.9134	0.7018	3.0565	0.3858
9	A	448.6293	1.1224	1.6830	2.9842
10	A	451.6936	1.3704	1.6187	4.3684
11	A	512.9340	1.8152	5.2929	10.7821
12	A	547.3105	1.9228	3.5684	1.1481
13	A	629.5833	2.8301	0.0833	0.0084
14	A	648.2061	1.3378	18.3511	1.5067
15	A	704.6820	4.3459	14.3877	2.9079
16	A	751.9599	2.9869	13.2502	24.4327

17	A	852.3948	0.5386	36.7973	0.0274
18	A	905.4392	1.9578	62.3773	0.4267
19	A	1168.2363	3.3880	7.2965	1.9211
20	A	1183.6192	1.9313	314.7575	1.6765
21	A	1216.0189	2.0151	74.1823	0.1656
22	A	1303.1286	2.3192	145.0454	1.3666
23	A	1430.8519	13.2386	4.5872	10.8637
24	A	1452.2011	9.9256	18.7399	7.8176
25	A	1478.2241	9.5763	85.6505	0.2774
26	A	1543.2412	10.7335	694.5266	3.2376
27	A	1664.9793	13.0780	4.4452	8.6643
28	A	1691.3714	15.9207	15.9662	5.3908
29	A	3251.9918	6.8180	3.6225	93.0678
30	A	3827.0351	9.1906	128.9766	93.2726

py-15_A_o3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.2020	0.1009	0.3117	0.0719
2	A	200.1517	0.2594	0.4786	0.3264
3	A	282.9959	0.6509	1.9062	0.6951
4	A	296.0932	0.4352	0.8688	1.4884
5	A	306.6497	0.6253	1.8513	0.1089
6	A	354.3374	0.6989	7.4189	0.0606
7	A	430.0817	0.2242	52.1483	1.4094
8	A	449.3160	1.3879	1.2764	4.3354
9	A	462.6933	0.4219	19.0582	1.8745
10	A	494.4986	0.3248	51.1192	0.9879
11	A	511.7259	1.7787	6.2406	12.2139
12	A	650.6765	1.3340	18.0960	1.4486
13	A	689.4534	4.1410	15.9219	1.2730
14	A	694.7619	3.2560	1.2543	0.2691
15	A	726.4508	2.7383	10.7026	0.8543
16	A	750.8024	2.9668	11.2815	25.2030
17	A	883.6309	0.6397	26.5307	0.1975
18	A	900.6287	1.9338	71.9792	0.3679
19	A	1150.5774	3.2347	31.0742	4.1564
20	A	1173.0168	2.0108	324.6465	1.3259
21	A	1200.0942	1.8237	72.8339	0.3820
22	A	1275.9266	2.8763	171.6703	1.8512
23	A	1380.3888	5.3792	1.8395	0.6590
24	A	1417.0923	13.1199	9.9286	13.3701
25	A	1466.9829	10.1663	82.3068	0.1853
26	A	1527.1955	10.2304	709.1932	1.6121
27	A	1653.7105	12.3191	0.5669	7.3804
28	A	1675.6215	15.8553	28.9601	7.1139
29	A	3222.6974	6.6915	1.9855	99.4989
30	A	3811.8777	9.1175	112.7603	101.7558

py-15_A_pbe0

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.0964	0.1079	0.3128	0.0633
2	A	203.4963	0.2671	0.4613	0.3051
3	A	282.3582	0.6375	2.0927	0.6298
4	A	302.0479	0.4498	0.9892	1.4397
5	A	305.9385	0.6226	1.7822	0.0907
6	A	359.3403	0.7130	8.1501	0.0518
7	A	432.3674	0.2110	59.3190	1.3846
8	A	456.2584	1.3991	1.4824	4.1917
9	A	468.7240	0.4640	18.2439	1.9470
10	A	501.2223	0.3462	49.8770	0.8912
11	A	520.3516	1.8291	6.3269	10.7345
12	A	657.4633	1.3288	19.6787	1.4169
13	A	704.0637	4.3047	15.6260	1.2355
14	A	706.9103	3.4256	0.9383	0.2166
15	A	740.2994	2.9616	12.2742	0.8182
16	A	767.5415	3.0991	10.4600	25.3316
17	A	897.3056	0.6558	28.9192	0.1860
18	A	918.2721	1.8327	62.3880	0.3657
19	A	1174.8919	2.0552	64.7517	3.3264
20	A	1192.9326	1.9934	312.4779	0.8675
21	A	1219.8547	2.5649	39.6862	0.9289
22	A	1297.2934	3.7855	186.7049	1.5447
23	A	1387.1280	5.0226	1.4967	0.8787
24	A	1455.9463	13.9357	7.9636	13.9835
25	A	1501.0367	11.5395	83.3362	0.1119
26	A	1564.1784	11.4117	742.1562	1.9205
27	A	1691.6047	13.6068	0.3014	7.7775
28	A	1713.9897	16.9011	33.5453	7.4460
29	A	3238.1326	6.7592	3.1781	95.0977
30	A	3842.8767	9.2660	128.7101	93.8287

py-15_A_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	108.1938	0.0941	0.3109	0.0859
2	A	192.2085	0.2407	0.3460	0.3483
3	A	271.3951	0.5946	1.8721	0.8469
4	A	285.9617	0.4090	0.8447	1.4577
5	A	294.1573	0.5773	1.9210	0.1215
6	A	343.3548	0.6504	7.3199	0.0620
7	A	417.6796	0.2896	33.3918	1.6178
8	A	437.7961	1.3046	1.3987	4.5357

9	A	448.4777	0.3802	16.2497	1.2400
10	A	487.6253	0.2504	67.2171	1.4315
11	A	497.8842	1.6831	6.5877	13.7009
12	A	629.1338	1.2353	17.3460	1.6585
13	A	663.8704	2.9351	1.5021	0.3143
14	A	670.1670	3.9320	15.8727	1.2087
15	A	693.4781	2.6745	8.6654	0.6755
16	A	734.2166	2.8597	11.0103	26.3970
17	A	844.5694	0.5758	27.7103	0.2216
18	A	874.6631	1.8058	71.1609	0.4239
19	A	1110.4185	2.9398	31.2719	4.8135
20	A	1137.6323	1.8541	315.9841	1.2190
21	A	1163.8406	1.8338	81.7123	0.6261
22	A	1243.5616	2.4288	154.4353	2.0607
23	A	1366.3278	6.8258	1.0489	0.3604
24	A	1375.6165	11.4045	16.6545	11.8262
25	A	1423.6081	9.2661	77.0681	0.2793
26	A	1479.3008	9.3750	665.8879	1.3523
27	A	1601.9060	11.6338	0.6939	8.5459
28	A	1628.7412	14.7156	25.5158	5.0511
29	A	3151.0606	6.3935	2.6692	104.6343
30	A	3668.0453	8.4391	98.7977	117.6555

py-15_A_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	110.7286	0.0987	0.3053	0.0799
2	A	193.7192	0.2451	0.4448	0.3384
3	A	265.0012	0.5585	2.0175	0.8076
4	A	288.1753	0.5589	1.7104	0.1045
5	A	289.9705	0.4236	0.8265	1.4544
6	A	342.7714	0.6477	7.6604	0.0501
7	A	418.7903	0.3093	30.2356	1.6826
8	A	436.2065	1.2628	1.6099	4.4400
9	A	448.8215	0.3993	13.5314	1.0610
10	A	489.0804	0.2399	73.0018	1.5012
11	A	498.2446	1.6855	6.5890	13.2595
12	A	626.4381	1.2534	17.2338	1.7165
13	A	658.9200	2.9434	1.4872	0.3283
14	A	674.9574	4.0247	16.2616	1.6371
15	A	687.2258	2.8933	7.4322	0.6141
16	A	737.6365	2.8958	12.4931	26.6788
17	A	865.6881	0.5891	26.8899	0.1858
18	A	877.0407	1.9244	76.2013	0.4021
19	A	1115.2058	4.2115	17.5894	4.9319
20	A	1148.9875	2.0058	322.1895	1.6131
21	A	1183.3747	1.6903	113.8951	0.2036
22	A	1255.1212	2.3425	128.8395	2.1746

23	A	1367.0228	6.3508	2.8180	0.2231
24	A	1382.6274	11.6552	12.9000	11.7530
25	A	1433.3357	8.7318	87.5913	0.4409
26	A	1488.0390	9.0253	651.9173	1.6347
27	A	1613.9891	11.1401	2.6598	9.4715
28	A	1648.2633	14.5509	25.7785	3.1603
29	A	3182.2875	6.5214	0.6637	107.8474
30	A	3664.2069	8.4220	87.1975	113.7999

py-15_A_tpssh

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	113.2453	0.1030	0.3125	0.0728
2	A	198.9174	0.2569	0.5543	0.3222
3	A	272.9933	0.5906	2.1071	0.7477
4	A	295.9193	0.4375	0.8732	1.4575
5	A	296.2134	0.5864	1.7000	0.0996
6	A	349.5681	0.6744	8.0269	0.0503
7	A	427.4577	0.2590	42.7579	1.5786
8	A	445.8926	1.3310	1.5313	4.3366
9	A	460.1127	0.4014	18.7706	1.4659
10	A	494.6585	0.2904	61.5405	1.1327
11	A	508.6939	1.7600	6.4449	12.2847
12	A	640.6801	1.3028	18.2732	1.5675
13	A	682.3371	3.1808	1.1824	0.2616
14	A	688.3700	4.1772	16.3696	1.6307
15	A	713.0795	2.9465	9.5643	0.7168
16	A	750.0277	2.9724	12.5042	25.9270
17	A	887.0376	0.6274	27.9017	0.1661
18	A	893.7584	1.9497	73.4220	0.3546
19	A	1141.9929	4.0312	19.4378	4.2603
20	A	1167.6370	1.9728	337.0405	1.5200
21	A	1203.1599	1.7381	90.6472	0.1881
22	A	1272.7055	2.8993	151.3213	1.8480
23	A	1370.3923	5.0885	1.3417	0.6121
24	A	1408.6135	12.9443	9.8221	12.4906
25	A	1458.6093	9.6046	88.4167	0.3350
26	A	1517.4600	9.6942	686.5643	1.8560
27	A	1644.6691	11.7383	1.3314	9.1612
28	A	1673.2219	15.2551	29.6301	4.5111
29	A	3219.3032	6.6769	1.6888	101.8764
30	A	3749.9223	8.8226	105.9083	104.3328

py-15_A_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
-----	------	------------	-------------	-----------	-------------

1	A	117.0709	0.1097	0.3080	0.0574
2	A	204.8000	0.2694	0.5760	0.2876
3	A	286.0873	0.6559	2.1478	0.6284
4	A	302.5218	0.4515	0.9955	1.4317
5	A	309.1293	0.6404	1.7909	0.0839
6	A	360.4281	0.7187	8.1877	0.0513
7	A	432.0980	0.1892	69.5249	1.2520
8	A	459.0918	1.4418	1.3192	4.2564
9	A	470.8909	0.5035	17.7978	2.0902
10	A	500.7018	0.3801	43.4713	0.7313
11	A	521.8892	1.8553	6.1204	10.5184
12	A	661.1272	1.3583	20.3784	1.3307
13	A	704.3613	4.3069	16.9615	1.3377
14	A	711.4601	3.4960	0.7391	0.1863
15	A	746.4754	2.9874	13.3635	0.8106
16	A	767.7182	3.0879	10.9714	25.3810
17	A	910.3114	0.6764	29.1244	0.1915
18	A	918.1898	1.9357	68.5734	0.3058
19	A	1175.3855	2.6307	55.5220	3.5877
20	A	1195.9224	2.0216	330.4175	1.1099
21	A	1219.7978	2.0619	35.2723	0.4647
22	A	1285.3730	6.0849	196.9460	1.6767
23	A	1360.8958	3.1904	3.8815	1.0240
24	A	1450.4422	13.7513	8.8419	14.3810
25	A	1499.2783	11.0911	82.0132	0.1343
26	A	1562.8388	11.0419	738.7277	2.3747
27	A	1696.3129	13.3937	0.6042	7.9258
28	A	1717.8019	16.8622	36.3627	8.0833
29	A	3235.2686	6.7499	2.4131	92.5647
30	A	3870.9597	9.4036	130.4093	87.3287

py-15_A_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.8203	0.1075	0.3223	0.0674
2	A	201.2059	0.2616	0.7300	0.3149
3	A	282.2970	0.6525	2.0336	0.6843
4	A	298.6469	0.4440	0.8959	1.4769
5	A	304.7642	0.6154	1.7238	0.1124
6	A	354.6507	0.6914	8.1045	0.0575
7	A	427.3486	0.2107	58.4940	1.4215
8	A	455.1984	1.4192	1.2957	4.3417
9	A	463.4493	0.3877	26.7969	2.1142
10	A	496.6314	0.3696	42.9115	0.7222
11	A	516.9298	1.8332	6.1297	11.9657
12	A	651.6615	1.3218	19.1947	1.4139
13	A	696.0432	4.2386	18.0036	1.2336
14	A	700.4910	3.3558	1.0031	0.2314

15	A	735.1780	2.8352	12.5835	0.8672
16	A	759.0653	3.0258	11.8277	25.2676
17	A	898.7872	0.6615	27.5259	0.1769
18	A	902.5310	1.9582	73.9845	0.3153
19	A	1153.3724	3.6131	27.1793	3.9417
20	A	1177.3997	1.9217	345.2500	1.4521
21	A	1206.7029	1.7849	62.1011	0.2893
22	A	1275.1312	4.1717	173.3745	1.6252
23	A	1357.0747	3.7352	2.9337	0.8828
24	A	1419.1934	13.2247	8.3803	13.6815
25	A	1470.0501	10.1666	86.9143	0.2612
26	A	1529.3864	9.9832	696.3094	2.1337
27	A	1657.0931	12.1473	0.2688	8.7348
28	A	1681.7178	15.6590	32.7598	6.4290
29	A	3218.5217	6.6744	2.6984	97.2289
30	A	3796.0009	9.0424	124.4508	98.9401

py-15_B_b3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	116.0612	0.1104	0.2329	0.0800
2	A	200.8637	0.2794	1.4981	0.1856
3	A	283.9871	0.6420	3.9201	0.5314
4	A	297.5231	0.3953	4.3296	1.3805
5	A	305.9191	0.5351	5.0570	0.0630
6	A	359.8330	0.8579	0.4686	0.2965
7	A	412.0641	0.1120	114.6836	1.3491
8	A	441.1589	1.2110	1.1516	2.7260
9	A	458.1558	1.6514	0.3493	4.1016
10	A	473.6714	0.5572	2.4895	0.0549
11	A	515.9197	2.0616	2.0348	11.4440
12	A	657.4657	1.2947	3.0606	2.2677
13	A	689.6224	3.7025	15.9089	1.3289
14	A	694.2959	3.1807	0.5477	0.0443
15	A	722.6742	2.8302	11.7628	0.8872
16	A	759.2058	3.0084	11.1678	25.9351
17	A	887.6276	0.6366	30.9175	0.1598
18	A	901.6241	2.5565	182.4265	0.1473
19	A	1130.8611	3.5433	28.7318	4.0996
20	A	1187.5365	2.6125	44.4101	0.3582
21	A	1201.7316	1.4867	50.2686	0.5088
22	A	1272.1256	3.0913	178.4828	1.0796
23	A	1350.8920	3.8994	182.3812	2.0004
24	A	1420.3641	11.2811	9.8194	11.3979
25	A	1476.2732	8.8984	118.0692	1.0887
26	A	1511.2576	9.4920	669.8517	0.7293
27	A	1647.1486	13.5078	25.0993	2.8669
28	A	1669.9808	15.9285	24.8300	12.0041

29	A	3218.1883	6.6745	2.8412	96.3769
30	A	3805.1499	9.0918	120.4525	72.1399

py-15_B_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	120.3424	0.1180	0.2289	0.0705
2	A	205.4077	0.2897	1.4465	0.1783
3	A	286.6445	0.7216	2.7931	0.3597
4	A	304.1945	0.3985	5.2572	1.3417
5	A	312.0189	0.5310	5.9152	0.0817
6	A	366.9004	0.8856	0.5920	0.2690
7	A	383.1268	0.0959	121.6057	1.1278
8	A	451.7799	1.4327	0.0242	3.0720
9	A	462.2126	1.6480	0.4103	3.9635
10	A	476.7930	0.5739	2.3620	0.0920
11	A	519.4872	2.0583	1.7976	9.3136
12	A	663.9294	1.2910	3.2812	2.2321
13	A	702.9906	3.7392	13.7768	1.0194
14	A	703.6135	3.2840	0.2542	0.0193
15	A	735.7018	3.1233	11.6271	0.8155
16	A	772.1185	3.1532	8.6976	25.8487
17	A	901.4319	0.6508	34.4650	0.1765
18	A	927.5434	2.2904	157.9533	0.1926
19	A	1171.2844	1.9356	55.0304	2.3628
20	A	1209.3338	2.2486	9.1542	0.8246
21	A	1216.9748	2.3271	7.5193	0.7817
22	A	1286.3078	6.7642	172.3143	0.4206
23	A	1347.2566	2.7312	232.6895	2.7259
24	A	1473.0593	12.9102	1.8665	13.2917
25	A	1520.6334	11.3105	67.6422	0.3006
26	A	1558.9501	11.9660	785.9855	1.5854
27	A	1698.0600	15.6031	31.6683	1.9010
28	A	1719.9738	17.2425	20.9339	13.2196
29	A	3245.2209	6.7932	5.9519	88.7887
30	A	3870.2814	9.4080	143.5165	66.6115

py-15_B_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	112.1826	0.0983	0.3756	0.0743
2	A	199.8906	0.3159	5.4360	0.1175
3	A	280.3180	0.0540	103.4170	0.8494
4	A	284.7596	0.6225	3.9308	0.4533
5	A	289.2234	0.3732	2.9578	1.1389
6	A	307.4641	0.5563	4.5168	0.0379

7	A	359.9325	0.8738	0.5469	0.2409
8	A	424.4590	0.6369	6.8556	1.2761
9	A	446.8968	0.8982	3.4111	2.2073
10	A	454.6554	1.5929	0.4692	4.1239
11	A	511.4561	2.0239	1.6384	10.2011
12	A	536.7620	1.5053	0.3640	0.8829
13	A	625.8202	2.3997	2.4126	0.0951
14	A	655.6064	1.3144	3.2295	2.3535
15	A	700.3911	3.8535	11.7705	3.2339
16	A	751.6377	2.9189	11.5737	25.0429
17	A	846.2015	0.5301	41.7977	0.0287
18	A	905.9152	2.4443	149.6550	0.2502
19	A	1151.0530	3.0936	29.1736	2.6433
20	A	1195.8419	2.7530	46.2038	0.3053
21	A	1212.0364	1.6761	57.2121	0.2533
22	A	1300.5432	2.0377	191.5865	2.1655
23	A	1430.1943	13.2391	61.6309	9.4377
24	A	1449.3227	8.2068	149.3548	6.6958
25	A	1483.0348	9.0452	67.9506	0.4948
26	A	1531.5488	10.5329	644.9267	1.6423
27	A	1661.2472	14.1747	10.6062	3.2363
28	A	1681.3009	16.8018	16.1470	11.1550
29	A	3253.5739	6.8266	4.0199	92.2986
30	A	3847.9137	9.2977	123.9187	73.6659

py-15_C_b31yp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	115.0346	0.1060	0.3232	0.0685
2	A	200.1317	0.2588	0.7117	0.3141
3	A	282.5106	0.6525	2.0207	0.7061
4	A	297.2886	0.4403	0.9153	1.4708
5	A	304.7713	0.6159	1.7325	0.1131
6	A	353.9964	0.6898	8.0522	0.0559
7	A	426.1031	0.2170	55.5125	1.4536
8	A	454.9058	1.4201	1.2821	4.3596
9	A	462.1737	0.3802	26.4616	2.0025
10	A	495.4901	0.3565	45.2266	0.7712
11	A	517.4862	1.8410	6.1749	12.0407
12	A	650.7409	1.3234	18.9484	1.4290
13	A	695.1741	4.2332	18.2297	1.2479
14	A	697.0691	3.3215	0.9715	0.2275
15	A	731.6276	2.8171	12.4584	0.8353
16	A	759.3584	3.0354	12.1156	25.2609
17	A	894.8673	0.6548	27.4323	0.1785
18	A	900.9697	1.9729	75.6405	0.3149
19	A	1150.0795	3.6805	26.0524	3.9674
20	A	1175.7938	1.9189	344.4833	1.4269

21	A	1205.3350	1.7774	65.3334	0.2825
22	A	1274.1336	4.0337	170.1275	1.6509
23	A	1357.1574	3.7706	3.5087	0.9119
24	A	1417.4202	13.1283	9.2134	13.4129
25	A	1467.5324	10.0512	87.4464	0.2159
26	A	1525.2173	9.8662	688.0520	2.1159
27	A	1652.4223	11.9780	0.4086	8.9323
28	A	1677.4456	15.4750	32.4214	6.1339
29	A	3216.9221	6.6674	2.5548	97.0313
30	A	3788.9343	9.0082	121.4254	99.5879

py-15_C_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	119.2850	0.1139	0.3064	0.0586
2	A	204.5543	0.2657	0.6181	0.3083
3	A	283.1899	0.6575	2.0823	0.5248
4	A	304.2851	0.4595	0.8234	1.4194
5	A	306.2580	0.6208	1.5497	0.0936
6	A	361.0722	0.7214	8.5980	0.0546
7	A	420.1358	0.1463	91.1479	1.0834
8	A	458.8011	1.4188	1.4114	4.2822
9	A	465.9712	0.6420	13.3066	2.7186
10	A	493.5897	0.4521	29.2534	0.5364
11	A	521.2925	1.8440	5.6293	9.8076
12	A	657.3409	1.3239	20.2387	1.2877
13	A	707.1050	4.2806	16.7682	1.0107
14	A	708.4482	3.5091	0.5907	0.1612
15	A	745.0149	3.0998	12.7877	0.8095
16	A	771.9523	3.1318	9.3142	25.3853
17	A	907.8962	0.6669	30.8239	0.1977
18	A	925.4007	1.8126	58.3044	0.3761
19	A	1186.6215	1.6846	68.2081	2.2509
20	A	1197.2090	1.9363	320.5843	1.8472
21	A	1224.5119	3.7594	8.5642	1.0319
22	A	1288.0537	8.9312	183.0106	1.3184
23	A	1353.3522	2.8384	14.0009	0.7776
24	A	1471.5379	14.5017	3.3895	15.3513
25	A	1512.6781	12.3801	92.0440	0.2453
26	A	1574.4217	11.9033	750.9285	2.7169
27	A	1704.9408	14.0076	0.4439	7.2780
28	A	1725.1656	17.2243	34.5329	7.9502
29	A	3243.7236	6.7850	5.4585	90.0469
30	A	3855.4496	9.3299	149.3125	90.2658

py-15_C_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	110.5284	0.1063	0.0548	0.0455
2	A	199.9726	0.2306	0.0867	0.3172
3	A	282.8431	0.6338	2.0513	0.6140
4	A	288.5158	0.4021	0.0366	1.3296
5	A	306.0501	0.6454	1.3654	0.0635
6	A	354.0374	0.7002	8.1678	0.0533
7	A	365.6876	0.0874	124.2516	0.6334
8	A	440.9136	0.7018	3.0566	0.3858
9	A	448.6298	1.1224	1.6829	2.9842
10	A	451.6935	1.3704	1.6187	4.3684
11	A	512.9339	1.8152	5.2929	10.7821
12	A	547.3101	1.9228	3.5684	1.1481
13	A	629.5832	2.8301	0.0833	0.0084
14	A	648.2061	1.3378	18.3511	1.5067
15	A	704.6818	4.3459	14.3877	2.9079
16	A	751.9600	2.9869	13.2503	24.4326
17	A	852.3945	0.5386	36.7973	0.0274
18	A	905.4389	1.9578	62.3778	0.4266
19	A	1168.2355	3.3880	7.2968	1.9211
20	A	1183.6190	1.9313	314.7580	1.6765
21	A	1216.0189	2.0151	74.1823	0.1656
22	A	1303.1283	2.3192	145.0445	1.3666
23	A	1430.8510	13.2386	4.5873	10.8637
24	A	1452.2017	9.9258	18.7397	7.8178
25	A	1478.2235	9.5761	85.6504	0.2773
26	A	1543.2414	10.7334	694.5264	3.2375
27	A	1664.9792	13.0780	4.4449	8.6645
28	A	1691.3716	15.9206	15.9660	5.3906
29	A	3251.9923	6.8180	3.6225	93.0678
30	A	3827.0354	9.1906	128.9763	93.2724

py-15_D_b31yp

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	109.8245	0.1186	2.0531	0.2486
2	A	166.8035	0.2096	4.5357	0.9353
3	A	269.1859	0.3510	0.8477	1.2401
4	A	278.7797	0.8106	0.6191	0.7559
5	A	314.0197	0.9598	0.4216	0.3042
6	A	350.6515	1.0223	8.3570	0.9048
7	A	382.0755	0.5586	3.3061	2.3954
8	A	434.4338	1.4369	1.8543	3.5088
9	A	437.9640	0.4062	2.8476	0.0290
10	A	497.2071	1.9579	0.7251	11.5526
11	A	597.6177	0.2525	69.4050	0.3302
12	A	647.5156	2.5665	8.9478	2.3326

13	A	659.6918	1.3606	2.3093	2.2909
14	A	704.4516	2.7259	26.7674	6.1597
15	A	742.5652	3.1087	36.6859	14.4027
16	A	749.5507	3.4545	17.2944	0.6021
17	A	885.9168	1.5590	71.5300	0.3244
18	A	892.6502	0.6482	36.3415	0.8112
19	A	1143.9384	6.3349	108.8856	9.4130
20	A	1173.4876	1.7684	29.6793	5.2730
21	A	1221.8744	3.4888	83.1389	4.0022
22	A	1285.2628	7.6960	93.0816	18.2732
23	A	1299.8021	1.8486	100.1308	13.3880
24	A	1435.3360	7.2999	37.3619	10.5121
25	A	1492.3224	5.6737	50.5394	30.9566
26	A	1623.2080	10.3368	37.4208	54.4045
27	A	1717.5590	13.2433	554.2272	27.3459
28	A	1776.3681	20.1005	394.8272	33.7661
29	A	3205.7215	6.6155	2.3685	106.4393
30	A	3589.1366	8.1797	110.6068	78.0277

py-15_D_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	111.3125	0.1215	1.9784	0.2598
2	A	169.1135	0.2145	4.2826	0.9925
3	A	275.3379	0.3634	0.9696	1.1559
4	A	278.3401	0.8024	0.7483	0.6027
5	A	316.5101	0.9710	0.4047	0.3828
6	A	356.8831	1.0522	9.0215	0.9408
7	A	389.3743	0.4942	4.1954	2.1537
8	A	436.3422	1.4329	2.2551	3.1198
9	A	441.9539	0.4532	2.0955	0.0458
10	A	502.5267	1.9582	0.5067	9.8667
11	A	601.7392	0.2572	75.4065	0.4191
12	A	656.4894	2.7850	9.3782	2.5122
13	A	665.8371	1.3730	3.2151	2.2724
14	A	713.8199	2.7608	25.2603	5.5119
15	A	749.9932	3.1722	34.5322	11.6953
16	A	757.1951	3.6676	16.0003	0.7496
17	A	902.8703	0.6560	41.3509	0.9731
18	A	905.8418	1.4574	63.8551	0.6140
19	A	1191.3949	1.4882	59.9332	2.8293
20	A	1195.4426	4.2204	76.6677	13.0208
21	A	1251.8330	6.5070	71.5762	7.4443
22	A	1313.6726	2.4938	39.2568	1.0924
23	A	1323.7915	4.5249	146.2960	46.1141
24	A	1470.1260	8.0056	55.7302	7.1836
25	A	1530.5061	7.2862	64.0057	36.2363
26	A	1677.2015	12.4286	54.3424	69.2566

27	A	1776.9592	15.7662	583.3664	27.0081
28	A	1836.3361	22.3407	442.2118	34.6092
29	A	3234.0004	6.7388	5.4644	96.4956
30	A	3610.2224	8.2782	134.8425	73.4545

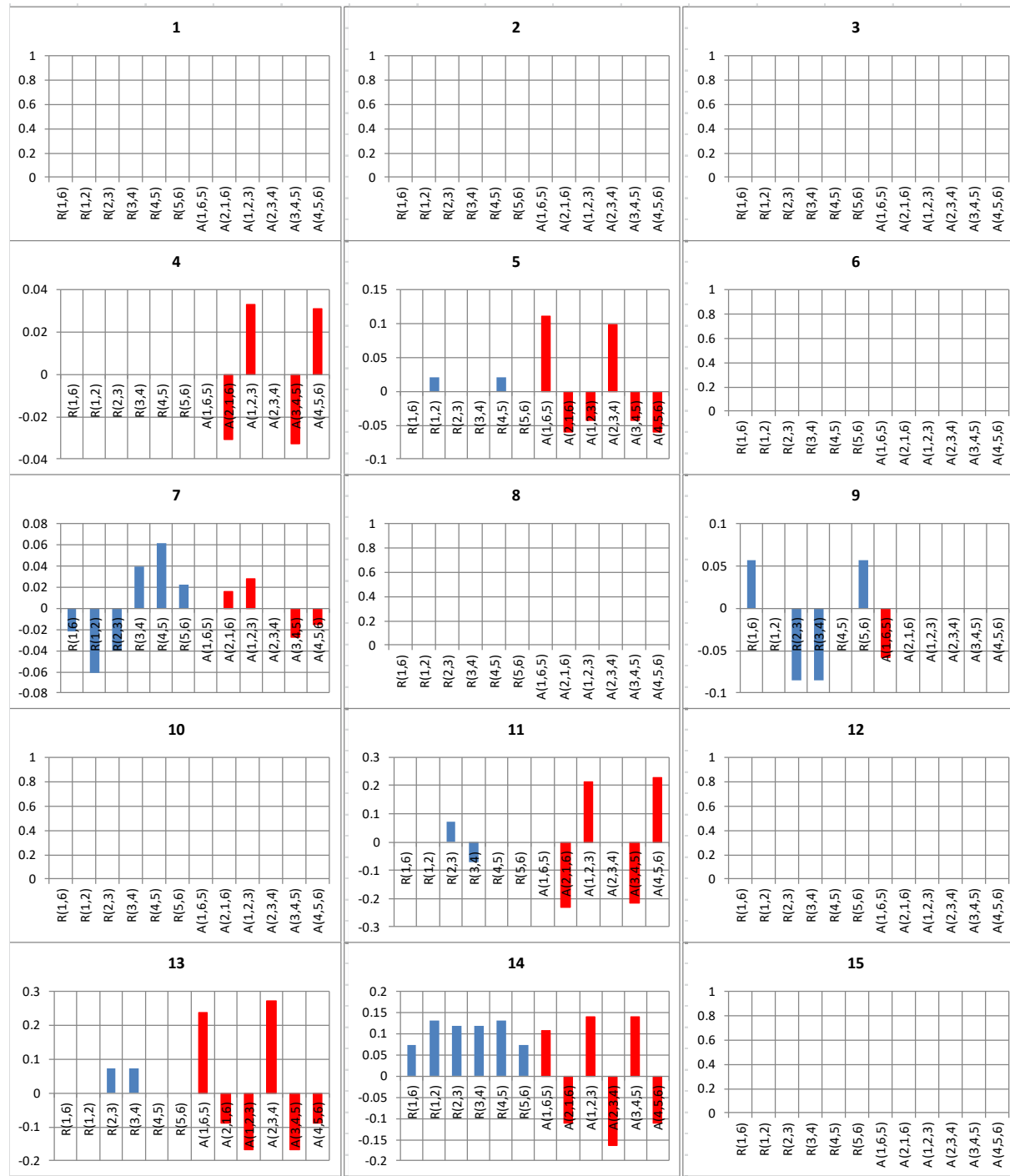
py-15_D_mp2

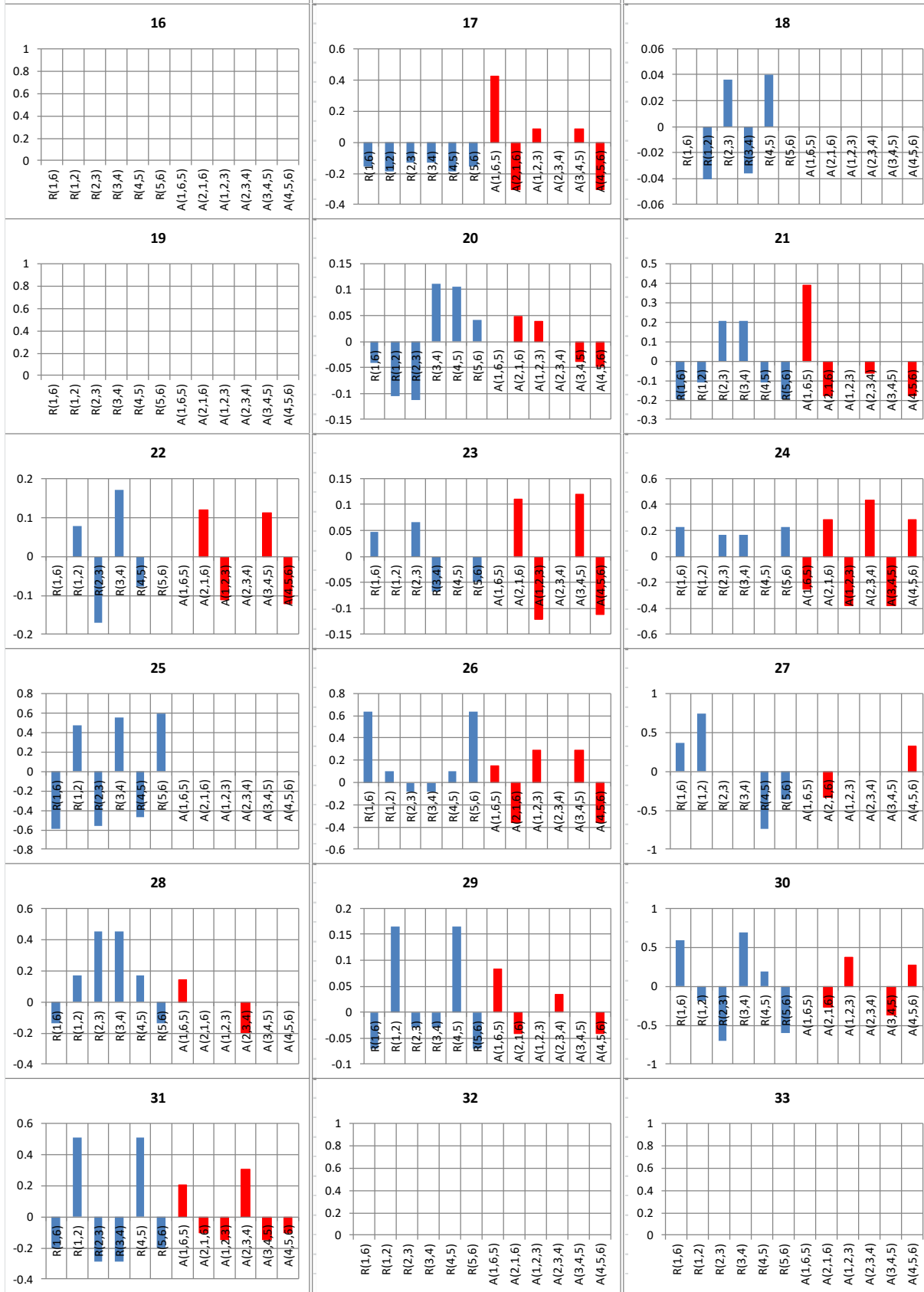
NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	24.8229	0.0053	0.1626	0.5989
2	A	136.4577	0.1833	0.0943	0.1151
3	A	222.2968	0.2261	9.1898	1.3052
4	A	277.2651	0.7974	0.7645	0.7148
5	A	315.8646	0.9684	0.4260	0.7851
6	A	348.6599	1.0097	8.3852	1.0636
7	A	358.5352	0.3919	8.3706	2.6525
8	A	409.6260	0.6156	0.5320	0.3420
9	A	431.4734	1.3782	1.8693	3.4401
10	A	453.5146	0.9615	3.4969	1.3903
11	A	495.2440	1.9335	0.8329	11.9608
12	A	572.6949	0.2326	73.5602	0.2219
13	A	648.3728	2.4694	1.8878	0.4412
14	A	654.2797	1.3846	2.1062	2.6407
15	A	702.9357	2.7192	24.8477	5.0211
16	A	739.2169	3.0888	30.3324	12.9107
17	A	850.5778	0.5506	47.1222	0.2496
18	A	889.4712	1.5482	60.3152	0.4417
19	A	1178.2075	3.0046	123.0514	9.0215
20	A	1194.7925	2.2227	20.0786	13.1482
21	A	1232.0010	3.6549	80.5646	2.9039
22	A	1306.0198	1.9793	52.7174	0.5071
23	A	1334.6369	6.8123	90.4349	66.8559
24	A	1458.6707	8.2644	28.5509	9.4499
25	A	1508.1041	6.7347	57.4169	64.7078
26	A	1634.0666	11.5184	4.8944	38.0370
27	A	1722.7948	13.2279	618.0570	95.9798
28	A	1787.2085	20.4016	284.7243	49.8074
29	A	3243.0781	6.7741	3.6727	101.7090
30	A	3603.2229	8.2449	118.5715	77.1010

D Composition of the vibrational normal modes as a function of the internal coordinates

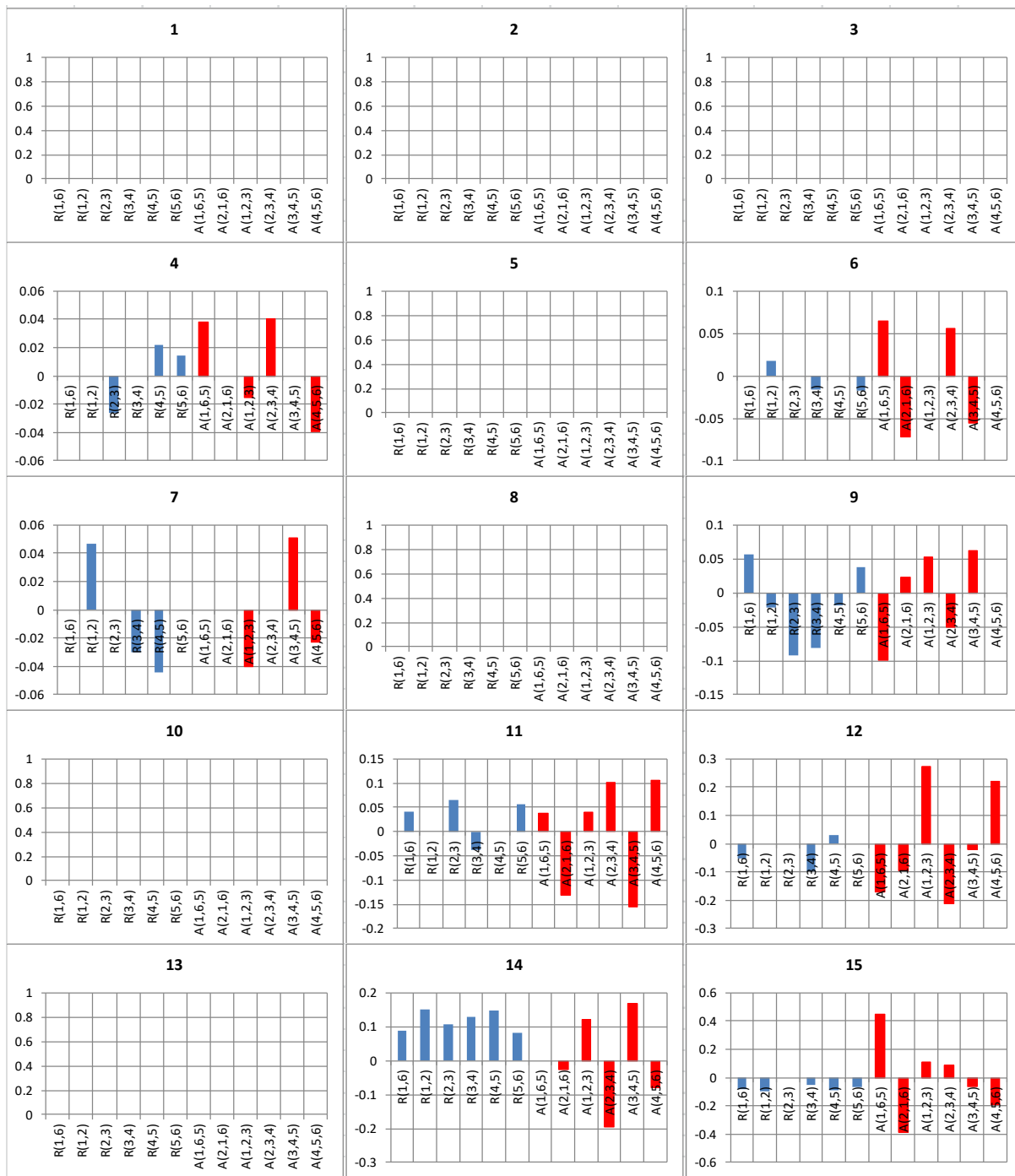
Level of theory: DFT B3LYP[GD3BJ] / 6-311++G**

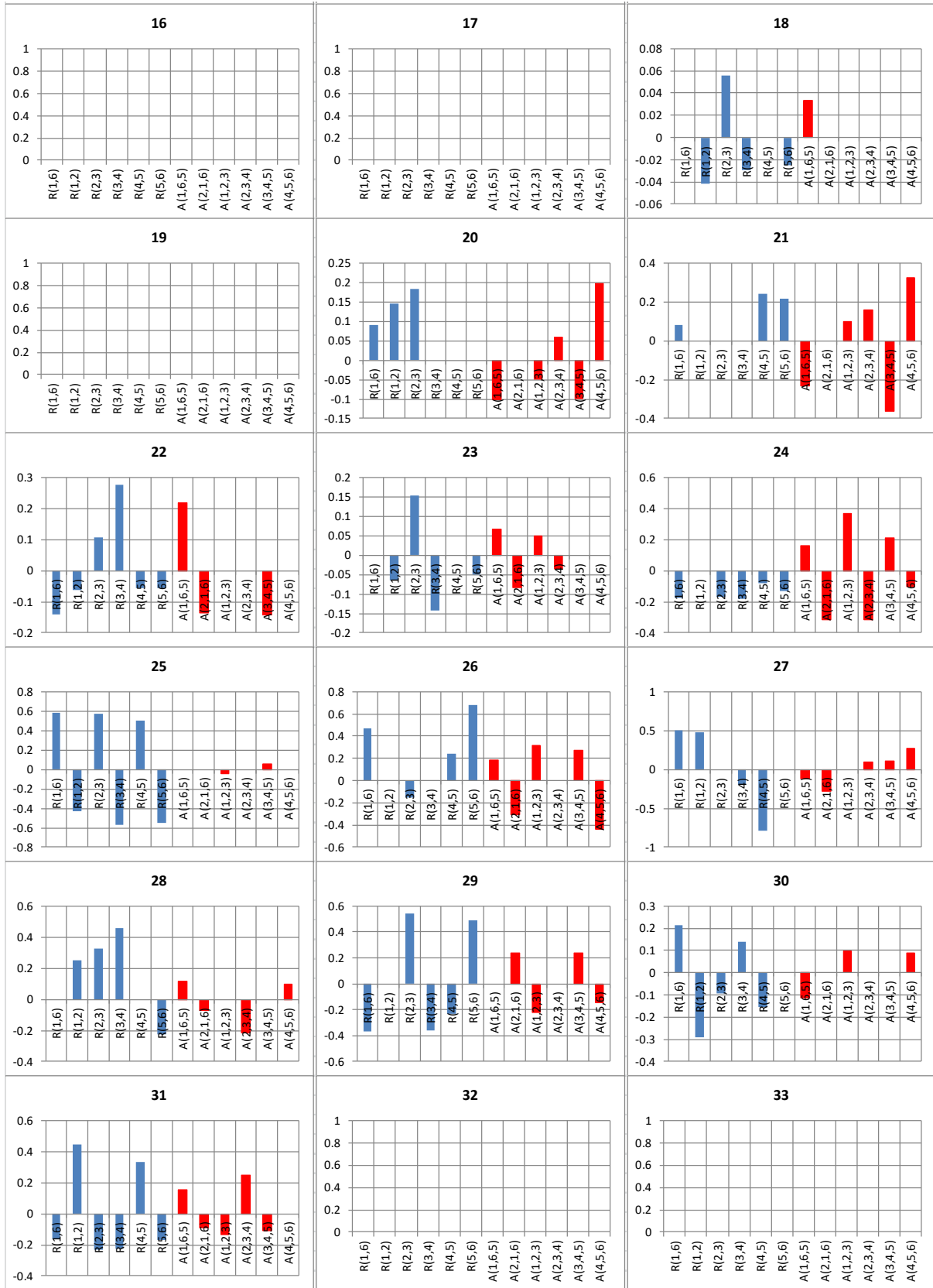
Molecule 1



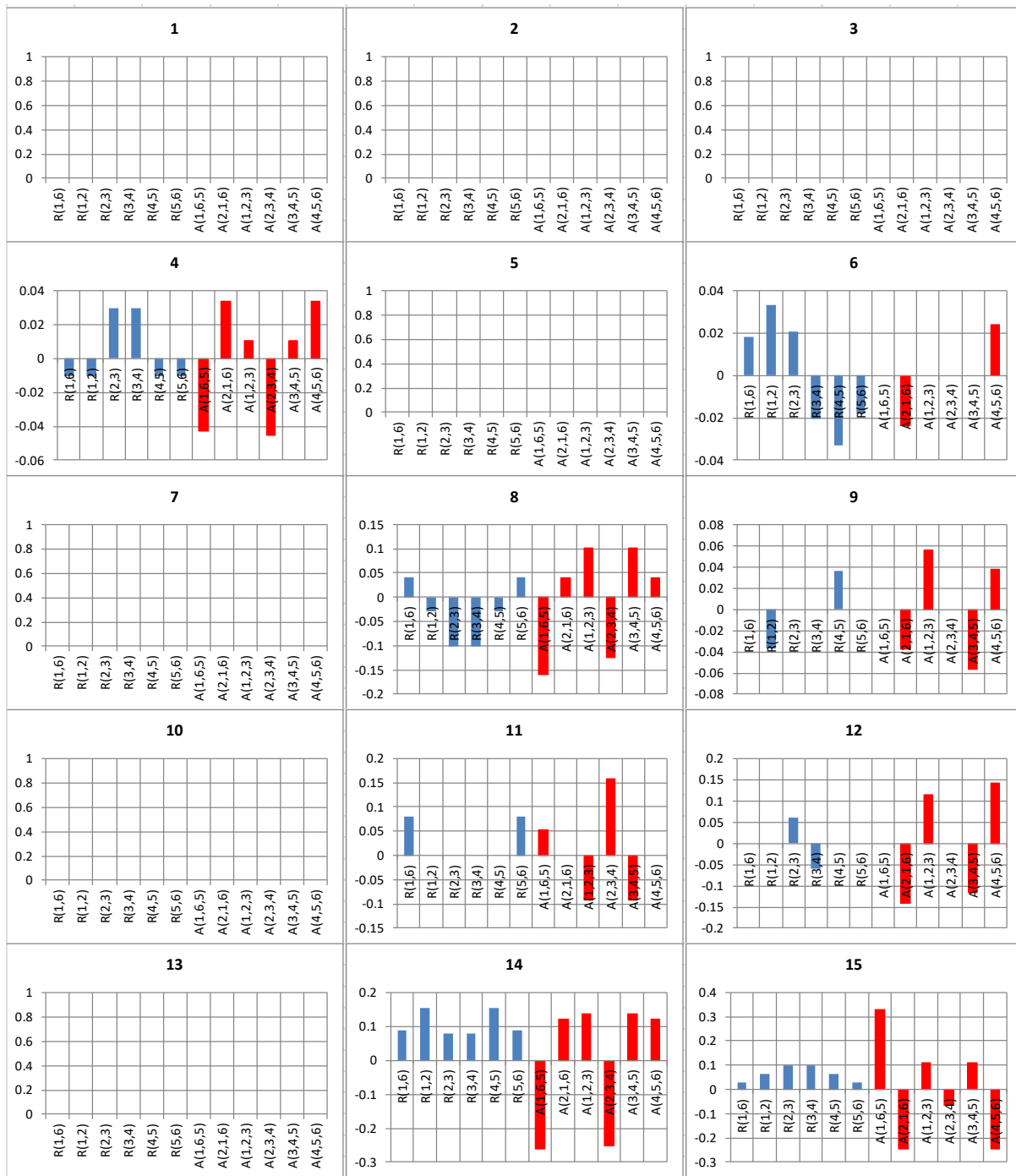


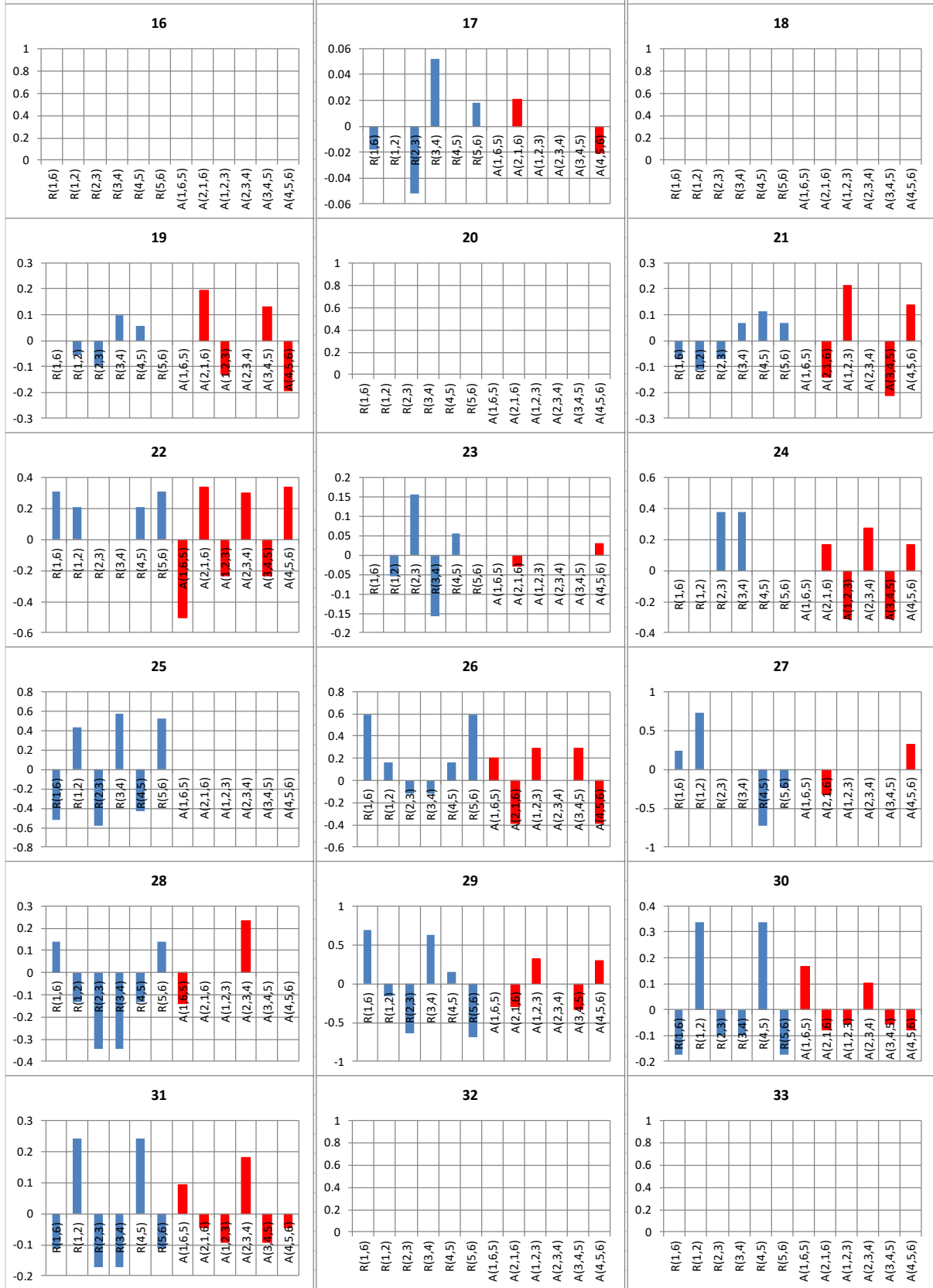
Molecule 2



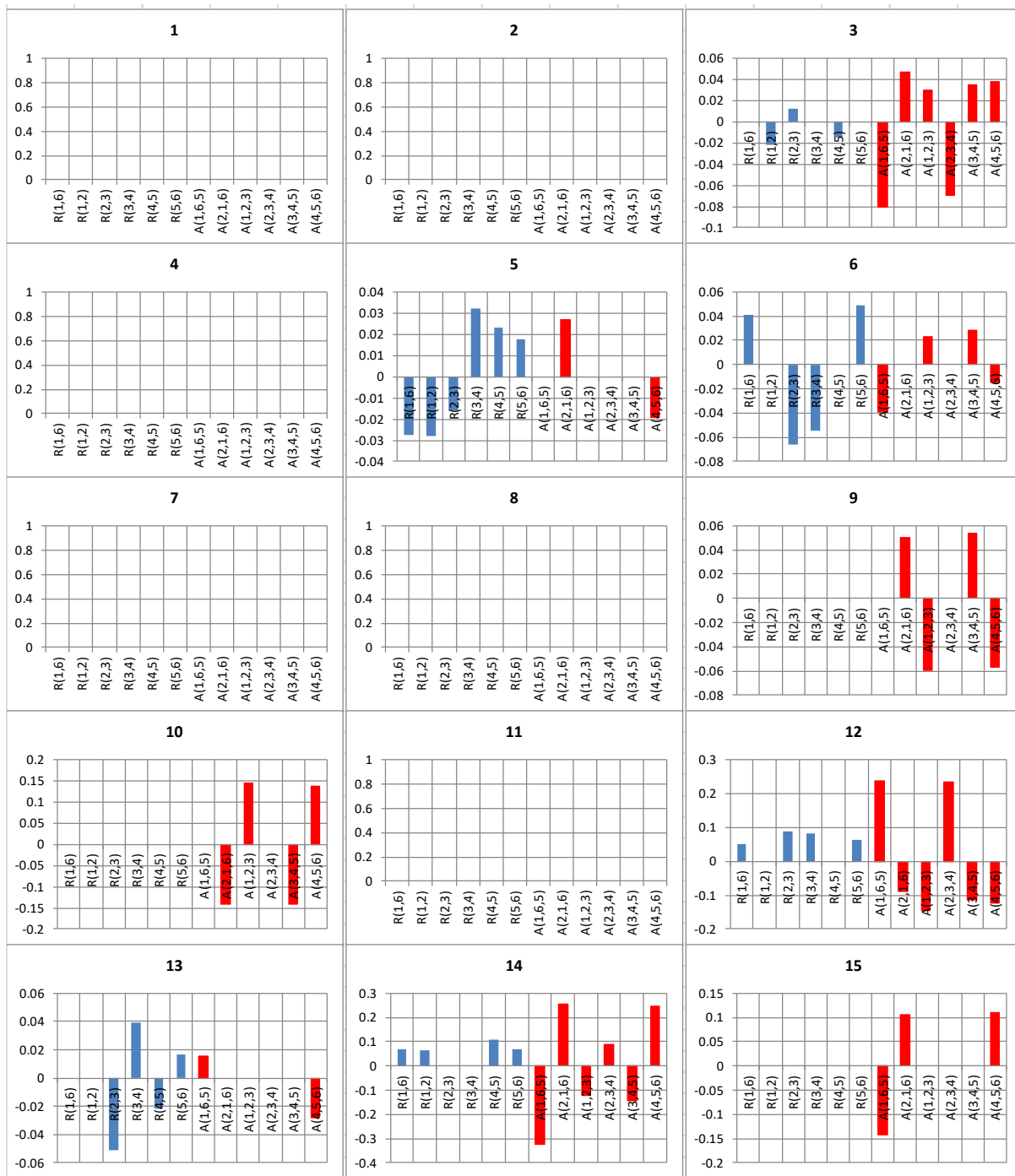


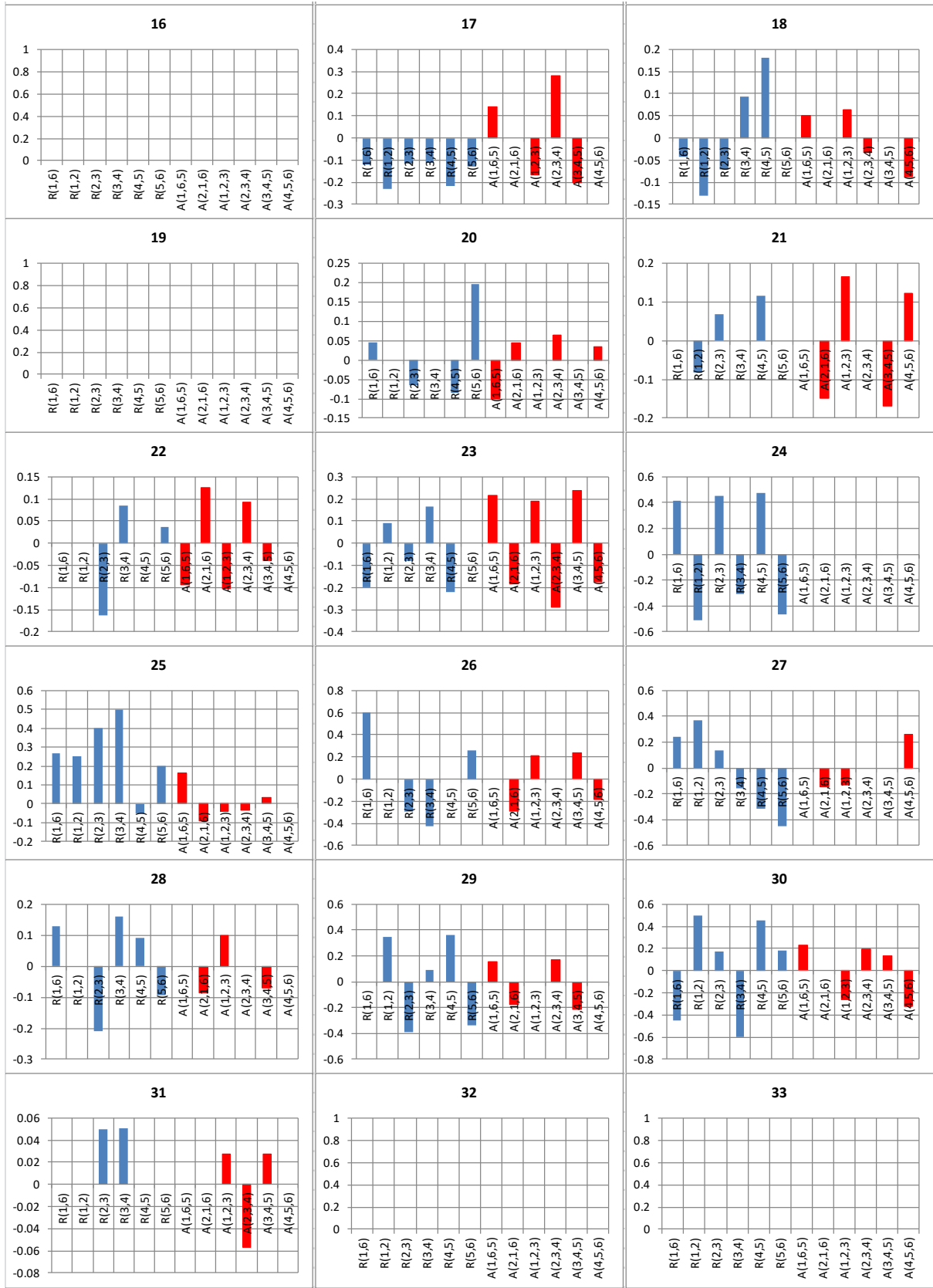
Molecule 3



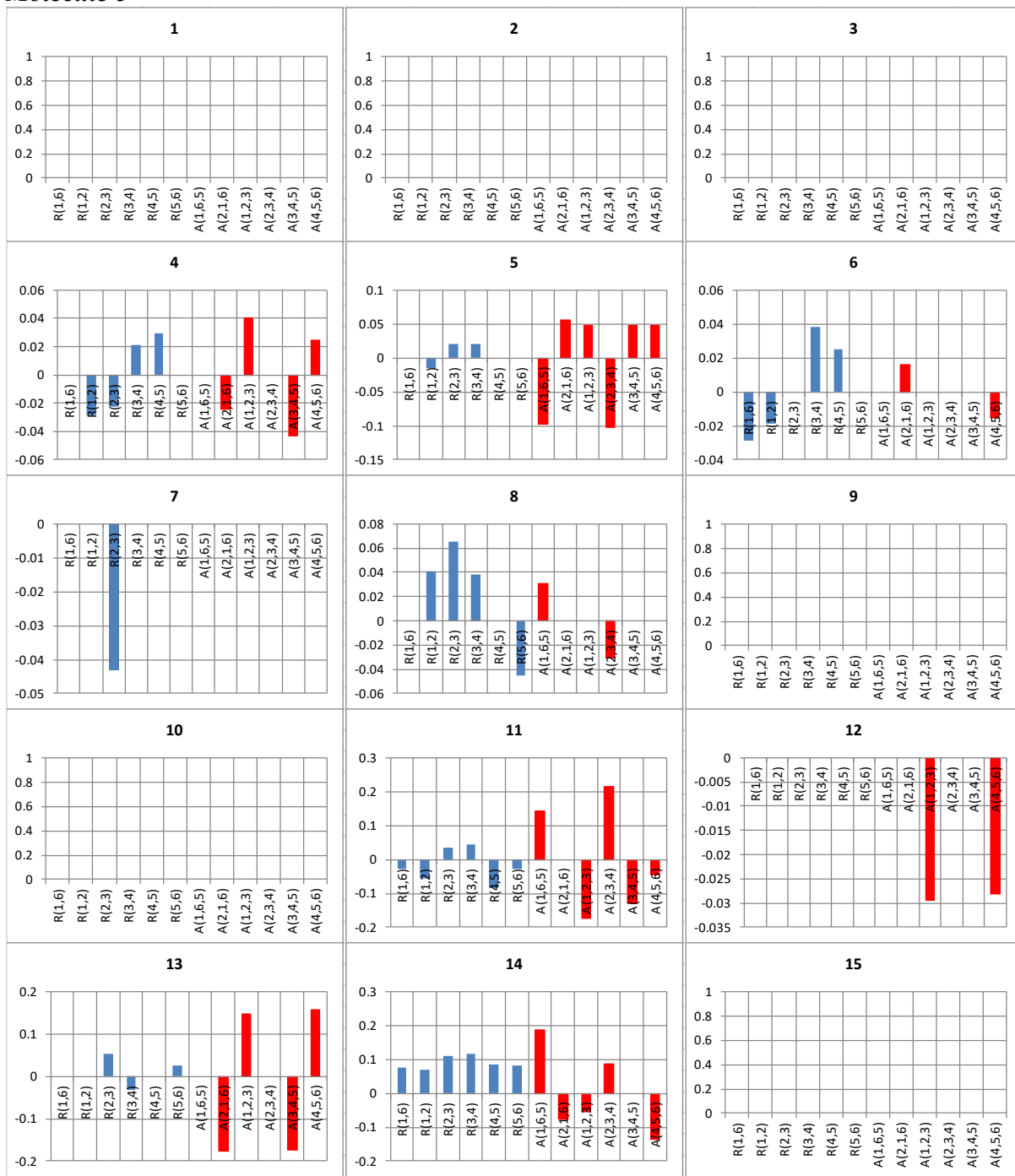


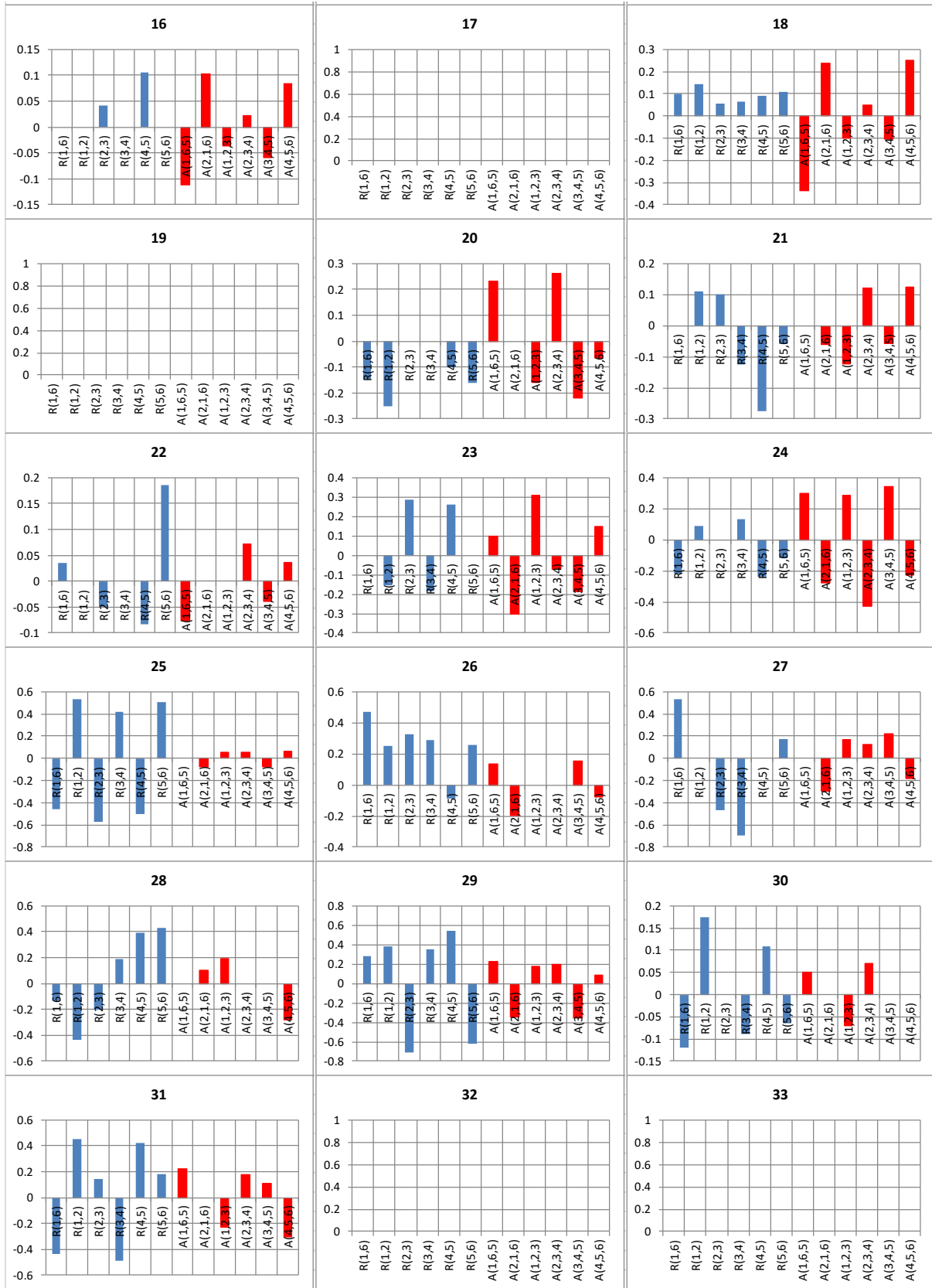
Molecule 4



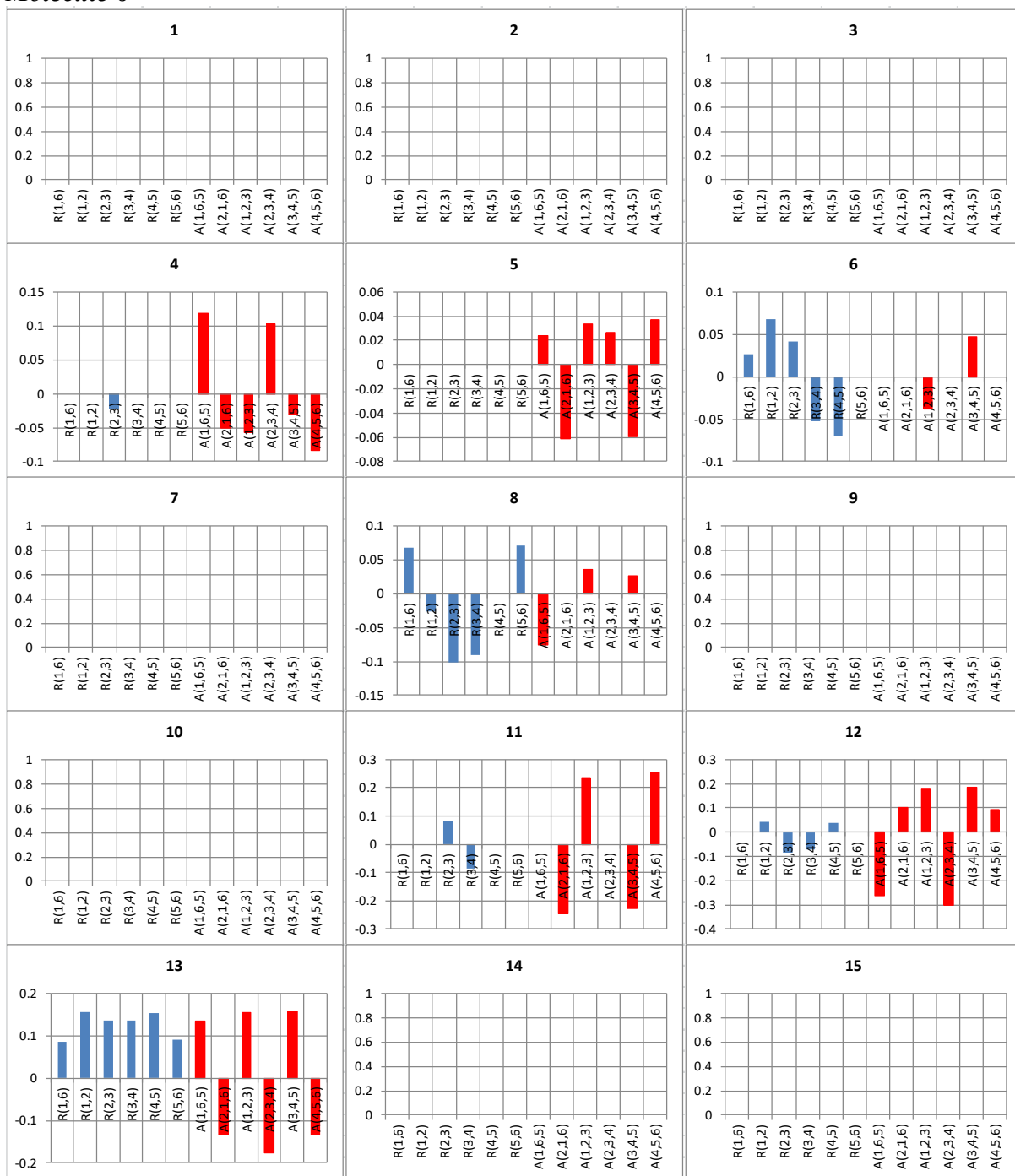


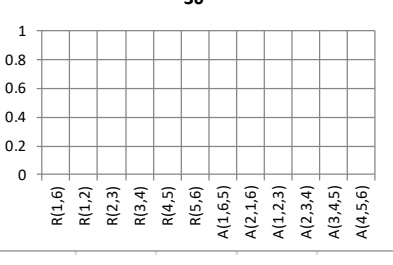
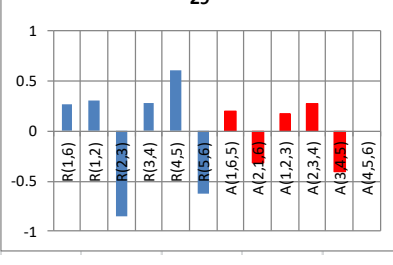
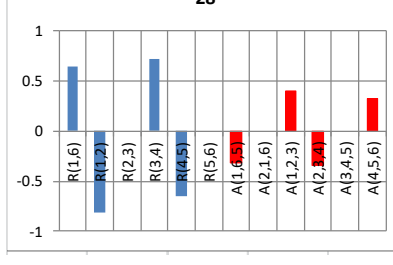
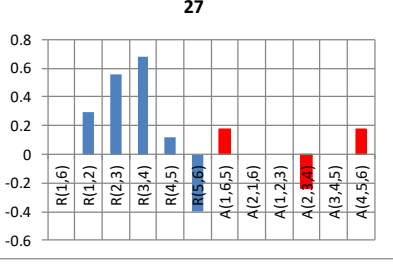
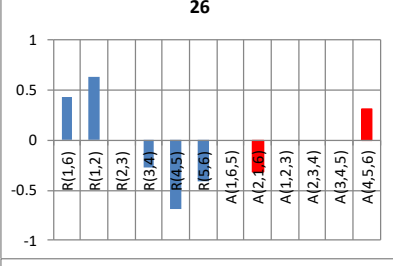
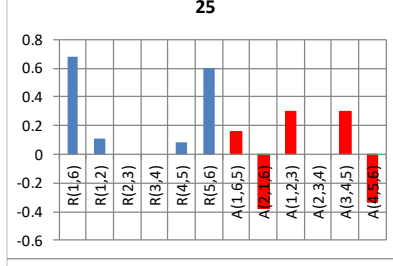
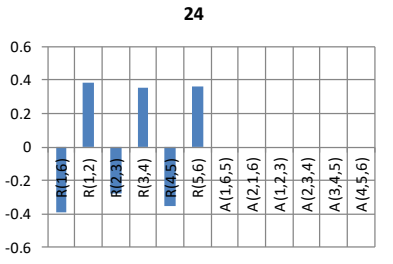
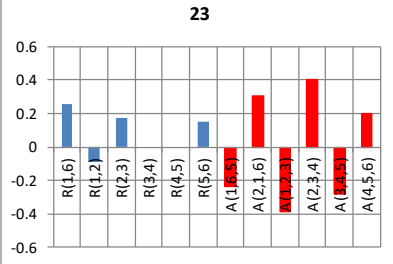
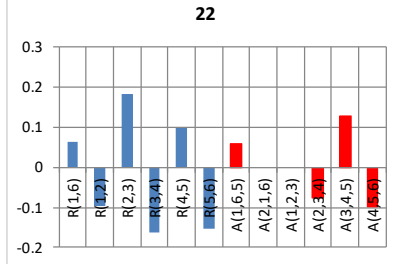
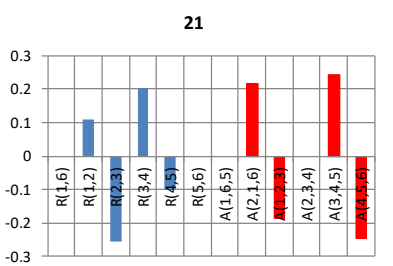
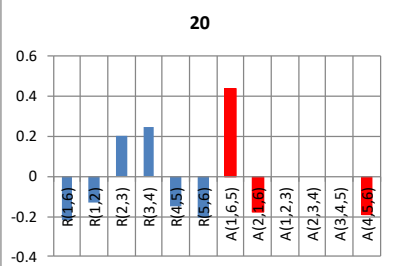
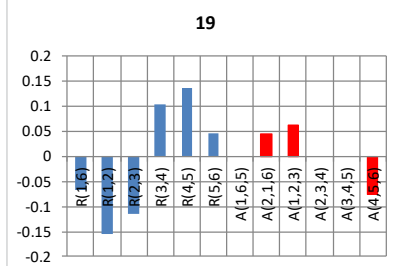
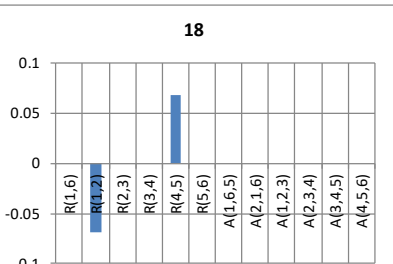
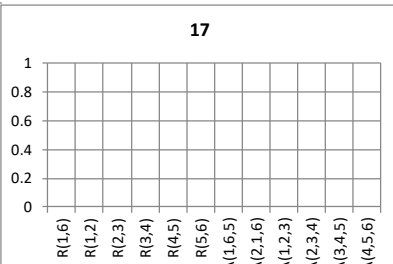
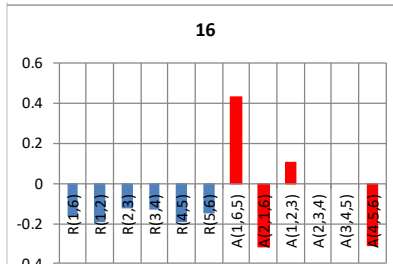
Molecule 5



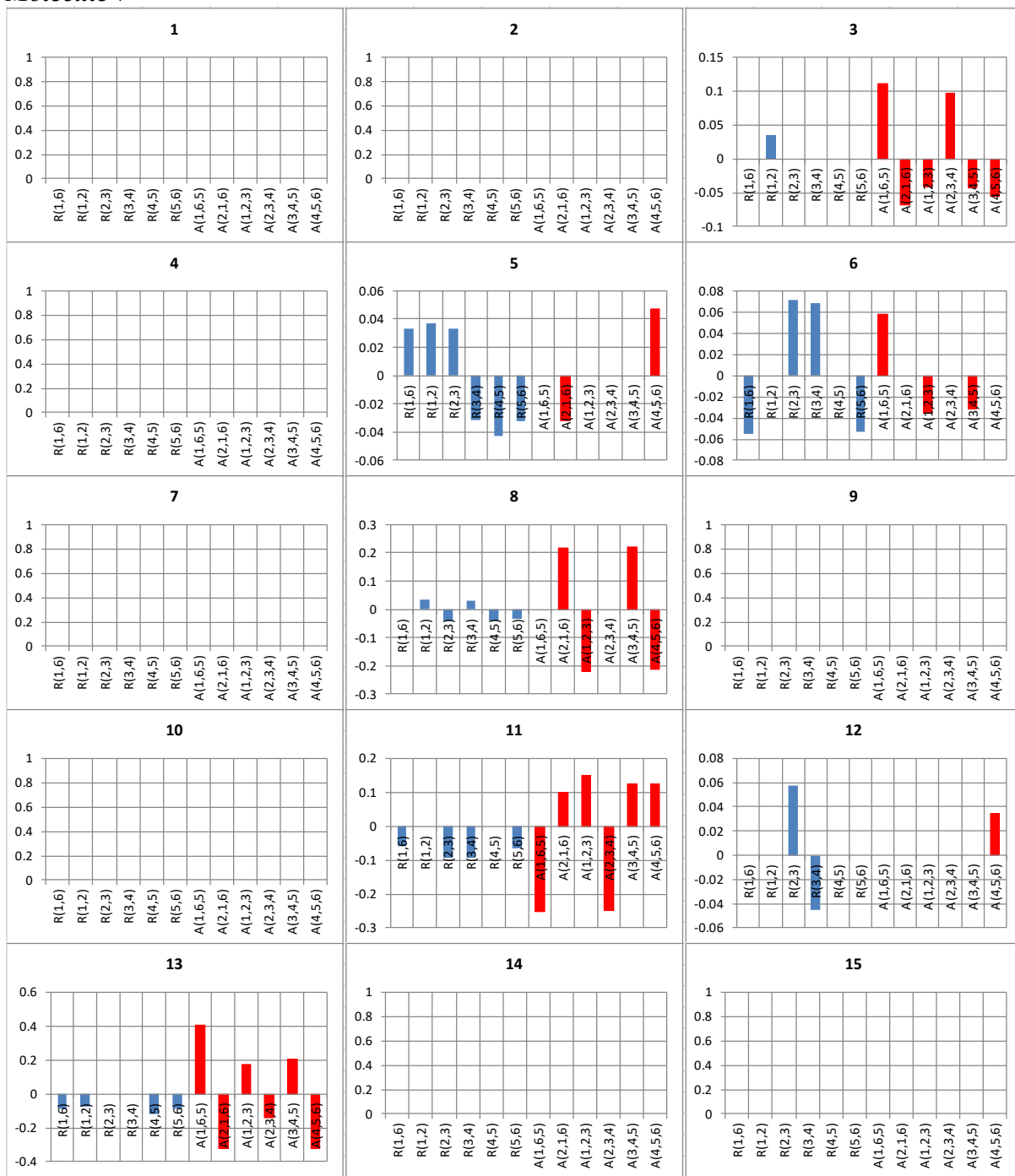


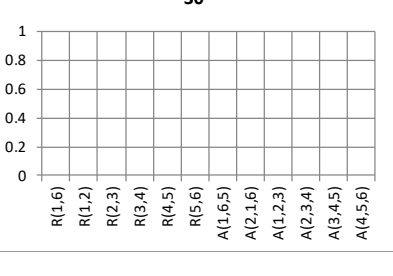
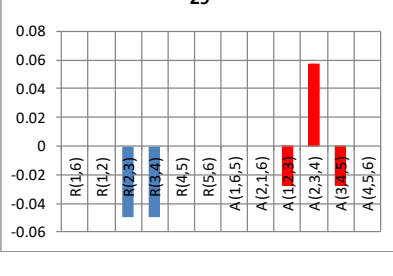
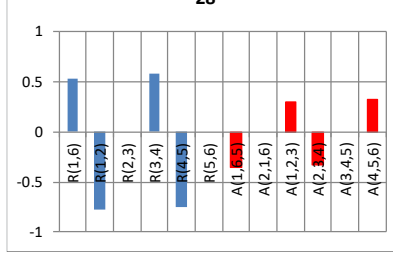
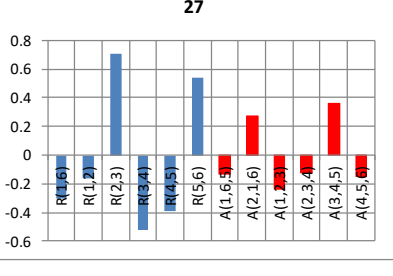
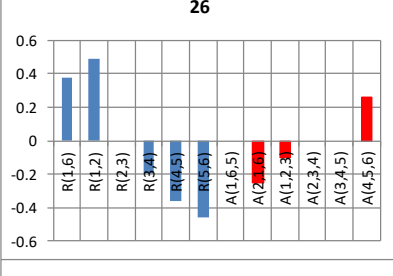
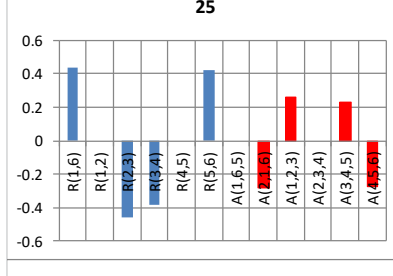
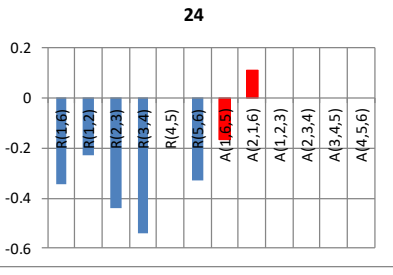
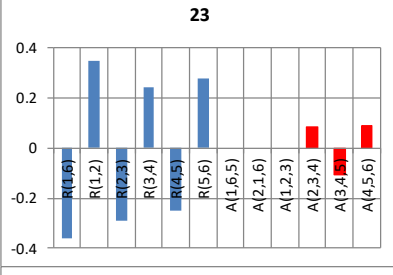
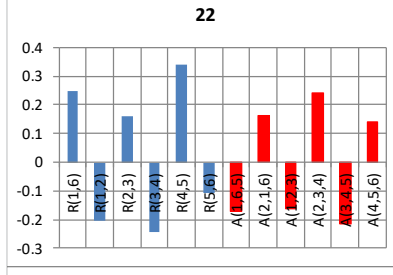
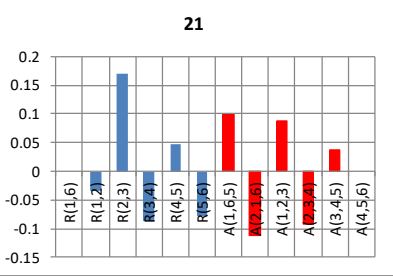
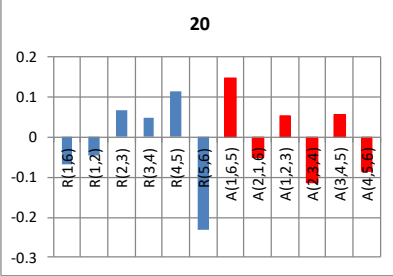
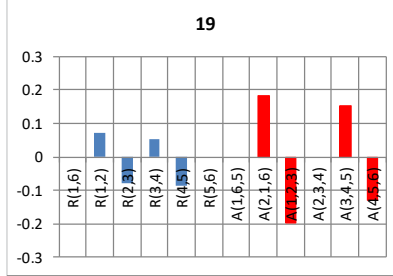
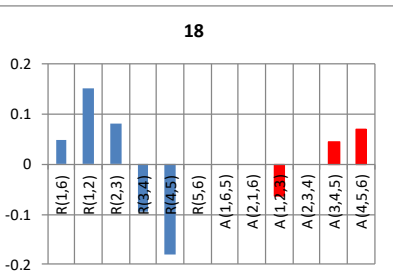
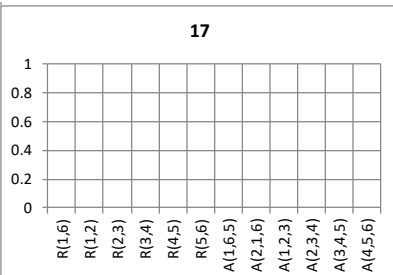
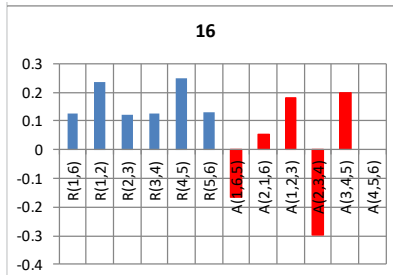
Molecule 6





Molecule 7





E Optimised Geometries of aggregates

01_hb

7	2.599090	10.164742	1.851303
7	1.645887	6.122583	2.205000
6	1.963192	7.432502	2.101524
6	1.092771	8.450918	2.522906
6	1.459368	9.772733	2.374414
6	3.429499	9.227694	1.451855
6	3.175898	7.874136	1.548004
9	4.065869	6.953721	1.124648
9	-0.091258	8.097196	3.070766
9	0.613521	10.725806	2.784314
9	4.591497	9.627072	0.920917
1	2.319799	5.396436	1.991574
1	0.805460	5.856551	2.689645
7	3.137472	3.468503	1.802269
7	4.212972	-0.547944	1.593087
6	3.854694	0.757973	1.645712
6	4.691008	1.781197	1.175508
6	4.288826	3.097933	1.277570
6	2.338041	2.521558	2.246045
6	2.633609	1.175983	2.196523
9	1.781062	0.241506	2.659992
9	5.874329	1.442249	0.628834
9	5.091018	4.057710	0.827139
9	1.172068	2.914529	2.771773
1	3.541514	-1.259231	1.828699
1	5.039650	-0.817342	1.086655

01_pi

7	2.422816	11.070939	2.225164
7	2.156287	7.057939	1.118371
6	2.243705	8.366877	1.480760
6	1.189146	9.039283	2.115331
6	1.333995	10.369758	2.456350
6	3.426712	10.452148	1.645706
6	3.403090	9.125945	1.266102
9	4.452074	8.546761	0.649911
9	0.044448	8.369990	2.346191
9	0.314908	11.001979	3.042106
9	4.523391	11.177664	1.390012
1	2.807834	6.732479	0.420051
1	1.230985	6.659667	1.066196
7	2.123756	8.857910	-1.876240
7	2.390283	12.870914	-0.769458
6	2.302868	11.561974	-1.131843
6	1.143482	10.802907	-0.917185
6	1.119860	9.476703	-1.296782

6	3.212577	9.559089	-2.107425
6	3.357426	10.889567	-1.766413
9	4.502123	11.558859	-1.997277
9	0.094499	11.382092	-0.300991
9	0.023183	8.751186	-1.041089
9	4.231666	8.926867	-2.693178
1	3.315585	13.269185	-0.717288
1	1.738742	13.196370	-0.071132

02_h1

17	-0.119911	5.377943	1.002960
7	2.099378	3.140191	3.442878
9	1.878307	5.365436	3.193924
6	1.523001	4.134722	2.807982
7	-0.668633	2.443363	0.410032
1	-1.134128	3.181437	-0.102691
1	-0.890153	1.492231	0.169783
9	0.538045	0.374267	1.739128
6	0.593087	3.998284	1.788792
9	2.346044	0.907138	3.719912
6	0.224157	2.695821	1.388132
6	0.852292	1.644948	2.079935
6	1.761302	1.923204	3.075786
17	-4.698218	1.474357	-4.003517
7	-2.524440	3.820699	-1.628755
9	-2.700019	1.586904	-1.814327
6	-3.083034	2.798067	-2.237832
7	-5.301089	4.384212	-4.676220
1	-5.738188	3.606580	-5.141040
1	-5.551454	5.321283	-4.941909
9	-4.136995	6.506982	-3.403280
6	-4.014027	2.888923	-3.258358
9	-2.319586	6.063673	-1.410465
6	-4.403268	4.175070	-3.689034
6	-3.798019	5.257176	-3.028637
6	-2.883170	5.026589	-2.025325

02_h2

9	8.991910	13.568271	2.692715
6	8.845659	12.460748	3.455650
6	9.981296	11.920253	4.081553
6	9.757673	10.767565	4.864732
17	11.089432	10.010925	5.694443
7	11.201102	12.476527	3.915576
1	11.987883	12.131457	4.439239
1	11.304250	13.351453	3.428931
17	11.246270	15.750388	2.196306
7	15.102215	15.917554	3.182103

7	12.411056	18.372717	1.162907
1	11.434623	18.139238	1.098126
1	12.714616	19.285097	0.867886
9	13.501450	14.369071	3.523477
9	15.017412	19.120375	1.535497
9	16.732691	17.451846	2.860547
6	14.605572	17.931164	2.021273
6	13.263698	17.562848	1.831757
6	13.853396	15.562634	3.014612
6	15.462858	17.084236	2.690853
6	12.887273	16.313044	2.364310
7	7.417931	10.787154	4.355604
9	8.247366	9.177070	5.690153
9	6.551028	12.395226	3.019814
6	8.466944	10.268103	4.950600
6	7.616645	11.862301	3.625762

02_p1

17	-0.125092	2.789400	5.114680
7	2.416788	0.625819	2.946052
9	2.515313	1.451163	5.035732
6	1.836286	1.325848	3.894296
7	-1.339896	2.332806	2.359083
1	-1.878702	2.619194	3.162140
1	-1.861987	2.020447	1.555332
9	-0.104715	0.882754	0.388305
6	0.586152	1.919491	3.789082
9	2.345715	-0.239090	0.855155
6	-0.117223	1.785726	2.575202
6	0.530158	1.054790	1.565558
6	1.766231	0.500533	1.810435
17	1.224065	-1.654460	5.880833
7	-2.206334	-0.408474	4.291789
9	-1.323664	-0.220513	6.351699
6	-1.209567	-0.678617	5.103989
7	1.101645	-2.578857	2.981169
1	1.956524	-2.538838	3.514846
1	1.198337	-2.705818	1.985833
9	-0.995305	-2.018777	1.307432
6	-0.067898	-1.384274	4.750500
9	-3.118315	-0.558790	2.225231
6	0.036521	-1.869069	3.431332
6	-1.049651	-1.591285	2.585274
6	-2.115383	-0.861109	3.060774

02_p2

17	-0.863005	4.094453	-1.158422
7	0.464036	4.880834	2.510723

9	-0.059202	6.194635	0.758763
6	0.041501	4.961155	1.272916
7	-0.573173	1.460004	0.366753
1	-1.111402	1.546529	-0.480872
1	-0.686807	0.607531	0.892486
9	0.298713	1.312138	2.955588
6	-0.318672	3.880336	0.483096
9	0.974468	3.594811	4.299142
6	-0.247599	2.589518	1.044812
6	0.211907	2.521137	2.369688
6	0.547780	3.678553	3.040087
17	-4.037100	2.615920	-0.057310
7	-2.905484	2.098152	3.723355
9	-3.498335	0.662414	2.093507
6	-3.300041	1.928560	2.485326
7	-3.419756	5.349474	1.166221
1	-3.489224	5.196557	0.172523
1	-3.034133	6.231665	1.464636
9	-2.584615	5.683842	3.749797
6	-3.503276	2.947824	1.567989
9	-2.280081	3.508273	5.376614
6	-3.254115	4.273629	1.976583
6	-2.837255	4.437757	3.307149
6	-2.683850	3.333797	4.119306

02_p3

17	10.512006	13.127173	5.787057
7	13.262880	13.784595	4.657422
1	12.636565	14.481092	5.031258
1	14.041962	14.128711	4.118598
9	14.646248	12.111613	2.982047
6	13.442282	11.717290	3.447521
6	12.732956	12.586529	4.288918
6	11.478919	12.127992	4.736281
17	13.206476	14.937359	1.310723
7	11.129946	16.179682	3.163466
1	11.876650	16.708313	2.738045
1	10.383677	16.723175	3.570196
7	10.054476	12.511964	1.498761
9	12.030853	12.362145	0.433706
9	8.667316	15.068034	3.620829
9	8.056212	12.625291	2.550411
6	9.535969	14.411587	2.826210
6	10.778173	15.002352	2.563077
6	11.214611	13.058252	1.227250
6	9.235504	13.180628	2.280330
6	11.640957	14.286767	1.713767
7	11.729500	10.073404	3.537276
9	9.860750	10.433741	4.737931

9	13.588439	9.681645	2.310362
6	11.049621	10.874768	4.321664
6	12.899300	10.494634	3.111320

02_p4

17	0.085456	3.906013	-0.165570
7	1.759557	4.906741	3.305161
9	0.884283	6.121792	1.625646
6	1.178328	4.915398	2.129897
7	0.991900	1.360288	1.258847
1	0.768150	1.392976	0.276864
1	1.451098	0.528937	1.596293
9	2.184735	1.355851	3.720871
6	0.875000	3.788829	1.381389
9	2.665897	3.721522	5.004997
6	1.228314	2.528413	1.905466
6	1.831953	2.534584	3.173279
6	2.071316	3.732004	3.811870
17	3.526848	3.050353	-0.947864
7	5.204335	1.961647	2.494080
9	4.445397	0.789756	0.726860
6	4.649298	1.981071	1.307525
7	4.088869	5.554866	0.701274
1	3.495116	5.545426	-0.112775
1	4.040775	6.368640	1.293998
9	5.229283	5.493005	3.189556
6	4.251540	3.125723	0.634038
9	5.960826	3.102075	4.294061
6	4.435538	4.371113	1.267424
6	5.031933	4.332071	2.537704
6	5.392436	3.120403	3.089563

02_p5

17	9.768098	18.052088	5.053147
7	10.420529	15.315106	6.250593
1	10.340055	15.474616	5.258764
1	10.816572	14.434125	6.538764
7	10.932329	18.552134	8.826284
9	10.311308	19.994494	7.212865
9	11.283873	14.969223	8.823347
9	11.585977	17.135501	10.462970
6	11.016307	16.216270	8.392329
6	10.585001	16.386445	7.067136
6	10.524182	18.727289	7.593446
6	11.168338	17.315597	9.210995
6	10.320601	17.712989	6.670700
17	12.944471	16.608751	3.912644
7	14.314100	15.807179	7.562807

7	13.226744	19.234431	5.454224
1	12.681010	19.149444	4.611254
1	13.111047	20.082074	5.987265
9	13.784853	14.501671	5.806450
9	14.122802	19.371004	8.035427
9	14.831193	17.084542	9.355511
6	14.040510	18.165587	7.441554
6	13.568592	18.102872	6.120769
6	13.880105	15.732207	6.328634
6	14.392818	17.006263	8.100126
6	13.503004	16.815597	5.550321

02_p6

17	14.610855	12.107660	0.826336
7	16.029164	11.720844	3.498325
1	16.511389	11.944666	2.641179
1	16.558793	11.829168	4.349400
9	14.747101	11.851326	5.917243
6	14.029479	12.024328	4.790489
6	14.696141	11.968879	3.555746
6	13.895330	12.158324	2.410592
17	12.928480	15.783794	0.051332
7	15.742300	15.165034	2.796514
7	11.617239	15.769715	2.803665
1	11.114433	15.661157	1.935951
1	11.127499	15.479131	3.636400
9	15.815223	15.364048	0.558133
9	13.011825	15.367555	5.133498
9	15.708002	14.938539	5.047068
6	13.683077	15.384573	3.964033
6	12.960820	15.576913	2.775423
6	15.086343	15.371690	1.676910
6	15.042739	15.174018	3.910109
6	13.717606	15.575319	1.585615
7	11.938446	12.477209	3.754895
9	11.778939	12.632890	1.516656
9	12.059049	12.342004	6.008627
6	12.545039	12.411396	2.592259
6	12.675384	12.277822	4.828028

03_hb

17	10.557260	1.734688	-0.026857
9	10.961974	1.726227	2.903717
7	8.808444	1.697603	3.550512
6	9.670634	1.712388	2.558363
17	5.332782	1.664944	1.608574
9	6.668960	1.668930	4.244417
7	7.566633	1.700836	-0.425203

1	8.221330	1.712087	-1.196829
1	6.584598	1.690052	-0.643347
6	9.337587	1.714505	1.215791
6	7.968906	1.699798	0.858686
6	7.047325	1.683934	1.932112
6	7.535402	1.683886	3.226258
17	11.260373	1.770932	-6.259892
9	10.807253	1.752595	-3.341836
7	8.558692	1.725657	-3.339744
6	9.674540	1.742119	-4.040361
17	5.785660	1.705080	-6.194602
9	6.312123	1.698506	-3.283138
7	8.509506	1.743465	-7.500773
1	9.372408	1.756126	-8.017832
1	7.635309	1.735238	-7.998498
6	9.735038	1.748958	-5.422300
6	8.525120	1.737698	-6.152564
6	7.331450	1.720054	-5.395197
6	7.430782	1.715148	-4.017357

03_pi

17	10.418116	0.895626	1.449294
9	10.518124	1.763708	4.271086
7	8.312008	1.970517	4.645977
6	9.273967	1.685023	3.795863
17	5.063350	1.538167	2.390613
9	6.116244	2.193955	5.072880
7	7.488180	0.874556	0.710497
1	8.225607	0.442373	0.175866
1	6.543686	0.606376	0.480946
6	9.078228	1.305207	2.479621
6	7.755548	1.231505	1.988558
6	6.728286	1.573178	2.896557
6	7.080967	1.913240	4.189994
17	4.343177	-0.895635	5.608784
9	4.243169	-1.763713	2.786988
7	6.449285	-1.970508	2.412096
6	5.487325	-1.685023	3.262212
17	9.697943	-1.538170	4.667461
9	8.645049	-2.193950	1.985191
7	7.273113	-0.874563	6.347580
1	6.535688	-0.442363	6.882201
1	8.217605	-0.606369	6.577123
6	5.683064	-1.305212	4.578455
6	7.005744	-1.231508	5.069516
6	8.033007	-1.573181	4.161517
6	7.680326	-1.913237	2.868078

04_hb

9	-0.019819	8.754746	3.863350
7	1.207542	6.500980	1.354509
6	0.928633	7.648239	1.995538
9	-0.107199	4.013382	3.600150
7	1.311977	8.824697	1.449182
1	1.677251	8.842849	0.497364
1	0.998657	9.683769	1.867802
6	0.261926	7.586403	3.236377
9	1.179173	4.251083	1.187057
6	-0.097772	6.386635	3.799585
1	-0.608383	6.345991	4.752705
6	0.216187	5.222665	3.103551
6	0.864977	5.351249	1.890648
9	3.673619	6.504454	-3.863350
7	2.446258	8.758220	-1.354509
6	2.725167	7.610961	-1.995538
9	3.760999	11.245818	-3.600150
7	2.341823	6.434503	-1.449182
1	1.976549	6.416351	-0.497364
1	2.655143	5.575431	-1.867802
6	3.391874	7.672797	-3.236377
9	2.474627	11.008117	-1.187057
6	3.751572	8.872565	-3.799585
1	4.262183	8.913209	-4.752705
6	3.437613	10.036535	-3.103551
6	2.788823	9.907951	-1.890648

04_p1

9	0.581580	9.148327	3.597390
7	0.292982	5.984683	1.921883
6	0.411756	7.302379	2.115982
9	0.169296	4.736510	5.291898
7	0.505307	8.126192	1.024187
1	0.165271	7.714274	0.166679
1	0.207301	9.079139	1.174546
6	0.468302	7.809074	3.424569
9	0.092193	3.873605	2.700048
6	0.393977	6.972236	4.514892
1	0.420905	7.360914	5.523947
6	0.265704	5.611639	4.271635
6	0.227579	5.182360	2.953928
9	-2.807847	7.716464	4.359050
7	-2.717430	7.338736	0.791439
6	-2.691274	7.904331	2.001137
9	-3.194550	3.872414	1.604798
7	-2.456177	9.261496	2.083862
1	-2.718653	9.782406	1.259744
1	-2.691962	9.705016	2.959066

6	-2.835030	7.111206	3.144971
9	-2.890517	5.528271	-0.545027
6	-3.008222	5.746579	3.048492
1	-3.118010	5.129078	3.929978
6	-3.030760	5.193134	1.777111
6	-2.876304	6.041964	0.690029

04_p2

9	-2.350048	5.033703	26.829671
9	-1.889370	5.339834	29.504569
9	2.354425	5.192858	26.211658
7	2.662948	5.463362	28.949285
1	2.688611	5.837118	29.885995
1	3.431198	5.717539	28.348241
7	0.347309	5.383332	29.181052
6	1.420741	5.353764	28.385042
6	-0.846561	5.269817	28.660649
6	-1.090553	5.110307	27.306001
6	1.251610	5.188974	27.001444
6	-0.002074	5.066589	26.446131
1	-0.136425	4.963040	25.377755
9	3.638984	8.622922	27.180450
9	2.582076	8.804633	29.692611
9	-0.808215	8.253279	25.560227
7	-1.730256	8.484764	28.160074
1	-1.973862	8.289327	29.119364
1	-2.348831	8.108131	27.458947
7	0.475074	8.655039	28.887967
6	-0.390933	8.514895	27.879427
6	1.757533	8.696066	28.637672
6	2.303292	8.608668	27.367021
6	0.088524	8.425774	26.563264
6	1.437290	8.470358	26.291388
1	1.810668	8.378334	25.280289

04_p3

1	3.928930	7.459974	26.056225
9	0.240286	2.336349	23.812391
9	-1.170596	4.583021	24.453108
9	3.203630	3.436456	27.355322
7	1.733174	5.726243	27.818226
1	1.020610	6.378294	28.108817
1	2.358672	5.399749	28.538219
7	0.261438	5.082557	26.129321
6	1.350917	4.822875	26.857853
6	-0.076943	4.263365	25.165807
6	0.628134	3.117166	24.837852
6	2.109502	3.673519	26.592131

6	1.760130	2.809321	25.578942
1	2.357354	1.935988	25.353731
9	5.689658	5.489223	25.919021
9	5.090894	3.624593	24.007136
7	3.242097	4.764423	23.385102
6	4.291901	4.691440	24.164587
6	4.600903	5.627340	25.138561
6	2.646029	6.781164	24.476292
6	3.746461	6.709653	25.299630
9	1.765288	7.802971	24.595004
7	1.319297	5.868971	22.669873
1	1.085448	5.019792	22.178421
1	0.541690	6.442337	22.957742
6	2.398010	5.793242	23.511040

04_p4

9	3.247180	6.053197	16.929157
7	1.335836	5.670132	18.883038
1	0.866196	5.529461	19.764553
1	1.813248	4.863232	18.511318
6	1.956004	6.883033	18.732289
9	3.729472	10.550686	18.367793
9	1.824780	10.024880	20.256358
7	1.615546	7.888653	19.544528
6	2.187475	9.056933	19.397411
6	3.148438	9.333505	18.440316
6	2.915962	7.092497	17.729584
6	3.526379	8.315739	17.575780
1	4.282652	8.473541	16.818647
1	2.094106	6.785659	23.486606
9	2.647286	4.708514	21.937459
9	4.551978	5.234320	20.048895
7	4.761211	7.370547	20.760725
6	4.189283	6.202267	20.907842
6	3.228320	5.925695	21.864937
6	3.460796	8.166703	22.575668
6	2.850379	6.943461	22.729473
9	3.129578	9.206003	23.376096
7	5.040922	9.589068	21.422215
1	5.510562	9.729739	20.540700
1	4.563510	10.395968	21.793934
6	4.420754	8.376167	21.572963

05_hb

17	-1.840447	2.725726	3.974996
9	-0.410455	5.104526	2.880559
7	1.455379	2.754488	0.911474
9	-0.625398	0.358163	2.606545

6	1.027135	3.922418	1.420327
7	1.582378	5.074874	0.987011
1	2.385685	5.045591	0.359743
1	1.329678	5.943622	1.425706
9	1.383083	0.506315	0.761529
6	-0.003339	3.920994	2.380673
6	-0.578476	2.737173	2.799739
6	-0.110008	1.540023	2.244646
6	0.904820	1.632156	1.312824
17	7.220375	4.900306	-3.974996
9	5.790382	2.521506	-2.880559
7	3.924549	4.871544	-0.911474
9	6.005325	7.267869	-2.606545
6	4.352793	3.703614	-1.420327
7	3.797549	2.551157	-0.987011
1	2.994242	2.580441	-0.359743
1	4.050250	1.682409	-1.425706
9	3.996845	7.119717	-0.761529
6	5.383267	3.705037	-2.380673
6	5.958404	4.888859	-2.799739
6	5.489936	6.086008	-2.244646
6	4.475108	5.993876	-1.312824

05_p1

17	6.038813	5.123674	-4.059612
9	4.929565	2.587072	-2.949580
7	3.331394	4.662006	-0.496390
9	4.980253	7.297155	-2.300176
6	3.721520	3.575488	-1.170632
7	3.282748	2.347690	-0.748767
1	2.434835	2.359720	-0.198039
1	3.354328	1.590780	-1.411360
9	3.320645	6.895914	-0.179652
6	4.576364	3.699114	-2.274266
6	5.017878	4.947028	-2.682137
6	4.596197	6.062752	-1.956663
6	3.754449	5.839759	-0.877975
17	2.260607	4.880592	-4.849742
9	1.237875	2.548038	-3.291037
7	-0.033659	4.981332	-0.980131
9	1.447824	7.296596	-3.290501
6	0.269449	3.808034	-1.536550
7	-0.054496	2.651892	-0.850410
1	-0.750296	2.791319	-0.130611
1	-0.198473	1.825936	-1.413682
9	0.028191	7.236627	-0.970980
6	0.962047	3.753688	-2.748689
6	1.376394	4.922089	-3.370375
6	1.069057	6.133528	-2.752283

	6	0.353893	6.086227	-1.562667
05_p2				
	7	4.201265	8.231256	7.262273
	6	5.322660	8.144254	6.539037
	7	6.409245	7.512703	7.079801
	1	6.393437	7.405923	8.082673
	1	7.310951	7.708984	6.673515
	9	2.055859	8.889806	7.514895
	6	3.148620	8.807965	6.738999
	17	4.311038	9.988751	3.120789
	9	6.525473	8.599407	4.554473
	6	5.368277	8.672926	5.240619
	6	4.258291	9.294035	4.695565
	6	3.097488	9.359572	5.471090
	7	4.638723	12.237107	6.445533
	6	4.926550	11.536851	7.547486
	7	3.971756	11.416304	8.519265
	1	3.033681	11.659889	8.238597
	1	4.050896	10.640045	9.158262
	9	5.214872	13.107335	4.444887
	6	5.552589	12.391541	5.521889
	17	8.726708	10.409283	6.890541
	9	6.462276	10.264045	8.827197
	9	1.991120	9.954991	5.013311
	6	6.199882	10.971388	7.709088
	6	7.161976	11.123230	6.724759
	6	6.831728	11.859261	5.585982
	9	7.713980	12.037793	4.597172
05_p3				
	7	3.841030	13.577333	7.550591
	6	4.610351	12.662307	6.953040
	7	4.234515	11.351890	7.013862
	1	3.295502	11.152632	7.318632
	1	4.700845	10.674785	6.433697
	9	3.428567	15.704221	8.183869
	6	4.229082	14.828334	7.565505
	17	7.685627	14.848365	5.584505
	9	6.548060	12.093295	5.720169
	6	5.807554	13.040574	6.327063
	6	6.214873	14.362549	6.343097
	6	5.401724	15.293276	6.993505
	9	4.168343	10.755905	10.505184
	17	3.545866	13.543409	11.395795
	9	5.872948	15.197823	10.523395
	6	5.963310	13.887066	10.218439
	6	4.956957	13.002411	10.570883

6	5.113484	11.661460	10.219357
7	7.211245	12.144498	9.192973
6	7.085714	13.437618	9.512255
7	8.044254	14.313311	9.083771
1	8.909380	13.913940	8.756629
1	8.080939	15.232340	9.493371
9	6.434008	10.025475	9.189020
6	6.266017	11.307886	9.537508
9	5.750757	16.584716	7.064492

05_p4

9	4.243382	9.193383	4.093247
17	2.399271	11.526339	3.782257
9	4.001362	13.632294	2.398889
6	4.656121	12.475311	2.615034
6	4.035119	11.413672	3.250038
6	4.778453	10.250510	3.461608
7	4.519384	13.449646	5.933229
6	5.202681	12.319967	6.143049
7	4.576424	11.283256	6.776438
1	3.569403	11.331224	6.804394
1	4.978466	10.362802	6.692350
9	4.381786	15.561578	5.146606
6	5.108588	14.455609	5.339641
7	6.679455	11.243351	2.422437
6	5.996151	12.373027	2.212618
7	6.622403	13.409741	1.579227
1	7.629424	13.361781	1.551274
1	6.220354	14.330193	1.663314
9	6.817065	9.131420	3.209060
6	6.090257	10.237386	3.016027
17	8.799568	13.166637	4.573415
9	7.197462	11.060688	5.956777
6	6.542712	12.217677	5.740635
6	7.163720	13.279312	5.105633
6	6.420392	14.442478	4.894062
9	6.955470	15.499604	4.262426

06_hb

6	5.442506	1.229005	5.235400
6	6.576873	1.822570	4.718166
6	6.451505	2.963156	3.920610
6	5.158709	3.441733	3.687248
6	4.095116	2.763433	4.258756
7	4.229220	1.687057	5.008162
9	5.553608	0.149825	6.002718
9	7.811685	1.344515	4.956686
8	7.500234	3.596470	3.385644

1	8.321861	3.155247	3.641674
9	4.967998	4.525958	2.936977
9	2.859135	3.207820	4.059355
6	2.474799	2.169964	9.739014
6	2.730566	1.879771	8.410814
6	1.902063	0.978745	7.730826
6	0.848992	0.427329	8.474604
6	0.698820	0.799241	9.799485
7	1.486714	1.646745	10.421672
9	3.276170	3.032787	10.372842
9	3.763743	2.452262	7.756123
8	2.049541	0.624479	6.457989
1	2.823755	1.049797	6.024437
9	0.012694	-0.442464	7.897578
9	-0.305750	0.270754	10.503147

06_p1

6	4.683389	1.646412	5.439708
6	5.229571	1.946165	4.204115
6	5.570219	3.268162	3.907618
6	5.333326	4.222857	4.900966
6	4.771559	3.797280	6.093413
7	4.458708	2.552147	6.362030
9	4.365710	0.384481	5.719320
9	5.442051	1.008885	3.261193
8	6.094447	3.642086	2.735590
1	6.115089	2.889526	2.128727
9	5.619711	5.509220	4.682366
9	4.503747	4.710398	7.034475
6	2.526213	5.816288	3.744500
6	1.980031	5.516535	4.980093
6	1.639383	4.194538	5.276590
6	1.876276	3.239843	4.283242
6	2.438043	3.665420	3.090795
7	2.750894	4.910553	2.822178
9	2.843892	7.078219	3.464888
9	1.767550	6.453815	5.923015
8	1.115155	3.820614	6.448618
1	1.094513	4.573174	7.055481
9	1.589891	1.953480	4.501842
9	2.705855	2.752302	2.149733

06_p2

6	5.602341	1.232204	4.863336
6	6.385167	1.434587	3.740727
6	6.635341	2.738131	3.310912
6	6.060725	3.771993	4.052485
6	5.302300	3.440423	5.163156

7	5.073179	2.211523	5.556836
9	5.368458	-0.014063	5.272632
9	6.939383	0.419523	3.050150
8	7.409468	3.028629	2.255931
1	7.783438	2.217433	1.885252
9	6.274006	5.048317	3.704829
9	4.774883	4.429749	5.891279
6	9.625061	6.230496	4.320872
6	8.842234	6.028113	5.443481
6	8.592061	4.724569	5.873296
6	9.166677	3.690707	5.131723
6	9.925102	4.022277	4.021052
7	10.154223	5.251177	3.627372
9	9.858943	7.476763	3.911576
9	8.288018	7.043177	6.134059
8	7.817934	4.434071	6.928277
1	7.443964	5.245267	7.298957
9	8.953396	2.414383	5.479379
9	10.452519	3.032951	3.292929

07_hb

9	-1.768523	1.174225	3.742917
7	-0.621439	-1.060957	1.186319
6	-0.888794	0.076701	1.836114
9	-1.838116	-3.549643	3.472856
1	-0.154675	1.149169	0.418897
6	-1.504613	0.028040	3.099420
9	-0.636810	-3.314310	1.020878
6	-1.833475	-1.181454	3.670495
1	-2.307504	-1.226668	4.642229
6	-1.540303	-2.343121	2.965430
6	-0.934994	-2.223446	1.730029
9	1.768523	-1.174225	-3.742917
7	0.621439	1.060957	-1.186319
6	0.888794	-0.076701	-1.836114
9	1.838116	3.549643	-3.472856
1	0.154675	-1.149169	-0.418897
6	1.504613	-0.028040	-3.099420
9	0.636810	3.314310	-1.020878
6	1.833475	1.181454	-3.670495
1	2.307504	1.226668	-4.642229
6	1.540303	2.343121	-2.965430
6	0.934994	2.223446	-1.730029
8	-0.583247	1.250359	1.309886
8	0.583247	-1.250359	-1.309886

07_p1

9	2.748523	2.171608	-0.515565
---	----------	----------	-----------

7	0.576092	-0.516467	-1.468404
6	1.140636	0.681698	-1.418562
9	2.420994	-2.285433	1.047506
1	-0.114487	1.328952	-2.659682
6	2.198287	0.949085	-0.543720
9	0.388454	-2.650428	-0.742886
6	2.652660	-0.044091	0.301148
1	3.453306	0.145525	1.003399
6	2.036837	-1.285568	0.236917
6	1.005370	-1.466142	-0.671313
9	0.180077	0.692144	2.606287
7	-1.850080	1.289223	-0.290301
6	-0.976189	1.480483	0.689323
9	-2.987178	-2.043212	0.392696
1	-0.512461	3.157182	-0.028358
6	-0.726837	0.482540	1.636365
9	-3.342775	-0.001246	-1.390930
6	-1.400744	-0.721037	1.559136
1	-1.215583	-1.510703	2.275301
6	-2.308765	-0.894534	0.525262
6	-2.488394	0.145570	-0.374110
8	0.667467	1.668362	-2.201380
8	-0.304500	2.641532	0.763381

07_p2

9	-0.095218	-1.796272	-3.177448
1	-3.164291	-2.099065	-1.173911
6	-1.699304	-1.011436	-1.615806
9	0.426834	2.416883	-1.082759
9	-1.909868	1.922404	0.251985
7	-2.130870	-0.081158	-0.775542
6	-1.437405	1.022713	-0.617992
6	-0.254760	1.277425	-1.292356
6	-0.513523	-0.837458	-2.339357
6	0.221219	0.319757	-2.176973
1	1.149994	0.467853	-2.711375
1	-1.149994	-0.467853	2.711375
9	-0.426834	-2.416883	1.082759
9	1.909868	-1.922404	-0.251985
7	2.130870	0.081158	0.775542
6	1.437405	-1.022713	0.617992
6	0.254760	-1.277425	1.292356
6	0.513523	0.837458	2.339357
6	-0.221219	-0.319757	2.176973
9	0.095218	1.796272	3.177448
1	3.164291	2.099065	1.173911
6	1.699304	1.011436	1.615806
8	-2.408453	-2.139846	-1.775466
8	2.408453	2.139846	1.775466

07_p3

9	-3.484058	-0.372604	-0.714203
9	-1.878867	0.709937	-2.642097
9	-0.598946	1.558675	2.506653
1	1.326818	2.792623	-0.371982
7	-0.521024	1.616463	-1.077318
6	-0.191371	1.834344	0.186882
6	-1.592203	0.909119	-1.354288
6	-2.413845	0.368350	-0.377371
6	-0.967501	1.330615	1.235939
6	-2.096418	0.587029	0.954895
1	-2.699236	0.166902	1.748631
9	3.484014	0.372696	-0.714127
9	1.878583	-0.709408	-2.642068
9	0.599225	-1.559202	2.506649
1	-1.326923	-2.792434	-0.372040
7	0.520887	-1.616216	-1.077325
6	0.191375	-1.834360	0.186866
6	1.592057	-0.908845	-1.354267
6	2.413820	-0.368299	-0.377330
6	0.967638	-1.330876	1.235942
6	2.096537	-0.587251	0.954927
1	2.699455	-0.167306	1.748683
8	0.920752	2.536835	0.468122
8	-0.920741	-2.536874	0.468077

F Computed IR and Raman Spectra of aggregates

01_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.4427	0.0001	0.0519	0.2390
2	A	10.9179	0.0009	0.4137	0.0473
3	A	17.5223	0.0022	0.2093	0.1013
4	A	22.0400	0.0034	0.4650	6.6189
5	A	40.8117	0.0135	0.4462	0.0422
6	A	64.1630	0.0306	1.8617	0.6608
7	A	122.1700	0.1595	0.0836	0.0113
8	A	123.3566	0.1624	0.0124	0.0034
9	A	144.9176	0.1645	13.9900	0.9475
10	A	147.0769	0.1768	6.7516	0.4027
11	A	195.1203	0.0302	146.2161	2.1811
12	A	207.3506	0.3427	4.8801	0.8773
13	A	211.7417	0.1221	84.0229	1.6385
14	A	275.2013	0.1971	4.1355	1.0273
15	A	280.5992	0.7376	1.7933	0.2413
16	A	280.8879	0.7303	2.5219	0.5640
17	A	288.9790	0.3193	5.9109	1.2475
18	A	313.0363	0.5388	0.1242	0.1093
19	A	319.4163	0.3787	2.2653	0.9890
20	A	333.8756	0.1848	58.9736	1.6521
21	A	341.4539	0.6739	0.3139	0.8745
22	A	348.5275	1.0502	7.6168	0.8192
23	A	351.0430	0.9460	0.7131	0.0695
24	A	356.1001	0.1274	95.6285	0.8966
25	A	413.2233	0.3038	0.5823	1.9044
26	A	434.1468	0.8461	10.4698	2.0771
27	A	463.5166	1.9098	0.3122	5.9188
28	A	464.3676	1.9162	0.2443	4.3727
29	A	484.8410	1.2201	0.7688	3.1369
30	A	485.0346	0.1998	2.0754	0.2260
31	A	488.2133	1.7539	5.5083	9.7663
32	A	604.1159	0.2836	7.3344	3.7151
33	A	611.1164	1.8861	1.1752	6.3861
34	A	612.2054	1.6951	19.9354	43.2045
35	A	644.6040	2.7225	0.0310	0.8470
36	A	653.7826	1.1039	32.8349	0.7073
37	A	671.3686	3.0919	0.2077	0.0077
38	A	673.3363	3.2340	0.0027	0.0150
39	A	696.9129	4.2442	1.4846	16.9522
40	A	708.5964	4.3795	0.0321	30.9542
41	A	718.1731	1.9282	1.0712	0.5899
42	A	721.0441	3.3693	8.2220	0.8965
43	A	723.1918	1.9856	0.2587	0.0627
44	A	727.9234	3.2900	3.5588	0.7828

45	A	907.6123	1.9803	35.7590	0.6973
46	A	913.7069	2.0455	220.6194	0.1648
47	A	1117.1141	3.3530	111.0556	0.7904
48	A	1119.5358	5.1095	346.2021	0.5024
49	A	1122.6890	4.5164	75.5952	0.7891
50	A	1130.1270	4.0013	94.7179	0.3307
51	A	1176.3749	2.1719	58.5883	4.5658
52	A	1182.8975	2.6381	39.2905	0.9006
53	A	1285.2533	9.2567	56.1517	11.9285
54	A	1289.4379	9.0314	104.1011	16.6648
55	A	1374.0424	9.1348	32.2539	12.8882
56	A	1375.8922	9.0905	46.0526	23.5670
57	A	1426.6262	14.3143	37.5378	4.3352
58	A	1430.2734	14.0824	14.0781	15.8561
59	A	1503.2025	15.6963	284.7698	3.1824
60	A	1512.3601	14.7962	800.2048	8.8076
61	A	1558.4149	6.8978	149.1349	0.3033
62	A	1561.8142	8.6408	84.7056	0.6995
63	A	1637.4457	9.1214	4.4908	0.3187
64	A	1638.2182	5.9451	2.4948	1.7607
65	A	1641.3922	3.3907	36.4479	1.7850
66	A	1657.1614	3.3502	1.3143	4.0200
67	A	1681.4426	6.3413	1037.2176	68.3644
68	A	1689.8050	5.9339	46.6644	6.8813
69	A	3512.2484	7.6851	859.0743	635.0141
70	A	3612.4392	8.0353	135.0547	157.2678
71	A	3695.7527	8.8127	112.3673	49.3691
72	A	3732.2215	9.0757	79.0888	39.4179

01_pi

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	19.8372	0.0028	1.5549	0.0000
2	A	36.5329	0.0082	0.0000	3.7975
3	A	42.5516	0.0145	0.0000	2.4971
4	A	46.5244	0.0186	0.9200	0.0000
5	A	56.6513	0.0155	10.1446	0.0000
6	A	77.0267	0.0417	0.0000	0.8049
7	A	124.2709	0.1620	0.1726	0.0000
8	A	128.6117	0.1726	0.0000	0.0598
9	A	158.5541	0.1057	0.0000	0.3207
10	A	159.6622	0.1184	7.3412	0.0000
11	A	211.5229	0.2619	3.3367	0.0000
12	A	222.8813	0.3138	0.0000	1.4252
13	A	276.5630	0.1973	0.0000	1.1579
14	A	277.0240	0.1961	8.4770	0.0000
15	A	280.6686	0.7960	1.6702	0.0000
16	A	281.3403	0.7880	0.0000	0.3216

17	A	312.7605	0.5067	0.7494	0.0000
18	A	313.2835	0.5154	0.0000	0.3666
19	A	345.3158	0.6332	0.0000	0.8031
20	A	346.4117	0.8258	5.9560	0.0000
21	A	349.3820	0.9128	0.0000	0.7834
22	A	350.9096	0.8987	0.2795	0.0000
23	A	394.0415	0.1330	0.0000	2.4440
24	A	395.1145	0.1290	30.2237	0.0000
25	A	462.3464	0.5324	7.7208	0.0000
26	A	463.3219	0.4095	0.0000	3.4055
27	A	464.3561	0.9909	5.9606	0.0000
28	A	464.5270	1.6064	0.0000	6.1057
29	A	480.0715	0.5986	162.5542	0.0000
30	A	482.8071	1.0560	0.0000	6.0403
31	A	502.4135	0.2417	596.2509	0.0000
32	A	516.8629	0.2261	0.0000	5.7781
33	A	611.6141	1.8450	32.4582	0.0000
34	A	611.9284	1.7875	0.0000	33.9210
35	A	641.8200	2.9878	0.0000	0.8356
36	A	644.1038	2.9328	13.4600	0.0000
37	A	674.9983	3.2694	0.2111	0.0000
38	A	675.2891	3.2635	0.0000	0.4690
39	A	700.6529	4.2357	8.5494	0.0000
40	A	700.8051	4.1960	0.0000	16.8820
41	A	720.9087	2.1121	0.3748	0.0000
42	A	721.5708	2.1222	0.0000	0.2074
43	A	726.5257	3.7805	0.0000	1.6920
44	A	727.4431	3.7834	25.5827	0.0000
45	A	915.9069	2.3163	0.0000	0.1958
46	A	920.8956	2.2529	230.7586	0.0000
47	A	1108.5577	6.4605	0.0000	0.3858
48	A	1121.1283	6.5427	252.9496	0.0000
49	A	1126.1502	4.5682	89.4154	0.0000
50	A	1130.3407	3.5135	0.0000	0.9135
51	A	1196.3537	1.8557	110.6066	0.0000
52	A	1198.6662	2.0679	0.0000	1.2873
53	A	1287.8871	9.3005	90.0309	0.0000
54	A	1289.8381	8.9715	0.0000	13.3196
55	A	1377.3442	7.9863	35.4616	0.0000
56	A	1378.9703	7.9781	0.0000	17.7600
57	A	1428.6035	14.2659	56.7690	0.0000
58	A	1429.6568	14.5959	0.0000	8.6879
59	A	1500.3352	15.5163	0.0000	5.1347
60	A	1510.7178	16.1200	1038.0541	0.0000
61	A	1551.2463	9.1286	154.9279	0.0000
62	A	1554.3856	8.5734	0.0000	1.5270
63	A	1641.6815	6.1088	3.8662	0.0000
64	A	1643.0815	7.3394	0.0000	2.0138
65	A	1644.3903	3.1965	6.1403	0.0000
66	A	1645.1681	3.2401	0.0000	1.3134

67	A	1681.3118	5.5909	0.0000	29.9373
68	A	1687.6251	6.4244	586.6268	0.0000
69	A	3582.8854	7.9140	175.1541	0.0047
70	A	3583.0478	7.9144	0.0041	197.8338
71	A	3690.0933	8.8456	0.0093	52.5223
72	A	3690.1896	8.8463	114.2279	0.0043

02_h1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.2129	0.0002	1.9036	0.1518
2	A	11.9727	0.0005	18.9595	0.1240
3	A	13.6468	0.0002	139.0861	0.0865
4	A	23.9462	0.0048	0.0355	0.2500
5	A	24.9930	0.0045	0.4287	6.9757
6	A	42.7451	0.0182	0.4578	0.0604
7	A	60.3720	0.0286	1.2308	0.5101
8	A	97.9702	0.1074	0.1094	0.0355
9	A	101.8126	0.0566	10.1666	0.0967
10	A	133.5242	0.1655	1.3151	0.1176
11	A	146.6950	0.0429	37.0029	0.1789
12	A	207.0977	0.3288	4.5905	1.7556
13	A	207.8604	0.2827	0.3336	0.1162
14	A	220.6175	0.5012	0.4411	2.3472
15	A	223.3779	0.4964	0.5115	0.7600
16	A	290.6509	0.4327	2.9379	0.4026
17	A	292.8978	0.6503	2.6900	0.1072
18	A	314.0104	0.3322	1.3424	0.6562
19	A	315.7584	0.5923	10.3181	0.0838
20	A	321.7133	0.3639	1.8660	0.4499
21	A	321.8164	0.5126	4.7632	0.4344
22	A	336.7097	0.8403	4.5364	3.0307
23	A	339.0814	0.7203	1.2905	1.3482
24	A	368.2903	0.0990	121.5713	0.2840
25	A	395.0585	0.4668	1.1485	0.7280
26	A	406.8249	1.2113	1.4637	6.4256
27	A	408.8079	1.2049	2.0525	4.2177
28	A	410.2465	0.5220	12.0030	0.8133
29	A	476.2225	1.8196	0.3762	1.2842
30	A	477.0491	1.8354	5.0094	9.6347
31	A	507.0869	0.1754	0.1809	0.0620
32	A	606.7000	0.2438	5.2957	0.1706
33	A	609.7521	2.0875	2.1786	0.9433
34	A	612.4722	2.1320	15.1541	67.5681
35	A	632.8412	3.6384	5.6019	5.5449
36	A	642.8598	3.6543	3.2794	17.7267
37	A	657.4651	2.5563	1.9307	0.1394
38	A	661.5257	1.8026	20.0283	1.2065

39	A	679.0444	3.2401	0.0293	0.0952
40	A	679.1780	3.1697	3.0370	0.0353
41	A	699.1146	1.6420	2.5286	1.1624
42	A	703.4229	1.6799	1.0950	0.1412
43	A	750.2851	3.8333	5.5449	0.3009
44	A	759.9737	3.8458	8.7805	0.1514
45	A	842.4246	2.5415	61.3171	8.1811
46	A	848.9125	2.6820	142.1028	1.6430
47	A	1074.4173	4.1415	54.0928	0.8434
48	A	1078.9893	4.8640	87.7291	3.1903
49	A	1109.8634	1.6204	109.8830	0.5312
50	A	1114.4217	1.8063	112.1935	1.3801
51	A	1120.9700	5.8825	114.6631	1.2006
52	A	1129.4565	4.6822	133.8826	0.6123
53	A	1239.1867	6.6549	61.5290	17.8855
54	A	1246.7934	6.7334	81.1847	9.2932
55	A	1364.7777	9.0867	68.6878	37.2860
56	A	1365.5224	8.8071	24.0782	14.6709
57	A	1419.7550	13.9387	120.5157	14.3585
58	A	1421.8598	13.5181	23.3859	3.0302
59	A	1475.6224	13.6614	297.8202	9.1245
60	A	1481.7988	13.0532	362.7582	13.1416
61	A	1534.3461	5.9631	192.2282	1.5663
62	A	1538.8755	7.0288	168.4253	0.5533
63	A	1619.8041	14.2672	28.2737	3.9371
64	A	1620.8152	11.2724	7.4218	4.8056
65	A	1635.0006	2.8439	15.8618	1.8545
66	A	1646.1069	4.0745	17.5087	7.5491
67	A	1668.7037	5.0592	1321.8966	56.5158
68	A	1678.4768	4.5929	40.7206	7.7576
69	A	3534.5870	7.7671	648.4857	522.0809
70	A	3613.4878	8.0384	126.5138	138.8076
71	A	3702.8312	8.8611	86.8067	38.4845
72	A	3736.5373	9.1001	83.1517	30.4501

02_h2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.6516	0.0001	0.1430	0.4387
2	A	10.2192	0.0009	1.4667	0.2054
3	A	16.3777	0.0021	0.3753	4.4941
4	A	19.7084	0.0032	2.0034	0.2047
5	A	33.7268	0.0093	0.1712	0.4845
6	A	45.7455	0.0175	0.1268	0.2318
7	A	94.9623	0.0451	30.9726	1.2295
8	A	97.7444	0.1061	0.2887	0.1039
9	A	110.2373	0.0209	89.2763	2.5051
10	A	134.7466	0.1648	0.9689	0.2497

11	A	153.7380	0.0257	85.3070	1.7049
12	A	206.2724	0.2659	0.0334	0.5967
13	A	207.5739	0.3503	4.7922	1.1862
14	A	223.0418	0.5069	0.9181	0.9518
15	A	226.9160	0.5248	2.0670	2.8112
16	A	286.7119	0.0658	143.2205	3.7041
17	A	288.9831	0.3402	11.9501	0.3313
18	A	290.0376	0.3525	7.7510	2.0071
19	A	313.5249	0.3140	3.5429	1.7507
20	A	314.8472	0.3294	1.5146	0.5948
21	A	316.3885	0.6504	0.4366	0.3251
22	A	321.8242	0.3047	16.3177	0.5533
23	A	334.1232	0.9759	0.7455	2.2605
24	A	336.6452	0.9860	2.9999	1.5477
25	A	395.2017	0.4378	3.2272	1.4899
26	A	397.3606	0.5187	3.3717	0.6063
27	A	406.9084	1.2210	3.1888	6.8853
28	A	407.3387	1.1922	1.8763	6.4446
29	A	475.7971	1.7975	0.5449	9.5705
30	A	477.1361	1.8159	3.0611	3.7558
31	A	497.1775	0.1721	1.2681	0.1550
32	A	516.8182	0.1785	1.1383	0.8489
33	A	609.2773	2.0872	3.0747	11.3179
34	A	611.3798	2.0838	12.0266	52.5503
35	A	632.2158	3.6137	10.2599	5.6391
36	A	632.5546	3.6267	1.2802	3.7121
37	A	652.0758	2.8038	5.8005	1.1435
38	A	656.2629	2.7636	7.4800	1.5798
39	A	675.9337	3.2423	0.9777	0.0818
40	A	681.0046	3.2501	0.9152	0.2923
41	A	697.6256	1.6466	1.8938	0.1706
42	A	699.5686	1.6887	1.2531	0.2666
43	A	744.4967	3.8336	7.0920	1.3796
44	A	753.3099	3.8638	11.6214	2.5374
45	A	841.5172	2.6312	124.1890	2.9038
46	A	844.3216	2.6549	101.3647	1.0945
47	A	1068.7259	5.3474	56.7990	0.7923
48	A	1075.9690	4.3685	43.4699	1.7592
49	A	1112.2560	1.7340	2.6258	0.5722
50	A	1114.3919	2.1214	202.3637	2.8401
51	A	1119.9593	4.1834	206.6658	0.5289
52	A	1124.9113	3.4144	104.7897	0.5504
53	A	1237.4922	6.6956	59.4212	5.2758
54	A	1243.5483	6.5251	46.0813	5.1216
55	A	1364.5716	8.8363	44.4941	29.2451
56	A	1367.4202	8.8694	36.2537	18.6770
57	A	1418.6166	12.7270	144.9300	5.8074
58	A	1423.7042	14.1524	64.7298	4.5307
59	A	1474.9410	13.2320	501.8402	8.9962
60	A	1476.0282	13.7686	307.2219	2.6454

61	A	1532.9099	6.6522	380.1149	1.3189
62	A	1534.0998	6.1837	42.3406	0.6128
63	A	1622.3881	9.8858	35.3491	4.8434
64	A	1625.2753	10.5070	57.3219	4.1305
65	A	1633.7812	2.8942	28.9758	3.8313
66	A	1635.5574	3.3506	14.3320	1.5721
67	A	1668.6472	5.9770	338.3055	5.3775
68	A	1672.3151	5.8240	612.4241	36.5452
69	A	3606.3683	8.0110	259.0994	307.5734
70	A	3612.2316	8.0339	106.5594	113.4693
71	A	3723.7848	9.0321	172.1382	93.0388
72	A	3733.8786	9.0843	79.3487	26.3159

02_p1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	11.5045	0.0012	0.0558	2.6866
2	A	13.2492	0.0015	1.4494	0.2294
3	A	26.7909	0.0055	0.0154	4.2808
4	A	60.7702	0.0210	9.7043	0.0742
5	A	60.9541	0.0373	0.0001	0.1418
6	A	72.6518	0.0484	0.0164	0.2994
7	A	104.2996	0.0828	0.0041	0.1788
8	A	110.2770	0.1280	0.6464	0.1175
9	A	139.5194	0.1053	3.6367	0.1287
10	A	149.6077	0.1055	0.0216	0.2197
11	A	208.5879	0.2150	2.1484	0.0024
12	A	221.0958	0.2827	0.1517	1.4774
13	A	222.1249	0.5033	0.2825	0.0463
14	A	222.6243	0.4993	0.5636	1.5683
15	A	289.6243	0.4805	0.8396	0.1986
16	A	289.8533	0.4941	2.6870	0.0949
17	A	313.7207	0.3038	0.0560	0.0047
18	A	313.7507	0.3055	3.4501	0.9140
19	A	319.1554	0.6115	1.2135	0.0119
20	A	326.8704	0.6189	0.4703	0.9289
21	A	335.3478	0.9333	1.9366	0.6946
22	A	335.6044	0.9553	0.5585	2.3778
23	A	388.2356	0.2861	9.4258	1.7409
24	A	396.1103	0.2454	2.9899	0.3294
25	A	406.3258	1.0245	19.4109	5.4136
26	A	408.5243	0.7935	0.1308	2.0502
27	A	435.5054	0.1637	572.4991	2.0702
28	A	454.8686	0.2094	23.6099	0.6122
29	A	473.5641	0.1921	21.1601	0.3217
30	A	473.8307	0.1921	23.0656	0.0995
31	A	479.0649	0.6947	75.7524	0.0373
32	A	480.3513	0.6710	7.0268	7.9882

33	A	610.5659	1.9079	3.1017	40.4409
34	A	610.6831	1.9202	13.5732	0.0192
35	A	634.9987	3.4936	2.0973	3.9200
36	A	635.1351	3.5701	10.4036	0.8005
37	A	644.2670	2.8560	0.0615	1.2332
38	A	646.6673	3.0382	7.5445	0.0540
39	A	676.4303	3.2843	0.3330	0.1906
40	A	677.9467	3.2260	1.8235	0.0453
41	A	702.2624	1.8280	0.3529	0.1044
42	A	702.4360	1.8424	0.5625	0.3179
43	A	735.6144	3.8139	28.6583	0.0826
44	A	737.5588	3.8947	0.0127	0.6210
45	A	849.1348	2.8447	16.5206	0.2536
46	A	853.0698	2.8243	151.7641	2.0168
47	A	1077.0385	6.2691	25.5919	0.3972
48	A	1084.4996	6.9431	52.2431	1.2562
49	A	1108.6679	6.9040	0.0046	0.6459
50	A	1116.8734	6.1283	162.7807	0.6483
51	A	1136.5185	1.4928	30.7270	0.0236
52	A	1140.4188	1.5047	105.8004	1.8037
53	A	1241.1003	6.1044	41.1756	0.1710
54	A	1252.3372	5.9208	35.2100	6.3431
55	A	1367.1504	7.9153	32.8769	11.3749
56	A	1367.7258	7.7811	11.5980	11.5113
57	A	1424.0177	14.0893	94.0965	0.0140
58	A	1425.4963	14.1714	13.6464	9.5614
59	A	1470.8931	12.9190	11.5920	0.3004
60	A	1476.2305	13.1508	569.1374	3.0930
61	A	1525.2171	7.6670	42.0442	1.2896
62	A	1532.1967	7.2751	286.1180	0.8258
63	A	1622.8818	12.9608	21.6027	2.6509
64	A	1623.6851	8.7488	13.7656	4.4172
65	A	1636.3296	3.2530	3.3128	0.4616
66	A	1638.6707	3.4496	12.6864	2.7501
67	A	1667.7827	4.0967	29.4185	13.1967
68	A	1677.1633	5.0180	631.8487	7.6597
69	A	3585.4324	7.9237	152.8526	7.7919
70	A	3585.5791	7.9237	9.9600	148.8493
71	A	3697.0376	8.8848	2.7161	26.0518
72	A	3697.2111	8.8857	115.5002	11.1609

02_p2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	5.9774	0.0003	0.5087	3.2734
2	A	18.3892	0.0029	0.6668	0.1030
3	A	44.6894	0.0154	0.0009	3.4517
4	A	53.7282	0.0187	5.1255	0.1676

5	A	54.5707	0.0289	0.0127	0.0587
6	A	80.7084	0.0482	0.1610	0.5639
7	A	100.9584	0.1016	0.7488	0.0062
8	A	111.1602	0.1357	0.0079	0.2038
9	A	146.6188	0.1006	0.0444	0.4572
10	A	146.9969	0.1196	4.8827	0.0820
11	A	210.7804	0.2350	0.7388	0.4286
12	A	219.1602	0.2802	1.3290	0.3314
13	A	221.7067	0.4938	0.8584	1.3159
14	A	223.7057	0.4306	0.0231	0.4079
15	A	289.9174	0.4580	1.3884	0.0119
16	A	290.0573	0.4727	2.5373	0.3197
17	A	312.3642	0.3283	2.7925	0.2030
18	A	313.5627	0.3183	1.5914	0.7136
19	A	320.4049	0.5785	2.4329	0.5431
20	A	328.3493	0.6693	0.3619	1.0953
21	A	335.4209	0.9056	0.9413	0.0912
22	A	335.9331	0.8866	2.0081	2.9056
23	A	383.6768	0.1741	167.5140	0.2948
24	A	389.3307	0.1833	39.9226	1.5610
25	A	406.9369	0.7886	17.8333	0.4794
26	A	407.1989	0.8178	0.1020	6.7227
27	A	418.9195	0.2031	406.3010	1.1165
28	A	419.4949	0.1905	52.1276	2.7932
29	A	473.8661	0.1791	35.9806	0.5152
30	A	476.2262	0.3780	6.4437	1.0233
31	A	477.5565	1.0857	5.0957	4.7643
32	A	479.4273	0.2830	1.2367	1.6371
33	A	610.1718	1.9646	12.5313	0.4661
34	A	610.3461	1.9292	0.4005	40.0558
35	A	633.1342	3.6096	10.0675	2.1345
36	A	633.4664	3.4942	2.6866	2.2908
37	A	645.9266	2.9258	5.1272	0.6547
38	A	648.3475	2.8723	0.4202	0.4727
39	A	678.2831	3.3033	1.0264	0.0502
40	A	682.3832	3.2609	0.3160	0.2806
41	A	701.5971	1.8204	0.9319	0.0391
42	A	702.1077	1.8272	0.0396	0.4072
43	A	736.3530	3.8100	27.8730	0.0844
44	A	741.0198	3.8893	0.0001	0.8040
45	A	848.7285	2.8428	43.2692	0.4372
46	A	850.5632	2.8082	113.0133	1.8713
47	A	1072.3546	5.8427	82.2363	0.2688
48	A	1075.6023	6.9459	12.9797	1.2550
49	A	1116.9413	5.6501	84.2861	0.0436
50	A	1118.2348	3.7256	34.0962	1.5549
51	A	1134.7712	1.5759	16.5524	0.4442
52	A	1139.3535	1.7782	162.5070	1.1190
53	A	1246.7218	6.0250	1.2681	3.6694
54	A	1251.3322	6.0165	76.6800	3.6976

55	A	1366.4866	8.0041	6.1859	5.7005
56	A	1368.5435	8.1058	36.0403	15.8109
57	A	1422.5587	13.8072	106.4233	2.2873
58	A	1426.8653	13.4607	5.2450	6.5142
59	A	1472.0945	13.0806	189.7359	2.8808
60	A	1478.2675	13.1261	380.4801	1.7439
61	A	1528.2073	7.7930	29.3461	1.6157
62	A	1532.8323	7.3935	272.4793	0.1309
63	A	1624.3133	14.5059	0.4805	0.5140
64	A	1628.1722	13.1234	24.7472	3.2412
65	A	1634.2524	3.2763	0.3670	0.9142
66	A	1636.1783	2.9993	26.6303	2.8395
67	A	1670.5928	4.8018	327.7037	5.7812
68	A	1671.1856	4.1918	422.2272	13.4422
69	A	3590.3043	7.9429	114.0539	8.5298
70	A	3590.5530	7.9435	39.9516	143.2643
71	A	3702.6042	8.9155	50.8269	5.6351
72	A	3702.9873	8.9172	61.2121	28.5403

02_p3

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	10.7445	0.0011	0.1409	1.0409
2	A	24.9881	0.0047	1.0241	2.6131
3	A	41.2527	0.0141	0.4304	2.4806
4	A	47.8755	0.0149	0.0492	0.6692
5	A	55.1925	0.0326	0.0376	0.0517
6	A	81.0826	0.0512	0.8016	1.1480
7	A	103.8028	0.1053	0.1223	0.0760
8	A	110.3804	0.1287	0.3916	0.1468
9	A	146.8439	0.1240	1.5649	0.1331
10	A	151.6333	0.1083	3.5974	0.3402
11	A	212.4058	0.2258	1.4943	0.5202
12	A	218.9328	0.2760	1.1265	0.6658
13	A	221.5282	0.5015	0.4311	1.1197
14	A	222.4138	0.5068	0.5100	0.3730
15	A	290.1894	0.4717	3.0006	0.1688
16	A	290.8807	0.5021	0.7249	0.1490
17	A	312.7957	0.3030	2.4311	0.3066
18	A	315.0226	0.3057	0.8437	0.8299
19	A	320.9826	0.6148	2.5569	1.0028
20	A	325.0283	0.6064	0.8983	0.1737
21	A	335.6174	0.9046	0.9216	0.9515
22	A	335.9527	0.8967	1.3347	2.1584
23	A	386.6218	0.1985	33.8549	0.8630
24	A	400.1697	0.2928	15.1548	1.8236
25	A	406.5171	1.1722	1.9573	5.2405
26	A	407.4796	0.9847	1.8478	2.9457

27	A	442.8610	0.2260	249.0122	1.2223
28	A	460.5214	0.1742	42.0045	0.2974
29	A	470.8113	0.2587	8.4312	2.0714
30	A	475.9798	1.0531	4.0829	4.2041
31	A	481.8736	0.3997	65.7139	2.1310
32	A	513.9357	0.2004	181.7985	2.7322
33	A	610.0469	1.7829	4.0859	7.6148
34	A	610.9794	1.8303	9.7209	34.1426
35	A	632.2526	3.4841	7.1005	1.6913
36	A	632.7906	3.3961	8.2870	1.9705
37	A	645.8752	2.9245	4.2296	1.2699
38	A	647.7877	3.0366	0.4306	0.1124
39	A	679.9451	3.2999	0.8888	0.2410
40	A	684.0333	3.3379	1.4034	0.1135
41	A	702.5351	1.8804	1.1762	0.1156
42	A	702.8669	1.8803	0.3658	0.2085
43	A	738.5610	3.8652	31.9103	0.2377
44	A	740.7865	3.9271	0.1565	0.2372
45	A	848.0631	2.9248	6.3992	2.2178
46	A	852.6413	2.8930	166.4709	0.1281
47	A	1078.2262	6.3266	39.3617	0.6444
48	A	1078.5830	6.3244	41.9311	0.8900
49	A	1113.5677	5.2548	23.6944	0.8627
50	A	1115.8949	5.6357	152.0938	0.5726
51	A	1142.9244	1.5617	21.3137	1.2654
52	A	1146.3041	1.6116	118.5702	0.5117
53	A	1242.9528	5.5419	28.3195	0.1812
54	A	1247.0326	5.7924	57.9748	6.5096
55	A	1363.9229	7.9033	9.5568	15.9204
56	A	1365.5147	7.7627	9.2166	6.6713
57	A	1426.9513	13.9994	11.4720	1.0997
58	A	1434.3168	13.9044	104.7091	7.8667
59	A	1470.5445	12.6605	9.0883	3.3396
60	A	1477.5696	12.2200	549.7685	0.4550
61	A	1521.0505	8.9792	285.7275	1.2398
62	A	1526.3446	8.1092	113.9155	1.5271
63	A	1628.8943	9.7312	10.1845	2.2268
64	A	1630.8472	3.4580	61.5058	4.3323
65	A	1633.9281	7.4633	13.9420	2.0433
66	A	1635.4056	3.4602	10.6926	1.8252
67	A	1664.5813	4.1635	5.7221	3.3782
68	A	1674.2591	4.8292	641.9369	16.9558
69	A	3577.0167	7.8871	73.5373	130.7751
70	A	3584.5296	7.9191	57.0227	66.7973
71	A	3686.5277	8.8272	52.5005	28.6575
72	A	3696.0848	8.8753	51.6346	16.6779

02_p4

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.7014	0.0005	0.8356	0.2464
2	A	19.7622	0.0030	0.6311	3.1017
3	A	37.6615	0.0111	0.0407	3.5722
4	A	53.4134	0.0168	5.8769	0.0855
5	A	58.8443	0.0339	0.2906	0.1338
6	A	78.4885	0.0466	0.2192	0.6757
7	A	101.0143	0.0967	0.6017	0.0137
8	A	112.2314	0.1431	0.0102	0.1737
9	A	143.5759	0.1108	1.1959	0.2449
10	A	147.6774	0.1175	2.5608	0.1484
11	A	210.7713	0.2386	1.0298	0.4183
12	A	218.2325	0.2592	1.0006	0.7213
13	A	222.0270	0.4631	0.7888	1.3499
14	A	222.3075	0.4825	0.1129	0.3019
15	A	289.6118	0.4519	0.9864	0.0168
16	A	289.7720	0.4657	2.9900	0.3164
17	A	313.0542	0.3251	1.5380	0.4478
18	A	313.3785	0.3169	2.2184	0.5207
19	A	321.5196	0.6196	3.6499	0.6700
20	A	326.0508	0.5995	0.2099	0.5840
21	A	335.3745	0.9379	0.7043	0.0539
22	A	335.5346	0.9070	2.0660	2.9564
23	A	380.0136	0.1479	279.7722	0.4430
24	A	389.9534	0.1656	71.0824	1.1619
25	A	405.4832	0.4234	1.8218	3.3734
26	A	407.4217	0.4932	48.6459	0.6098
27	A	411.5400	0.3040	189.6119	2.1113
28	A	412.7083	0.2467	82.7305	4.7955
29	A	475.1338	0.1936	13.2289	0.5184
30	A	476.9468	1.1013	7.0062	5.2325
31	A	477.4401	0.9963	4.1877	1.8027
32	A	482.3774	0.1823	4.6574	0.3381
33	A	609.8442	1.9600	4.7269	24.3323
34	A	610.5517	1.9836	8.1420	16.3146
35	A	633.0885	3.5590	4.0888	2.2908
36	A	634.4773	3.5692	8.0180	2.5195
37	A	645.8397	2.8325	0.4103	0.4053
38	A	646.6508	2.9524	6.3733	0.6367
39	A	677.5492	3.2860	1.0524	0.1585
40	A	680.4191	3.2629	0.2176	0.2064
41	A	701.0086	1.7998	0.8997	0.0854
42	A	701.8726	1.8138	0.2635	0.3170
43	A	734.8126	3.8036	17.3673	0.2354
44	A	741.4928	3.8910	11.6883	1.1185
45	A	848.6502	2.8275	32.0337	0.3801
46	A	850.7728	2.7881	128.1822	2.0046
47	A	1073.2116	6.0274	73.5352	0.2380
48	A	1075.3372	6.8692	16.9627	1.2713

49	A	1117.5552	3.7850	26.6851	1.5136
50	A	1117.8135	5.7039	99.1170	0.0483
51	A	1133.3670	1.5763	14.9596	0.4729
52	A	1137.3286	1.7338	162.6535	1.1901
53	A	1246.1998	6.1110	0.1640	3.5830
54	A	1251.4934	6.1542	80.8396	3.7153
55	A	1366.7726	8.0938	3.7870	9.7456
56	A	1368.8329	8.1806	41.7031	12.4780
57	A	1421.7488	13.8185	110.2775	2.4426
58	A	1425.4406	13.3571	3.3403	6.4674
59	A	1471.7380	13.2445	135.6619	3.5631
60	A	1478.9164	13.0936	432.3316	1.3436
61	A	1528.7165	7.4959	47.8614	1.4443
62	A	1532.2572	7.1810	240.8230	0.1645
63	A	1624.4312	13.3750	1.4286	0.6192
64	A	1627.2008	12.5154	24.8172	3.6117
65	A	1633.4962	3.0856	2.8918	0.5686
66	A	1635.8485	3.1072	24.1057	3.3524
67	A	1669.5337	4.8243	297.1616	9.9316
68	A	1672.0244	4.6436	469.1145	10.8308
69	A	3591.3958	7.9471	120.5407	21.3402
70	A	3591.6398	7.9478	38.1401	138.4927
71	A	3704.8047	8.9272	48.8925	15.0131
72	A	3705.2865	8.9300	68.0535	21.5523

02_p5

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.0121	0.0003	0.5087	3.2730
2	A	18.3932	0.0029	0.6666	0.1030
3	A	44.6893	0.0154	0.0009	3.4518
4	A	53.7301	0.0187	5.1214	0.1675
5	A	54.5759	0.0289	0.0170	0.0588
6	A	80.7098	0.0482	0.1611	0.5639
7	A	100.9594	0.1016	0.7489	0.0062
8	A	111.1614	0.1357	0.0079	0.2038
9	A	146.6191	0.1006	0.0445	0.4572
10	A	146.9966	0.1196	4.8831	0.0820
11	A	210.7810	0.2350	0.7390	0.4285
12	A	219.1610	0.2802	1.3293	0.3314
13	A	221.7065	0.4938	0.8585	1.3159
14	A	223.7074	0.4306	0.0232	0.4080
15	A	289.9173	0.4580	1.3887	0.0119
16	A	290.0573	0.4727	2.5371	0.3197
17	A	312.3644	0.3283	2.7925	0.2030
18	A	313.5628	0.3183	1.5911	0.7136
19	A	320.4068	0.5786	2.4331	0.5431
20	A	328.3515	0.6693	0.3623	1.0953

21	A	335.4211	0.9056	0.9414	0.0912
22	A	335.9331	0.8867	2.0078	2.9056
23	A	383.6733	0.1741	167.5568	0.2949
24	A	389.3289	0.1833	39.9348	1.5610
25	A	406.9383	0.7888	17.8008	0.4809
26	A	407.1996	0.8179	0.1069	6.7219
27	A	418.9203	0.2031	405.7615	1.1190
28	A	419.4954	0.1906	52.6239	2.7897
29	A	473.8714	0.1791	36.0067	0.5159
30	A	476.2277	0.3786	6.4473	1.0255
31	A	477.5568	1.0852	5.0884	4.7636
32	A	479.4322	0.2826	1.2327	1.6348
33	A	610.1716	1.9646	12.5313	0.4663
34	A	610.3460	1.9291	0.4005	40.0554
35	A	633.1340	3.6096	10.0674	2.1345
36	A	633.4664	3.4942	2.6868	2.2909
37	A	645.9262	2.9258	5.1267	0.6548
38	A	648.3485	2.8724	0.4203	0.4726
39	A	678.2827	3.3033	1.0262	0.0502
40	A	682.3841	3.2609	0.3160	0.2806
41	A	701.5975	1.8204	0.9318	0.0391
42	A	702.1078	1.8272	0.0396	0.4072
43	A	736.3533	3.8100	27.8730	0.0844
44	A	741.0197	3.8893	0.0006	0.8039
45	A	848.7292	2.8428	43.2695	0.4371
46	A	850.5629	2.8082	113.0128	1.8714
47	A	1072.3544	5.8427	82.2353	0.2688
48	A	1075.6023	6.9460	12.9786	1.2550
49	A	1116.9413	5.6502	84.2867	0.0436
50	A	1118.2351	3.7259	34.1026	1.5549
51	A	1134.7714	1.5759	16.5527	0.4442
52	A	1139.3541	1.7781	162.5028	1.1191
53	A	1246.7219	6.0250	1.2681	3.6696
54	A	1251.3330	6.0165	76.6796	3.6976
55	A	1366.4867	8.0041	6.1867	5.7006
56	A	1368.5436	8.1057	36.0404	15.8110
57	A	1422.5582	13.8072	106.4203	2.2873
58	A	1426.8650	13.4607	5.2459	6.5143
59	A	1472.0945	13.0806	189.7348	2.8808
60	A	1478.2680	13.1261	380.4824	1.7438
61	A	1528.2075	7.7930	29.3453	1.6156
62	A	1532.8327	7.3935	272.4771	0.1309
63	A	1624.3128	14.5058	0.4802	0.5141
64	A	1628.1716	13.1228	24.7503	3.2414
65	A	1634.2529	3.2763	0.3672	0.9142
66	A	1636.1788	2.9994	26.6277	2.8394
67	A	1670.5931	4.8017	327.7104	5.7822
68	A	1671.1863	4.1919	422.2192	13.4411
69	A	3590.3030	7.9429	114.0461	8.5487
70	A	3590.5517	7.9435	39.9599	143.2460

71	A	3702.6028	8.9155	50.8238	5.6356
72	A	3702.9859	8.9172	61.2143	28.5392

02_p6

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	17.5884	0.0027	1.2839	0.2894
2	A	32.6045	0.0077	0.0243	3.4818
3	A	40.5596	0.0136	0.0558	3.2474
4	A	52.2753	0.0262	1.7319	0.0260
5	A	60.6688	0.0191	8.8631	0.0367
6	A	76.0339	0.0526	0.0009	0.7043
7	A	105.5836	0.0888	0.3615	0.1922
8	A	110.1517	0.1228	0.5436	0.1132
9	A	143.0554	0.1003	1.2668	0.1738
10	A	147.7348	0.1147	3.2082	0.1270
11	A	211.6020	0.2306	3.0353	0.0632
12	A	221.4443	0.2868	0.0254	1.6441
13	A	222.2003	0.5025	0.3880	0.7032
14	A	223.0882	0.4870	0.2788	0.9423
15	A	289.6339	0.4697	0.5197	0.1642
16	A	290.1954	0.4743	3.1099	0.1255
17	A	313.6533	0.3095	2.4661	0.5858
18	A	314.8028	0.3124	1.2534	0.3617
19	A	324.4273	0.5700	0.7673	0.3965
20	A	325.8537	0.6219	0.7647	0.2917
21	A	335.6419	0.8993	1.2137	1.2572
22	A	335.8296	0.9306	1.2801	1.8912
23	A	389.8998	0.2219	7.1190	1.7302
24	A	392.7669	0.2162	14.9971	0.5086
25	A	407.1864	1.1691	1.3919	4.1498
26	A	407.7579	1.0424	2.1064	4.2385
27	A	456.7581	0.2259	266.9875	0.7068
28	A	462.2665	0.2053	7.8705	0.6161
29	A	468.3012	0.2184	151.1948	0.4652
30	A	472.4647	0.6084	9.2682	2.0300
31	A	481.3110	0.4849	162.2942	2.3106
32	A	495.8773	0.2235	116.6165	4.8232
33	A	610.5213	1.8981	10.6777	17.6676
34	A	611.0041	1.8379	9.3129	24.2543
35	A	635.5128	3.5690	7.2524	0.0531
36	A	636.0519	3.4370	5.0629	4.3959
37	A	646.8714	3.0349	0.4523	0.7951
38	A	649.6794	3.0503	10.0118	0.1406
39	A	679.2632	3.2884	0.5951	0.1922
40	A	680.5979	3.3105	0.7211	0.2216
41	A	702.8311	1.8615	0.2489	0.1579
42	A	703.4809	1.8622	1.1896	0.1722

43	A	739.2998	3.9166	1.3215	1.4278
44	A	741.4423	3.9119	33.2775	0.1494
45	A	849.8427	2.9044	0.6914	0.2816
46	A	854.3396	2.8685	174.5239	2.1898
47	A	1075.0089	6.7240	9.4173	0.8246
48	A	1083.0901	7.0251	75.8217	0.6034
49	A	1111.1596	6.2402	18.6376	0.7422
50	A	1120.5832	5.6943	130.6112	0.4626
51	A	1140.3031	1.5522	21.6018	0.2305
52	A	1145.2769	1.5208	115.7768	1.6671
53	A	1247.4417	5.8145	24.5512	5.6031
54	A	1249.9197	5.9217	57.8597	2.3844
55	A	1367.6198	7.6825	39.6797	1.2383
56	A	1369.2330	7.6266	2.2173	22.8923
57	A	1422.2039	13.8693	41.5688	5.4376
58	A	1424.3660	14.0571	72.0331	4.1484
59	A	1472.8816	13.1096	13.0783	2.5880
60	A	1479.6744	13.0628	605.2300	3.3055
61	A	1526.4934	7.7476	100.5247	1.3196
62	A	1530.7310	7.4899	202.0786	0.5751
63	A	1624.1610	12.4389	32.4667	3.8739
64	A	1624.9179	12.5027	10.9694	3.3357
65	A	1636.2539	3.0707	14.5634	1.6554
66	A	1638.5491	3.4983	14.0074	2.4691
67	A	1669.6820	3.9207	15.5845	22.0370
68	A	1676.8592	4.7296	653.6384	0.6352
69	A	3580.6855	7.9032	79.6928	79.3080
70	A	3584.3100	7.9189	75.4428	93.4323
71	A	3689.3687	8.8432	55.4671	18.8783
72	A	3694.9392	8.8724	61.2282	21.8780

03_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.4984	0.0004	0.0225	0.1102
2	A	11.0621	0.0014	0.1328	0.0042
3	A	22.2452	0.0049	0.0513	0.0452
4	A	30.3226	0.0081	0.1109	6.7612
5	A	42.1074	0.0182	0.4475	0.3965
6	A	55.1253	0.0287	0.9255	0.4921
7	A	89.6153	0.0272	52.0389	0.0127
8	A	94.2475	0.1116	0.0107	0.0115
9	A	96.0995	0.1143	0.0301	0.1104
10	A	103.4980	0.0869	0.1294	0.1854
11	A	127.9344	0.0127	136.8692	0.1379
12	A	203.6780	0.5558	0.7735	3.1482
13	A	205.9100	0.5476	0.0610	1.0420
14	A	208.0864	0.2563	0.5113	1.7548

15	A	208.8682	0.2823	3.1849	0.0807
16	A	248.4600	0.6080	0.4742	0.6513
17	A	250.6209	0.5907	1.2846	1.4620
18	A	304.3106	0.6102	7.2774	0.0806
19	A	309.2982	0.5830	3.9608	0.4463
20	A	321.2853	1.3542	0.3228	2.9365
21	A	324.1013	1.2769	0.7942	4.9226
22	A	328.3952	0.3042	2.6607	0.0177
23	A	337.9043	0.3488	2.8754	0.0550
24	A	354.6684	0.2133	29.5688	0.0362
25	A	358.3679	0.3958	5.1735	0.0586
26	A	400.7820	0.1509	85.5126	0.0024
27	A	407.8669	1.4703	4.5697	8.4292
28	A	408.6289	1.4025	1.8598	2.7739
29	A	411.5312	1.0282	2.3333	4.3426
30	A	413.1726	0.9377	1.2141	3.7404
31	A	519.6488	0.1746	0.0048	0.0115
32	A	599.3068	2.0805	1.5817	8.2492
33	A	606.2030	2.0490	3.0310	60.7054
34	A	617.8199	2.9509	15.4142	23.4818
35	A	619.3931	0.2622	6.3217	0.0262
36	A	623.5837	3.4612	0.2604	5.3888
37	A	658.8698	2.7733	0.0470	0.0360
38	A	665.6054	1.4256	15.7352	0.5470
39	A	677.3474	1.3940	1.3887	0.8739
40	A	680.8824	3.2616	0.2186	0.1167
41	A	681.1862	1.3999	0.1737	0.1939
42	A	685.6128	3.0869	0.3968	0.5531
43	A	746.0820	3.0425	45.0594	0.3962
44	A	751.3564	3.1832	117.3126	0.1249
45	A	752.9136	3.7429	0.0086	0.0515
46	A	755.2300	3.9842	30.5319	0.4238
47	A	1065.4710	2.3963	2.3187	3.2602
48	A	1072.2127	2.8230	4.4400	0.2600
49	A	1088.6335	8.1258	293.3870	3.1157
50	A	1096.4455	7.0257	164.2578	5.6031
51	A	1107.8927	1.7676	109.3665	4.0201
52	A	1117.2948	1.7824	63.3069	0.1564
53	A	1138.5543	6.7646	0.2492	7.3754
54	A	1139.8107	6.6148	3.3414	9.9957
55	A	1352.2227	7.9735	53.5254	43.8073
56	A	1353.7382	7.7627	40.9585	26.3161
57	A	1417.0993	14.2758	143.7124	10.7160
58	A	1419.6460	13.9937	48.4897	12.4736
59	A	1455.7728	13.5694	275.0841	2.4158
60	A	1461.4185	12.9940	326.5917	4.6365
61	A	1506.9254	5.1748	24.1209	1.4520
62	A	1513.6329	6.0506	19.8469	3.8616
63	A	1597.7069	12.6481	45.0377	6.0840
64	A	1598.3694	14.7930	113.1348	3.2992

65	A	1624.2513	3.9702	90.5478	10.0158
66	A	1629.4224	6.5223	123.2748	10.9900
67	A	1656.6720	3.2830	1238.9708	42.9779
68	A	1670.9740	3.1756	121.9080	7.2259
69	A	3535.0437	7.7614	616.2475	527.9765
70	A	3606.7787	8.0087	105.4163	119.9354
71	A	3693.3437	8.8217	97.2167	28.2315
72	A	3728.8778	9.0602	80.1734	20.4215

03_pi

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	16.1328	0.0026	1.1454	0.0000
2	A	25.8398	0.0056	0.0000	3.9533
3	A	38.2349	0.0131	0.0000	3.5679
4	A	50.5552	0.0250	3.9281	0.0000
5	A	68.4860	0.0289	7.1205	0.0000
6	A	75.1837	0.0593	0.0000	0.6522
7	A	97.2865	0.1136	0.0735	0.0000
8	A	109.8005	0.1261	0.0000	0.2209
9	A	115.4347	0.0743	3.0430	0.0000
10	A	118.2804	0.0603	0.0000	0.4168
11	A	204.6573	0.5633	0.1505	0.0000
12	A	205.0043	0.5650	0.0000	2.3497
13	A	212.5971	0.2142	3.0372	0.0000
14	A	220.5130	0.2570	0.0000	1.9945
15	A	248.6102	0.5959	1.0750	0.0000
16	A	248.6625	0.5883	0.0000	1.1253
17	A	311.1278	0.6580	0.7889	0.0000
18	A	313.5650	0.5282	0.0000	0.5667
19	A	322.2435	1.3483	1.3755	0.0000
20	A	322.4445	1.3582	0.0000	6.7797
21	A	328.9835	0.3044	0.0000	0.0374
22	A	329.2049	0.3066	4.7677	0.0000
23	A	362.7365	0.3452	0.0000	1.0785
24	A	366.7200	0.3500	7.8415	0.0000
25	A	405.0252	0.9781	0.0014	6.7409
26	A	405.2330	0.8504	39.1715	0.0002
27	A	411.2921	1.0285	3.1079	0.0000
28	A	411.6669	1.0236	0.0000	6.1469
29	A	439.2972	0.1553	581.2260	0.0000
30	A	453.0764	0.1632	0.0008	3.9063
31	A	475.2926	0.1609	27.6130	0.0000
32	A	476.8966	0.1642	0.0000	0.5802
33	A	600.5925	1.9845	3.1502	0.0000
34	A	600.7358	2.0214	0.0000	34.1398
35	A	619.5531	2.9185	15.8022	0.0000
36	A	619.6900	2.8808	0.0000	12.7310

37	A	653.1255	2.9669	0.0000	0.6864
38	A	656.2972	3.0467	6.3806	0.0000
39	A	681.0338	1.7489	0.0000	0.1431
40	A	681.2853	1.6427	0.1619	0.0000
41	A	683.6794	3.0908	0.4076	0.0000
42	A	684.8543	2.7258	0.0000	0.4242
43	A	749.3812	3.4100	0.0000	0.6502
44	A	751.3625	3.6243	0.0000	1.1704
45	A	752.7729	4.0135	47.3364	0.0000
46	A	754.3879	3.1023	136.0807	0.0000
47	A	1071.7502	4.6268	10.7742	0.0000
48	A	1078.2997	5.1600	0.0000	1.1779
49	A	1085.4712	6.9052	0.0000	1.8650
50	A	1093.5465	7.7522	231.6120	0.0000
51	A	1133.2539	1.4976	0.0000	0.5758
52	A	1136.9362	6.9165	3.1513	0.0000
53	A	1138.4527	1.4239	137.8484	0.0000
54	A	1140.9329	5.3280	0.0000	5.6337
55	A	1356.0951	6.9020	42.9539	0.0000
56	A	1357.5970	6.8445	0.0000	29.7692
57	A	1419.7404	14.4341	0.0000	12.5161
58	A	1421.2864	14.3257	152.1915	0.0000
59	A	1455.0468	12.7595	0.0000	2.1058
60	A	1458.5328	13.0108	577.3470	0.0000
61	A	1500.2339	6.3004	32.0330	0.0000
62	A	1504.0336	6.0374	0.0000	1.5383
63	A	1601.1642	13.9175	0.0000	5.1006
64	A	1602.5573	13.6389	108.3049	0.0000
65	A	1621.7413	6.1764	0.0000	12.2080
66	A	1623.6043	4.0561	65.9623	0.0000
67	A	1658.7916	2.6639	0.0000	15.4529
68	A	1666.2676	3.3680	712.5070	0.0000
69	A	3582.8482	7.9111	136.9725	0.0425
70	A	3583.0295	7.9115	0.0403	144.9273
71	A	3694.1702	8.8707	0.0865	26.9735
72	A	3694.3232	8.8716	117.0706	0.0199

04_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	13.3790	0.0011	0.0854	0.0000
2	AU	19.1715	0.0023	1.6263	0.0000
3	AG	41.4822	0.0117	0.0000	6.4793
4	AU	50.8448	0.0166	5.3343	0.0000
5	AG	62.0690	0.0295	0.0000	0.7036
6	AG	102.6315	0.0662	0.0000	1.3917
7	AG	113.8876	0.1015	0.0000	0.6874
8	AU	114.7576	0.1094	1.2678	0.0000

9	AG	196.8076	0.2707	0.0000	1.9145
10	AU	196.8734	0.3030	9.2578	0.0000
11	AG	284.5989	0.7317	0.0000	2.1272
12	AU	285.4491	0.7694	5.4466	0.0000
13	AU	290.7044	0.4144	4.3992	0.0000
14	AG	296.2013	0.3840	0.0000	3.2387
15	AU	317.4624	0.4118	34.9299	0.0000
16	AG	320.6310	0.3531	0.0000	5.1363
17	AG	349.1464	0.0951	0.0000	3.2568
18	AU	356.1098	0.0987	235.0049	0.0000
19	AG	362.5053	0.3257	0.0000	3.0996
20	AU	366.7296	0.3099	37.1167	0.0000
21	AG	428.7920	0.7589	0.0000	5.2249
22	AU	430.5832	0.6457	25.5118	0.0000
23	AG	454.7228	1.3094	0.0000	8.1188
24	AU	457.8128	1.3656	2.9284	0.0000
25	AU	463.2936	0.4902	0.4886	0.0000
26	AG	470.0111	0.5313	0.0000	0.2266
27	AU	519.0313	1.7309	21.5821	0.0000
28	AG	519.3174	1.6765	0.0000	20.9828
29	AG	637.0038	0.8633	0.0000	5.2055
30	AU	646.5545	1.0232	13.1314	0.0000
31	AG	660.9022	0.3181	0.0000	1.7808
32	AU	691.8939	1.9756	3.4934	0.0000
33	AG	693.9474	2.6340	0.0000	1.6151
34	AG	697.9067	2.9630	0.0000	5.4765
35	AU	701.5891	2.5516	22.7659	0.0000
36	AU	717.9327	0.3757	81.9417	0.0000
37	AU	731.0210	2.2068	41.8457	0.0000
38	AG	736.2629	1.7385	0.0000	1.5598
39	AU	761.6809	2.7945	28.6361	0.0000
40	AG	764.7648	2.8450	0.0000	84.6876
41	AG	891.6484	0.7570	0.0000	0.6678
42	AU	891.8961	0.6427	53.2433	0.0000
43	AG	893.3499	1.2334	0.0000	0.6294
44	AU	902.4526	1.8934	184.9767	0.0000
45	AU	1102.2716	1.3352	88.1298	0.0000
46	AG	1116.6486	1.4052	0.0000	3.2215
47	AU	1136.4339	2.9588	114.4276	0.0000
48	AG	1137.7563	2.8435	0.0000	11.1821
49	AG	1201.5041	2.0515	0.0000	0.9944
50	AU	1202.9643	1.8874	119.4247	0.0000
51	AU	1258.4012	4.2921	349.6943	0.0000
52	AG	1259.4600	4.1214	0.0000	1.1803
53	AU	1342.6789	5.6274	74.4852	0.0000
54	AG	1343.8231	5.2651	0.0000	19.1840
55	AG	1425.2498	8.1450	0.0000	28.3914
56	AU	1428.3892	10.1718	235.0301	0.0000
57	AG	1458.4810	9.4508	0.0000	14.4405
58	AU	1467.1567	10.8846	139.7167	0.0000

59	AG	1533.5459	10.2443	0.0000	7.8800
60	AU	1536.2582	5.6068	992.1691	0.0000
61	AU	1621.2546	8.9122	43.6110	0.0000
62	AG	1621.8248	12.3135	0.0000	23.0278
63	AU	1662.6821	3.0033	165.1859	0.0000
64	AG	1674.6348	2.4225	0.0000	4.5159
65	AG	1696.8419	6.7179	0.0000	32.5997
66	AU	1701.9313	6.3325	363.9168	0.0000
67	AG	3215.5429	6.6615	0.0000	268.5909
68	AU	3215.5475	6.6616	3.2006	0.0000
69	AG	3386.9957	7.2049	0.0000	958.8319
70	AU	3415.5243	7.3274	2111.3591	0.0000
71	AG	3692.8116	8.7425	0.0000	103.6969
72	AU	3692.9345	8.7453	229.0849	0.0000

04_p1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	18.0043	0.0020	0.2860	1.2574
2	A	33.8916	0.0081	0.1101	2.0214
3	A	44.9263	0.0144	0.2440	0.8541
4	A	50.4702	0.0141	0.1487	1.5824
5	A	62.3751	0.0240	0.5825	1.6486
6	A	88.0485	0.0498	0.1218	1.7917
7	A	122.5669	0.0796	5.0708	0.4683
8	A	130.6033	0.0699	1.2448	0.8344
9	A	202.3122	0.2193	1.4709	0.5291
10	A	214.3456	0.2450	0.9186	0.5018
11	A	281.1407	0.3530	6.1793	0.6052
12	A	281.8652	0.3687	2.3980	0.6724
13	A	295.9642	0.2474	6.6977	0.4341
14	A	299.8049	0.3136	2.6489	0.0953
15	A	302.0991	0.3530	5.2853	0.5891
16	A	306.0376	0.3646	15.2467	1.9180
17	A	347.0853	0.3956	0.8708	0.0445
18	A	349.6987	0.3594	3.2870	0.2003
19	A	363.8389	0.1067	32.8754	0.4286
20	A	401.3779	0.1376	17.6428	1.2755
21	A	445.5964	0.7442	7.7530	1.9040
22	A	448.9836	0.5246	8.0912	4.0116
23	A	455.2911	1.3217	0.6974	3.4398
24	A	457.1762	0.9302	1.9721	2.0128
25	A	469.8934	0.5018	10.7304	0.9381
26	A	473.8978	0.5360	1.7830	0.1488
27	A	516.1052	1.6519	5.4778	6.1028
28	A	517.2320	1.6211	6.4649	11.6537
29	A	561.5435	0.2559	305.2122	2.8773
30	A	598.8584	0.3146	291.4066	2.0067

31	A	637.3871	1.0692	1.3354	1.7515
32	A	638.0618	1.0694	6.0359	0.8917
33	A	689.0360	3.1005	7.0955	0.8108
34	A	693.8514	2.9170	9.8186	0.6788
35	A	698.3278	2.2553	15.7419	0.6330
36	A	700.0388	2.8441	5.2067	1.1819
37	A	738.4058	2.7949	66.7627	3.1313
38	A	739.6762	2.7241	7.4236	0.9885
39	A	760.4996	2.6180	16.1292	32.6100
40	A	761.9559	2.5408	16.7365	12.8988
41	A	888.5342	1.4987	31.1193	0.5001
42	A	890.7659	1.4428	97.6068	0.3702
43	A	893.1553	0.7154	45.9502	0.2414
44	A	895.6699	0.6774	16.2604	0.2399
45	A	1111.0518	1.4106	31.7969	0.8277
46	A	1120.4812	1.4632	54.7099	0.9762
47	A	1134.3983	3.1600	50.4344	4.2726
48	A	1136.1332	3.0137	30.6305	4.8249
49	A	1201.4116	1.8039	78.3127	0.8646
50	A	1203.6571	1.8124	29.0423	0.3256
51	A	1252.7102	4.1012	53.8591	0.3029
52	A	1254.7838	3.9629	148.6628	1.2285
53	A	1342.2765	5.7465	28.8177	0.3506
54	A	1348.9340	5.5500	29.5757	1.4294
55	A	1414.8786	10.1359	25.4517	2.1401
56	A	1422.5157	10.4789	54.0555	23.7414
57	A	1467.2073	9.1148	48.2773	1.4040
58	A	1470.4577	8.7365	45.2074	2.2668
59	A	1512.0961	8.0654	284.7565	2.0368
60	A	1524.0813	7.8816	784.6372	1.0131
61	A	1631.4572	5.7662	27.6155	4.4211
62	A	1633.2853	2.5572	104.8093	1.8578
63	A	1636.0803	11.2354	9.8008	4.6291
64	A	1643.2804	2.2597	43.3781	0.9824
65	A	1680.8272	9.4246	34.3744	20.6166
66	A	1685.1791	9.1612	99.2409	17.7158
67	A	3217.1216	6.6697	3.2708	65.5438
68	A	3218.6910	6.6754	1.9278	96.6961
69	A	3568.7445	7.8535	52.4957	105.1515
70	A	3573.2693	7.8736	57.6545	159.2819
71	A	3674.3831	8.7538	37.0831	21.8854
72	A	3683.0358	8.8008	42.7606	40.7504

04_p2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	10.3147	0.0006	0.6634	0.2506
2	A	13.5061	0.0011	0.7555	3.5954

3	A	35.9988	0.0095	0.0557	2.8484
4	A	47.4825	0.0136	1.2855	0.1638
5	A	57.3089	0.0192	0.2083	0.2329
6	A	77.5871	0.0350	0.0133	1.1489
7	A	118.7719	0.0725	0.0098	0.7264
8	A	121.5851	0.0796	4.4284	0.1173
9	A	204.6003	0.2329	1.3847	0.2987
10	A	210.9571	0.2492	0.5867	0.8791
11	A	280.1766	0.3520	1.9335	0.4554
12	A	281.4670	0.3874	7.9412	1.0478
13	A	295.5411	0.3566	11.0587	1.7119
14	A	299.8562	0.3483	0.8985	0.0646
15	A	300.1789	0.3075	3.9845	0.2057
16	A	305.8123	0.3811	0.0007	0.1870
17	A	348.6655	0.5378	2.4843	0.1695
18	A	348.7847	0.5644	0.0107	0.2278
19	A	405.3940	0.1588	2.7678	0.2200
20	A	406.1623	0.1477	17.1809	1.5027
21	A	438.2996	0.1937	330.4299	0.0507
22	A	450.8599	0.2815	0.2505	3.6302
23	A	453.0445	0.9881	3.5356	1.7729
24	A	454.9170	0.9492	2.0187	3.7662
25	A	462.0581	0.4195	97.2441	0.9735
26	A	464.3089	0.3662	5.7263	0.4157
27	A	490.2864	0.2831	338.5528	0.4206
28	A	501.4679	0.2644	50.2178	0.6125
29	A	515.9617	1.3467	29.9824	0.6030
30	A	516.3165	1.3200	12.7379	18.8143
31	A	634.6327	1.0661	1.2501	1.5610
32	A	635.0351	1.0621	1.1493	0.9536
33	A	689.6291	3.0326	6.6214	0.4799
34	A	691.4764	2.9205	17.6682	1.4137
35	A	693.8493	3.2261	0.8684	0.5438
36	A	696.5266	3.1602	5.8075	0.6065
37	A	733.9974	2.9763	31.6137	0.8901
38	A	738.1039	2.9884	0.0121	1.1422
39	A	760.4053	2.7186	8.5758	0.6489
40	A	761.0322	2.6670	16.7028	41.2880
41	A	885.2563	1.6701	15.6605	0.4098
42	A	887.8635	1.5025	117.5325	0.5307
43	A	893.1797	0.6770	55.8204	0.2851
44	A	896.0052	0.6598	0.3251	0.0982
45	A	1100.4599	1.3703	5.6870	0.4884
46	A	1104.0590	1.3796	66.7280	0.6860
47	A	1129.0982	3.3462	0.2498	3.9196
48	A	1132.8722	3.1822	80.0216	5.4058
49	A	1198.7845	1.8963	26.7287	0.0127
50	A	1198.7886	1.7503	84.2195	1.0966
51	A	1247.6017	3.6955	0.4242	0.3644
52	A	1253.1925	4.0830	202.1199	1.1844

53	A	1342.1292	6.0316	13.7348	1.5433
54	A	1345.3128	5.9759	43.8004	0.2435
55	A	1416.0049	10.0010	78.4288	0.1735
56	A	1422.5853	9.6316	5.6842	16.4405
57	A	1467.0960	9.1873	21.5690	1.3543
58	A	1469.7734	8.7375	52.8497	4.3264
59	A	1512.4373	7.6863	7.4105	2.0431
60	A	1528.0257	6.9719	956.0088	0.3499
61	A	1631.5635	7.5851	38.2134	2.5063
62	A	1631.8813	12.5715	10.6720	4.7258
63	A	1636.0933	2.4817	175.0821	0.4893
64	A	1636.1880	2.1308	5.7257	1.4784
65	A	1685.8902	10.7502	69.9313	18.3096
66	A	1686.6551	10.1673	115.3898	9.7078
67	A	3217.5471	6.6709	0.3665	18.7576
68	A	3217.8639	6.6720	4.4641	146.4586
69	A	3586.2893	7.9280	124.4407	8.8385
70	A	3586.4720	7.9280	24.7032	188.8129
71	A	3700.3775	8.8966	11.1828	32.4677
72	A	3700.5288	8.8974	83.6417	18.7030

04_p3

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	9.3746	0.0005	0.7959	0.3452
2	A	17.4698	0.0019	0.1330	3.6026
3	A	39.7394	0.0112	0.1096	3.3478
4	A	50.5117	0.0186	1.5048	0.1634
5	A	57.5086	0.0173	0.1016	0.2585
6	A	78.0173	0.0365	0.0199	1.1204
7	A	119.8554	0.0779	0.2638	0.5863
8	A	125.1391	0.0819	3.3758	0.1639
9	A	205.0683	0.2257	0.6615	0.2472
10	A	212.3929	0.2454	1.3070	0.9350
11	A	280.4265	0.3597	2.8482	0.7699
12	A	281.0213	0.3334	5.0551	0.7722
13	A	298.8445	0.3225	1.0825	0.7655
14	A	299.4758	0.3317	2.9388	0.2403
15	A	300.1803	0.3370	1.4478	0.8882
16	A	304.6494	0.3661	15.1704	0.4549
17	A	348.0018	0.5167	1.1585	0.1187
18	A	349.2142	0.5691	0.9472	0.1830
19	A	401.6470	0.1363	5.9610	0.9977
20	A	411.2912	0.1541	9.2657	0.6789
21	A	439.4093	0.2301	102.0548	1.1361
22	A	445.0981	0.2549	95.6484	1.5078
23	A	453.9496	0.9988	4.7127	1.7714
24	A	454.0524	1.0704	3.9947	3.5680

25	A	463.3195	0.4420	30.0848	1.0732
26	A	466.1235	0.4230	49.4468	1.4836
27	A	491.8202	0.2779	109.7146	0.8933
28	A	503.6556	0.2644	261.9909	0.7190
29	A	515.9984	1.5282	7.2432	11.4229
30	A	517.0129	1.2168	29.3674	7.9735
31	A	635.3718	1.0689	1.2776	1.0029
32	A	636.1141	1.0669	2.0256	1.4914
33	A	691.4313	2.9725	10.8592	0.7028
34	A	692.5582	2.9898	14.3714	0.4356
35	A	694.4920	3.1888	5.3822	0.6450
36	A	697.8092	3.1696	0.4921	1.2457
37	A	734.7330	2.9093	12.1262	0.8961
38	A	737.2337	2.8564	25.0136	0.8871
39	A	760.4149	2.6975	6.9974	35.7152
40	A	760.9306	2.7168	19.7145	7.5986
41	A	885.7253	1.0997	34.3471	0.4141
42	A	886.3894	0.9286	35.0516	0.2256
43	A	890.4140	1.2963	90.1666	0.4562
44	A	898.0339	0.6718	29.4832	0.1836
45	A	1103.5677	1.3735	57.5573	0.9146
46	A	1104.5857	1.3684	17.0403	0.9624
47	A	1132.9255	3.3606	18.5073	3.7701
48	A	1136.1979	3.3057	58.1106	4.5446
49	A	1199.1552	1.7721	48.7238	0.4475
50	A	1201.1920	1.8116	70.8815	0.4974
51	A	1251.4463	3.9230	36.3624	0.9095
52	A	1254.0223	4.0722	161.0022	0.1766
53	A	1341.4806	5.9814	13.7540	1.4071
54	A	1345.3376	6.1643	42.4076	0.2430
55	A	1417.2630	9.8109	70.9596	1.9584
56	A	1422.1905	9.6612	22.8283	15.6742
57	A	1466.6678	8.9849	19.9616	4.3544
58	A	1467.5963	9.2587	60.5901	1.1512
59	A	1514.3121	7.6340	207.7918	2.3505
60	A	1524.1222	7.2289	802.7652	0.5126
61	A	1630.5825	2.9457	130.2827	0.9521
62	A	1631.7083	5.6812	12.0088	2.2084
63	A	1634.5762	3.2179	28.0917	3.1427
64	A	1637.2579	3.6588	78.3780	3.7123
65	A	1684.4132	11.0142	34.0570	18.9120
66	A	1686.3194	10.7221	117.6848	12.6469
67	A	3219.5392	6.6804	3.9696	75.6446
68	A	3224.8349	6.7002	1.9911	77.0405
69	A	3584.7064	7.9193	76.6561	137.2304
70	A	3586.7663	7.9294	63.6109	114.8137
71	A	3700.0583	8.8943	39.8242	36.4317
72	A	3700.5870	8.8968	54.2912	28.4130

04_p4

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	14.8533	0.0013	1.1163	0.0000
2	AG	30.8168	0.0063	0.0000	2.9863
3	AG	40.3763	0.0096	0.0000	3.0824
4	AU	44.9772	0.0127	1.1090	0.0000
5	AU	52.0790	0.0147	2.0206	0.0000
6	AG	81.5733	0.0365	0.0000	2.6002
7	AG	120.2340	0.0789	0.0000	0.5598
8	AU	121.2688	0.0748	5.5949	0.0000
9	AU	200.5101	0.2290	1.8700	0.0000
10	AG	210.1624	0.2524	0.0000	0.9247
11	AU	281.0059	0.3516	10.5086	0.0000
12	AG	281.5297	0.3586	0.0000	1.2591
13	AG	298.0350	0.2633	0.0000	1.2552
14	AU	299.5817	0.2828	12.0790	0.0000
15	AG	301.7243	0.3811	0.0000	2.2430
16	AU	302.1708	0.3734	11.3593	0.0000
17	AU	348.0242	0.4844	2.7456	0.0000
18	AG	348.7802	0.4927	0.0000	0.3805
19	AU	388.3617	0.1196	25.4375	0.0000
20	AG	389.8204	0.1193	0.0000	0.9266
21	AU	443.8393	0.3523	124.3589	0.0000
22	AG	444.9154	0.5030	0.0000	4.5922
23	AU	454.8845	1.3398	1.0985	0.0000
24	AG	455.2699	1.3438	0.0000	5.6979
25	AG	466.8211	0.4243	0.0000	0.5109
26	AU	468.2686	0.4773	43.5794	0.0000
27	AU	511.2555	0.3554	399.6744	0.0000
28	AG	515.4986	1.5721	0.0000	17.0456
29	AU	517.5393	0.5304	273.2521	0.0000
30	AG	526.0153	0.2380	0.0000	4.3179
31	AG	635.3238	1.0743	0.0000	2.7252
32	AU	635.8140	1.0724	2.0014	0.0000
33	AU	689.3836	3.0009	21.6592	0.0000
34	AG	691.3222	2.8765	0.0000	2.1300
35	AU	694.8663	3.0506	19.5254	0.0000
36	AG	696.0595	3.0943	0.0000	1.2303
37	AU	736.9218	2.8402	44.4366	0.0000
38	AG	739.8571	2.8809	0.0000	6.7140
39	AU	760.3508	2.7289	29.3055	0.0000
40	AG	761.1533	2.6704	0.0000	43.9920
41	AG	885.4413	1.7111	0.0000	0.8069
42	AU	889.3085	1.6131	124.3308	0.0000
43	AU	894.8370	0.6663	54.8920	0.0000
44	AG	895.1717	0.6612	0.0000	0.2938
45	AG	1105.0680	1.3732	0.0000	2.4343
46	AU	1107.7758	1.4024	83.1264	0.0000

SI-207

47	AU	1129.6940	3.4822	65.3281	0.0000
48	AG	1134.6013	3.2043	0.0000	9.2709
49	AG	1196.6943	1.8626	0.0000	1.2030
50	AU	1199.8545	1.6776	102.4788	0.0000
51	AG	1251.0365	3.7896	0.0000	1.3303
52	AU	1253.9517	4.2633	233.0050	0.0000
53	AG	1344.6293	5.9006	0.0000	2.4862
54	AU	1346.4672	5.9491	43.7663	0.0000
55	AU	1413.2902	9.7058	70.7453	0.0000
56	AG	1423.7746	9.8441	0.0000	20.0618
57	AG	1468.2726	9.0049	0.0000	6.5048
58	AU	1468.2736	9.1981	68.5103	0.0000
59	AG	1512.0723	7.7067	0.0000	2.9758
60	AU	1527.5161	7.2042	990.5199	0.0000
61	AG	1631.7646	4.4526	0.0000	4.2115
62	AU	1632.9152	7.3908	45.8835	0.0000
63	AG	1636.8854	3.1034	0.0000	5.9286
64	AU	1638.6282	2.4410	176.5665	0.0000
65	AG	1686.3621	9.8823	0.0000	28.8483
66	AU	1686.6964	10.9222	154.7627	0.0000
67	AU	3218.3374	6.6744	3.9140	0.0000
68	AG	3218.3403	6.6744	0.0000	203.1013
69	AU	3584.7772	7.9220	129.7849	0.0000
70	AG	3584.7782	7.9213	0.0000	212.6517
71	AG	3695.9901	8.8699	0.0000	57.1446
72	AU	3696.0556	8.8703	91.7066	0.0000

05_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	8.9920	0.0006	0.0909	0.0000
2	AU	14.5716	0.0023	0.3347	0.0000
3	AG	27.3762	0.0064	0.0000	7.0337
4	AU	42.7810	0.0146	4.0465	0.0000
5	AG	60.1157	0.0294	0.0000	0.1399
6	AG	91.4634	0.0650	0.0000	0.8186
7	AG	112.4887	0.1061	0.0000	0.6286
8	AU	112.7558	0.1121	1.5039	0.0000
9	AU	121.8932	0.1619	0.2075	0.0000
10	AG	122.1166	0.1670	0.0000	0.3195
11	AU	197.5236	0.3302	13.9647	0.0000
12	AG	198.8283	0.3019	0.0000	0.9360
13	AU	204.8865	0.5177	1.6548	0.0000
14	AG	205.5374	0.5107	0.0000	3.2336
15	AG	283.8220	0.8336	0.0000	0.5812
16	AU	285.0538	0.8994	5.2465	0.0000
17	AU	311.9053	0.2467	54.5682	0.0000
18	AG	318.0335	0.1329	0.0000	2.2487

19	AU	318.0885	0.7425	18.9415	0.0000
20	AG	319.5776	0.3961	0.0000	0.9403
21	AG	334.8280	0.1847	0.0000	2.3124
22	AU	338.1430	0.1131	171.9521	0.0000
23	AG	341.8597	0.2476	0.0000	18.4126
24	AU	343.4181	0.2272	57.6847	0.0000
25	AG	410.2274	0.5939	0.0000	4.4590
26	AU	411.9345	0.5212	32.6784	0.0000
27	AU	432.5705	1.7572	3.6767	0.0000
28	AG	433.9653	1.9833	0.0000	10.3874
29	AG	464.9374	1.5957	0.0000	10.6641
30	AU	466.5338	1.6470	1.8407	0.0000
31	AU	555.0853	1.8228	32.7267	0.0000
32	AG	555.8499	1.7843	0.0000	51.0012
33	AG	582.9808	1.5954	0.0000	1.2848
34	AU	585.1477	2.0152	6.2483	0.0000
35	AG	664.2649	0.3157	0.0000	1.7626
36	AG	682.9634	1.3536	0.0000	1.6575
37	AU	689.5817	2.3330	1.1412	0.0000
38	AG	690.1921	2.6493	0.0000	2.0677
39	AU	692.9912	1.3520	5.6062	0.0000
40	AU	709.0777	0.7303	46.1662	0.0000
41	AG	709.5902	3.1987	0.0000	26.1749
42	AU	720.1501	0.7399	22.7951	0.0000
43	AU	731.3022	1.4836	43.0238	0.0000
44	AG	733.1889	2.3059	0.0000	1.4349
45	AU	912.9799	5.0980	289.4434	0.0000
46	AG	913.4781	5.0600	0.0000	23.9413
47	AG	962.5469	4.8991	0.0000	3.1823
48	AU	966.4986	5.1346	240.5522	0.0000
49	AU	1105.8434	1.3487	36.4720	0.0000
50	AG	1119.2446	1.4282	0.0000	6.6356
51	AU	1170.7214	7.6505	22.3057	0.0000
52	AG	1173.7776	7.8714	0.0000	12.0530
53	AG	1261.7321	6.7495	0.0000	3.5583
54	AU	1264.3004	6.4929	181.6167	0.0000
55	AU	1336.0294	6.9761	48.9199	0.0000
56	AG	1336.4325	6.6332	0.0000	24.7602
57	AG	1434.4740	8.0642	0.0000	23.7842
58	AU	1440.2012	11.9614	466.0276	0.0000
59	AG	1475.9181	13.4002	0.0000	23.6330
60	AU	1479.5418	14.1049	126.2010	0.0000
61	AG	1526.9323	11.7347	0.0000	7.2071
62	AU	1530.9210	6.1794	857.5098	0.0000
63	AG	1601.9251	15.4176	0.0000	36.7700
64	AU	1602.3672	10.3769	53.0180	0.0000
65	AU	1656.0249	3.7015	198.9572	0.0000
66	AG	1670.4972	3.5330	0.0000	5.7501
67	AG	1687.5790	3.7153	0.0000	24.3366
68	AU	1692.7424	4.5751	690.8701	0.0000

69	AG	3386.2776	7.2024	0.0000	1309.0710
70	AU	3414.5131	7.3236	2515.2076	0.0000
71	AG	3696.0225	8.7605	0.0000	102.4611
72	AU	3696.1028	8.7628	246.4965	0.0000

05_p1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	14.2049	0.0020	0.1919	1.2070
2	A	31.0474	0.0062	0.3214	2.5985
3	A	37.9058	0.0126	0.0456	1.4959
4	A	48.9664	0.0226	0.0253	0.0817
5	A	57.6175	0.0318	0.1018	1.7391
6	A	84.9126	0.0473	0.0874	1.1770
7	A	119.8774	0.1146	1.4218	0.2614
8	A	122.8385	0.1228	0.0718	0.1254
9	A	127.7396	0.0917	0.7376	0.2973
10	A	135.2693	0.1197	2.4721	0.7719
11	A	203.4382	0.4430	0.7166	1.7046
12	A	204.3381	0.4713	0.0573	0.3235
13	A	206.6724	0.2329	1.0020	0.4088
14	A	215.8623	0.2389	1.4190	0.4839
15	A	281.1806	0.4321	3.8290	0.2599
16	A	283.4320	0.6787	2.2342	0.1805
17	A	302.3899	0.2364	3.6406	0.8012
18	A	309.8912	0.2757	2.0091	0.3365
19	A	322.7933	0.6342	1.4410	2.0942
20	A	323.6364	0.4554	0.5490	0.1148
21	A	330.3168	0.6077	6.3959	1.3134
22	A	332.3211	0.5607	6.0112	1.1143
23	A	383.3479	0.1389	10.9467	0.3693
24	A	403.4135	0.2515	9.5504	3.0999
25	A	428.7411	1.8246	0.4575	4.9263
26	A	429.0106	1.8769	0.1008	0.1091
27	A	437.6359	0.2910	3.6649	0.4874
28	A	443.9443	0.2259	38.4284	1.3985
29	A	464.5699	1.4131	5.0965	3.9387
30	A	465.1834	1.5766	0.4004	2.5206
31	A	544.4072	0.5890	106.8501	6.9554
32	A	550.7862	1.7661	5.6735	20.4661
33	A	566.1386	0.4306	143.8082	8.7381
34	A	577.9313	1.1164	24.2400	1.3553
35	A	592.7949	0.9051	141.5397	2.8134
36	A	620.8462	0.3686	237.0766	4.6737
37	A	682.1183	1.6481	2.9027	1.0148
38	A	683.4439	1.6159	0.1540	0.1407
39	A	688.8171	3.2467	3.4068	1.6392
40	A	698.2439	3.2280	2.3001	0.5772

41	A	704.7208	2.7761	15.2952	4.0178
42	A	706.6530	2.1513	11.3707	1.4119
43	A	734.8256	3.7348	26.4804	3.1870
44	A	745.3442	3.3510	15.3535	0.8922
45	A	909.9018	5.0734	1.4264	0.0996
46	A	915.6809	5.0671	203.8087	8.0051
47	A	952.7524	4.6024	11.9388	0.2054
48	A	961.2463	4.5796	145.3045	0.4787
49	A	1123.2404	1.4402	2.6267	0.1103
50	A	1124.7207	1.4860	34.0602	2.5066
51	A	1162.6274	6.7099	1.0017	0.5692
52	A	1168.3001	6.8072	22.0965	9.2438
53	A	1256.8946	6.1911	3.7012	0.2497
54	A	1262.7418	6.0509	119.6470	1.7859
55	A	1334.8267	6.8823	12.0575	1.4646
56	A	1338.4108	6.3708	13.4634	3.5931
57	A	1432.0730	10.4067	2.8768	0.4895
58	A	1445.3338	10.4027	106.5092	12.2133
59	A	1477.3300	11.3559	2.0925	0.0761
60	A	1479.5353	11.3093	135.3445	6.5391
61	A	1495.5828	10.8776	44.6038	0.6146
62	A	1514.2559	9.6123	913.2778	1.8025
63	A	1614.6225	14.0474	15.4255	2.5407
64	A	1619.8904	8.1982	63.9160	3.1874
65	A	1634.0213	2.4685	59.3771	3.2826
66	A	1641.3728	2.5178	33.1547	0.2155
67	A	1664.5834	8.2455	59.1157	9.0698
68	A	1674.7868	6.3551	318.3685	22.1335
69	A	3560.6493	7.8237	133.4090	293.4295
70	A	3563.1417	7.8349	15.5071	7.9876
71	A	3668.9045	8.7292	41.7168	48.7367
72	A	3679.1149	8.7737	56.2292	31.9078

05_p2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	14.3252	0.0019	0.3620	1.5143
2	A	22.9725	0.0037	0.1204	2.4858
3	A	38.8721	0.0120	0.0333	2.8262
4	A	52.8980	0.0285	0.6608	0.1522
5	A	59.1921	0.0278	0.4926	0.3408
6	A	86.5823	0.0423	0.1500	1.4119
7	A	120.0406	0.0874	0.4534	0.4076
8	A	121.9042	0.1406	1.5059	0.0788
9	A	127.6662	0.1180	1.5491	0.2083
10	A	135.1827	0.1006	3.9872	0.2451
11	A	203.6036	0.4683	0.4551	1.6000
12	A	204.1580	0.4793	0.2940	0.3749

13	A	206.8880	0.2211	0.9732	0.1457
14	A	216.4706	0.2412	1.0866	0.5216
15	A	281.3083	0.5164	3.2897	0.1970
16	A	282.7778	0.5516	2.9075	0.2404
17	A	304.2293	0.2575	3.5016	0.5661
18	A	305.2121	0.2367	4.1676	0.5149
19	A	321.8426	0.5583	1.6442	1.0357
20	A	323.6097	0.6836	0.6910	1.4299
21	A	326.7252	0.5305	6.1677	0.4888
22	A	329.9519	0.5981	6.2969	0.7764
23	A	386.7603	0.1610	9.0529	1.2999
24	A	395.2168	0.2059	8.1917	1.5914
25	A	427.7711	1.7939	0.9565	2.0228
26	A	428.8156	1.7466	3.0971	3.1409
27	A	436.5071	0.2117	76.0552	1.0502
28	A	441.8390	0.2334	27.4705	2.1140
29	A	462.8573	1.2740	2.7106	0.4266
30	A	463.7548	1.3282	19.4675	5.4669
31	A	496.7637	0.2118	444.8280	2.0930
32	A	514.6900	0.2293	201.8668	0.7902
33	A	552.8745	1.2800	20.4508	35.6827
34	A	553.1667	1.3118	33.3652	2.2214
35	A	583.2830	1.8502	15.1863	1.3692
36	A	584.6617	2.2961	44.3290	0.2070
37	A	679.2917	1.5967	1.3027	0.4211
38	A	680.8140	1.5696	2.3455	0.4405
39	A	686.8485	3.1949	0.6484	0.7160
40	A	690.6313	3.2198	1.5748	0.5777
41	A	701.6132	3.1516	6.6931	3.3023
42	A	703.2382	3.2350	4.7009	3.7531
43	A	732.2733	3.8364	19.6696	0.8931
44	A	733.6862	3.8452	2.6364	0.6862
45	A	908.5424	5.0489	70.9515	6.0296
46	A	913.2406	5.0546	99.5841	1.0430
47	A	956.8736	4.4471	93.4665	0.3547
48	A	958.5710	4.5812	92.6915	0.2956
49	A	1113.0803	1.4068	26.2497	0.3834
50	A	1114.2554	1.4068	17.3363	1.9488
51	A	1162.1577	7.4092	6.9181	2.2608
52	A	1168.9165	7.7838	11.9711	8.4131
53	A	1256.3294	6.5178	39.6492	1.8460
54	A	1259.4554	6.5064	58.1453	0.9430
55	A	1334.1672	7.0407	16.4328	1.7233
56	A	1336.7785	6.9629	17.2743	2.4760
57	A	1436.6316	10.1336	117.4153	4.3725
58	A	1441.8919	9.8664	70.5490	5.5078
59	A	1477.8222	11.7197	42.1517	3.4201
60	A	1479.0386	12.7558	49.7470	4.8251
61	A	1508.0322	9.1787	372.0842	0.6109
62	A	1511.9632	8.4094	533.4018	0.2520

63	A	1611.7531	12.4979	23.2329	3.3441
64	A	1613.7742	14.0554	42.7920	4.2245
65	A	1635.4924	2.4142	58.6209	0.3933
66	A	1636.7461	2.3333	53.4564	0.7808
67	A	1671.4086	7.9907	188.4539	7.8220
68	A	1675.7374	8.0134	225.8320	18.6509
69	A	3582.9652	7.9137	82.6958	95.3764
70	A	3585.9888	7.9262	70.8374	119.5573
71	A	3695.1754	8.8692	44.1438	23.7226
72	A	3698.0790	8.8823	49.9146	31.9387

05_p3

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	9.0001	0.0006	0.7131	0.2310
2	A	21.4159	0.0039	0.0172	3.0378
3	A	35.6651	0.0107	0.1057	2.9940
4	A	44.2657	0.0217	0.9431	0.1031
5	A	55.3837	0.0198	1.5649	0.0311
6	A	79.8126	0.0357	0.0446	2.5539
7	A	120.2591	0.1158	0.0687	0.4950
8	A	121.6985	0.1207	1.3610	0.0501
9	A	127.9635	0.0973	1.4164	0.3934
10	A	129.2609	0.1095	0.8556	0.2251
11	A	203.5226	0.4596	0.6621	0.8536
12	A	203.7983	0.4652	0.3136	1.2379
13	A	207.6110	0.2217	0.8330	0.0783
14	A	213.4674	0.1438	2.8727	0.8814
15	A	250.1917	0.0530	114.5976	1.0329
16	A	281.9318	0.5188	4.3748	0.2157
17	A	283.0017	0.4761	5.6190	0.1396
18	A	303.5186	0.2344	21.2117	0.5804
19	A	306.0266	0.2519	3.7518	0.5807
20	A	323.0305	0.6913	7.0336	0.9373
21	A	323.3453	0.3598	35.5759	0.2100
22	A	323.8110	0.4476	19.7698	1.9652
23	A	329.9144	0.2660	30.4386	0.2881
24	A	337.4347	0.1182	254.6877	0.2391
25	A	398.1576	0.2253	0.2998	3.2819
26	A	401.5931	0.2636	0.7521	0.7837
27	A	428.6814	1.8609	0.6807	2.6625
28	A	429.4116	1.8460	0.7271	2.3489
29	A	452.7179	0.2261	5.4861	1.5402
30	A	461.1062	0.2476	4.8073	1.6779
31	A	465.8596	1.0775	3.4318	2.0527
32	A	467.1112	0.5459	0.4832	3.5830
33	A	552.3545	1.6662	2.4508	34.0548
34	A	552.4861	1.6273	18.2510	2.8525

35	A	582.0474	2.4473	4.8158	0.0830
36	A	584.2826	2.4622	16.2807	0.0339
37	A	676.2130	1.4858	0.4451	0.5299
38	A	677.4098	1.5056	0.5718	0.3003
39	A	689.0888	3.1764	2.7633	0.8568
40	A	691.1999	3.2025	1.3546	0.4287
41	A	700.3394	3.4607	5.5946	5.9461
42	A	700.8156	3.4892	10.2111	2.7926
43	A	732.5596	3.7463	6.3186	0.4776
44	A	734.6203	3.8288	8.9691	0.5348
45	A	909.6443	4.7567	31.1692	6.4303
46	A	913.4909	4.8135	171.4362	0.7072
47	A	955.3776	4.3954	20.0210	0.8412
48	A	959.3297	4.3617	154.3111	0.0615
49	A	1094.6530	1.3620	28.8120	1.1602
50	A	1099.5056	1.3683	28.4346	1.0860
51	A	1163.8730	7.6826	11.2149	3.4225
52	A	1167.5482	7.9480	3.4465	6.6984
53	A	1254.9712	6.8647	9.1065	2.5109
54	A	1257.8603	6.7057	99.0893	0.1693
55	A	1332.5983	7.6659	2.6871	4.5964
56	A	1336.0291	7.9695	29.2129	1.5800
57	A	1436.2733	9.8492	162.7032	1.4097
58	A	1442.9107	9.7847	19.5008	9.1741
59	A	1477.5140	12.6455	19.6090	8.3935
60	A	1479.4773	12.1330	91.3386	1.8784
61	A	1502.9604	8.1750	81.8356	2.0780
62	A	1516.0038	8.1582	811.5178	0.0938
63	A	1613.9001	14.2575	28.1743	3.2524
64	A	1615.2984	12.9786	38.0562	3.5739
65	A	1628.4596	2.3533	121.1950	0.7756
66	A	1629.7530	2.3076	48.3255	2.8309
67	A	1670.7807	9.1627	47.6536	20.7427
68	A	1674.9877	9.6798	389.7220	5.9802
69	A	3599.2208	7.9800	90.1127	128.8238
70	A	3604.8389	8.0034	96.1100	146.9844
71	A	3719.9233	9.0023	52.6011	35.2554
72	A	3728.4564	9.0495	58.3969	35.0336

05_p4

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	20.0409	0.0030	0.5280	0.0000
2	A	33.2115	0.0090	0.0000	3.6237
3	A	43.9794	0.0155	0.0000	2.8599
4	A	48.5004	0.0219	1.5998	0.0000
5	A	65.8178	0.0294	1.2759	0.0000
6	A	79.0508	0.0390	0.0000	1.4179

7	A	118.6578	0.0886	2.9758	0.0000
8	A	122.4900	0.1039	0.0000	0.4640
9	A	129.5976	0.1318	1.7934	0.0000
10	A	131.6686	0.1238	0.0000	0.3787
11	A	203.7343	0.4680	0.9666	0.0000
12	A	204.6405	0.4836	0.0000	1.8404
13	A	206.8147	0.2232	1.6927	0.0000
14	A	215.8146	0.2409	0.0000	0.6570
15	A	281.9430	0.5177	6.3404	0.0000
16	A	281.9621	0.5306	0.0000	0.3734
17	A	304.2907	0.2488	8.5645	0.0000
18	A	304.9704	0.2455	0.0000	1.0392
19	A	322.8061	0.6274	0.0000	2.2291
20	A	323.3608	0.6038	1.9766	0.0000
21	A	327.2383	0.6682	0.0000	1.2965
22	A	330.8533	0.5659	11.3329	0.0000
23	A	389.0312	0.1989	0.0000	3.2897
24	A	395.7527	0.2088	23.5241	0.0000
25	A	427.3926	0.6337	84.3396	0.0000
26	A	427.5736	1.3728	0.0001	4.6581
27	A	430.6006	0.1894	272.2336	0.0000
28	A	441.6511	0.1863	0.0000	2.4176
29	A	457.6922	0.4056	145.6083	0.0000
30	A	461.3087	0.6517	0.0000	4.6447
31	A	473.1936	0.3280	301.0328	0.0000
32	A	477.9952	0.2351	0.0000	3.9822
33	A	552.5566	1.5399	35.1747	0.0000
34	A	553.0728	1.4655	0.0000	38.2207
35	A	581.5431	2.3166	0.0000	0.7017
36	A	581.8993	2.3616	37.2904	0.0000
37	A	679.2039	1.5760	0.0000	0.9534
38	A	679.3136	1.5607	1.8616	0.0000
39	A	689.2546	3.1861	3.4646	0.0000
40	A	689.7167	3.2656	0.0000	1.5523
41	A	700.6590	3.2520	0.0000	6.1998
42	A	701.1322	3.2626	12.2867	0.0000
43	A	733.6263	3.8644	20.3314	0.0000
44	A	734.5539	3.8689	0.0000	1.1637
45	A	910.4834	5.0048	0.0000	7.2062
46	A	912.5459	4.9078	200.1779	0.0000
47	A	953.2732	4.5918	0.0000	0.8913
48	A	959.9958	4.4961	152.5122	0.0000
49	A	1108.2882	1.3721	0.0000	2.4821
50	A	1111.3429	1.3996	41.5793	0.0000
51	A	1161.2475	7.8554	13.0611	0.0000
52	A	1167.9800	8.0723	0.0000	10.7235
53	A	1254.7078	6.5804	0.0000	2.8909
54	A	1258.3914	6.2808	108.7650	0.0000
55	A	1336.3905	7.3578	35.1091	0.0000
56	A	1338.0391	6.9965	0.0000	4.0790

57	A	1437.0249	10.6057	184.0684	0.0000
58	A	1442.9729	10.2528	0.0000	11.2698
59	A	1478.5269	11.9265	0.0000	7.5362
60	A	1479.5843	11.0605	117.4654	0.0000
61	A	1502.0863	8.9364	0.0000	1.6560
62	A	1515.8156	8.4699	888.2821	0.0000
63	A	1614.0119	14.1546	73.4434	0.0000
64	A	1615.3548	13.3563	0.0000	6.3168
65	A	1631.8932	2.4146	0.0000	1.6019
66	A	1634.4303	2.3873	115.7403	0.0000
67	A	1671.1939	7.4917	0.0000	26.4053
68	A	1671.5407	8.1010	429.1364	0.0000
69	A	3588.8572	7.9373	0.4210	205.4252
70	A	3588.8693	7.9382	156.8671	0.5513
71	A	3703.4895	8.9134	0.0060	50.6797
72	A	3703.5951	8.9141	92.6243	0.0033

06_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.1103	0.0004	0.1041	3.3875
2	A	13.3058	0.0013	0.5400	1.5943
3	A	13.7521	0.0017	0.0674	1.2487
4	A	50.6141	0.0236	0.0495	0.7101
5	A	70.0409	0.0415	0.8960	1.2377
6	A	81.5081	0.0567	2.8431	0.0432
7	A	120.8950	0.1596	0.0104	0.0052
8	A	123.4893	0.1638	0.0668	0.0033
9	A	159.3622	0.1918	0.3418	0.0250
10	A	159.6305	0.2199	0.0412	0.0039
11	A	213.0498	0.3827	3.9567	0.1815
12	A	213.8157	0.3200	1.1654	0.2784
13	A	277.5429	0.6889	3.8267	0.3516
14	A	279.3787	0.4549	2.8981	0.4096
15	A	281.4913	0.8205	2.9227	0.4678
16	A	295.9949	0.7339	1.9083	0.6154
17	A	318.6762	0.6224	3.1557	0.1074
18	A	336.8309	0.6334	1.5130	1.1045
19	A	346.4085	0.9625	2.1928	0.7601
20	A	346.8890	1.1520	4.7577	0.7450
21	A	352.0751	0.9873	0.6379	0.8774
22	A	357.6738	0.7892	0.3492	0.1765
23	A	419.0924	0.2902	42.0628	2.6015
24	A	431.2060	1.3493	0.0405	2.5972
25	A	450.3916	0.1939	84.2515	0.5395
26	A	462.3661	1.9476	0.5004	4.4579
27	A	464.5708	1.9805	0.4368	6.4726
28	A	484.3080	1.9721	1.5744	5.7237

29	A	491.7756	2.0431	4.3091	5.7105
30	A	605.9186	2.9569	2.7991	8.2383
31	A	607.4689	2.9730	3.1136	34.7656
32	A	641.6377	2.7950	4.8262	0.6425
33	A	643.8221	2.8353	0.9037	0.5524
34	A	676.2722	3.2121	0.2211	0.1035
35	A	679.0256	3.2876	0.7596	0.0214
36	A	698.4989	4.3988	4.3675	14.6481
37	A	713.6634	3.3933	3.8175	2.3658
38	A	719.4406	3.2304	6.3341	17.3307
39	A	722.3826	1.6417	22.1322	1.7130
40	A	731.8916	2.4433	2.0112	0.1965
41	A	741.1517	3.4627	3.2652	0.1053
42	A	814.6499	0.4969	40.6796	0.1969
43	A	961.1172	3.7361	142.5088	0.6039
44	A	962.1868	4.6590	297.6147	0.3087
45	A	1106.2473	9.5555	456.9519	0.2098
46	A	1117.0613	9.7378	197.9950	0.3910
47	A	1141.6885	8.4439	3.5757	1.7912
48	A	1159.4078	6.3037	17.9454	1.4517
49	A	1271.5788	1.8844	106.4971	1.0756
50	A	1288.2718	5.6392	3.1643	1.0986
51	A	1303.0340	8.1897	119.3227	6.5595
52	A	1307.1168	3.1016	108.2758	3.4959
53	A	1371.9650	4.5047	40.4783	7.6497
54	A	1384.5380	2.9316	96.9584	17.6674
55	A	1434.4294	15.0284	25.0804	4.3231
56	A	1440.1189	12.1626	2.3023	8.4866
57	A	1499.6019	15.1502	717.4610	2.2384
58	A	1517.7059	16.0191	588.3961	3.2223
59	A	1546.4803	14.4211	210.3194	2.8000
60	A	1549.0128	13.1322	145.5649	1.9892
61	A	1651.7744	14.1353	58.1683	7.1047
62	A	1663.0667	13.9933	30.3615	5.3201
63	A	1666.5762	17.1755	213.2088	8.1115
64	A	1676.6636	19.5285	154.9034	11.8650
65	A	3415.7826	7.3654	1947.1672	600.5494
66	A	3785.0592	8.9996	158.2047	81.6718

06_p1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	8.5624	0.0006	0.8965	0.0000
2	AG	25.1868	0.0045	0.0000	3.2133
3	AG	38.3899	0.0134	0.0000	2.1463
4	AU	42.3863	0.0174	1.0958	0.0000
5	AU	50.5317	0.0171	2.8300	0.0000
6	AG	70.1279	0.0434	0.0000	0.8323

7	AU	121.5406	0.1608	0.0515	0.0000
8	AG	125.5942	0.1686	0.0000	0.0458
9	AU	160.2789	0.1895	0.9977	0.0000
10	AG	161.0233	0.1827	0.0000	0.0962
11	AU	215.4598	0.3377	4.5378	0.0000
12	AG	223.2183	0.3449	0.0000	0.8986
13	AU	277.1313	0.7055	4.8881	0.0000
14	AG	277.7546	0.6807	0.0000	0.3570
15	AG	278.9423	0.4495	0.0000	0.4685
16	AU	279.0179	0.4355	6.0658	0.0000
17	AU	318.2634	0.6236	4.4952	0.0000
18	AG	319.3009	0.6263	0.0000	0.3225
19	AG	346.4894	1.1194	0.0000	0.5655
20	AU	346.8603	1.0996	4.1254	0.0000
21	AG	350.9051	0.7347	0.0000	0.9404
22	AU	352.5001	0.7487	0.0477	0.0000
23	AG	418.7443	0.1866	0.0000	4.5035
24	AU	424.1302	0.1953	157.6609	0.0000
25	AU	451.8653	0.2902	124.8564	0.0000
26	AG	454.6503	0.3009	0.0000	2.4378
27	AU	463.1092	1.7983	2.8472	0.0000
28	AG	463.4775	1.9629	0.0000	6.7902
29	AU	486.1665	1.9805	1.0180	0.0000
30	AG	486.7011	1.9807	0.0000	9.1155
31	AU	605.8358	2.9724	2.0484	0.0000
32	AG	606.1776	2.9702	0.0000	29.1729
33	AG	637.1173	2.7794	0.0000	0.7699
34	AU	638.4507	2.8305	11.6222	0.0000
35	AU	677.5341	3.2845	0.0485	0.0000
36	AG	677.8486	3.2613	0.0000	0.3627
37	AG	698.7411	4.3864	0.0000	16.7346
38	AU	698.9931	4.4119	6.4515	0.0000
39	AU	722.0538	3.6927	17.4410	0.0000
40	AG	722.1784	3.6991	0.0000	1.3417
41	AG	736.1690	3.1219	0.0000	0.3386
42	AU	736.2253	3.1042	9.8846	0.0000
43	AG	949.7677	3.8305	0.0000	0.5161
44	AU	956.4472	3.7071	350.3172	0.0000
45	AG	1098.3389	9.4235	0.0000	0.1376
46	AU	1109.1434	9.6256	424.1413	0.0000
47	AU	1139.1716	6.8701	51.8522	0.0000
48	AG	1147.8078	6.2331	0.0000	2.8339
49	AU	1271.5448	1.8791	175.9178	0.0000
50	AG	1272.9212	1.8740	0.0000	1.6869
51	AU	1294.4036	9.2339	82.7567	0.0000
52	AG	1295.0606	9.4023	0.0000	5.7494
53	AU	1374.6219	4.4915	67.1025	0.0000
54	AG	1375.3366	4.6899	0.0000	13.6720
55	AU	1435.7119	14.8994	45.4867	0.0000
56	AG	1436.7553	14.8422	0.0000	5.6131

57	AG	1498.4265	15.3394	0.0000	2.9664
58	AU	1509.1559	16.3651	1101.6670	0.0000
59	AU	1542.9380	14.4122	255.7161	0.0000
60	AG	1545.7329	14.5339	0.0000	3.8389
61	AG	1663.4920	19.5034	0.0000	9.9184
62	AU	1663.8397	15.0566	100.2788	0.0000
63	AG	1666.0674	13.8644	0.0000	4.1350
64	AU	1667.2955	17.3641	210.5580	0.0000
65	AU	3787.5734	9.0108	286.8439	0.0000
66	AG	3787.8878	9.0123	0.0000	123.0975

06_p2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	4.4718	0.0002	0.9776	0.0000
2	AG	21.1594	0.0038	0.0000	1.8106
3	AG	29.3108	0.0070	0.0000	1.9754
4	AU	31.7274	0.0092	0.0473	0.0000
5	AU	43.2082	0.0141	2.4440	0.0000
6	AG	77.3042	0.0453	0.0000	2.7432
7	AG	125.0635	0.1700	0.0000	0.0496
8	AU	125.8855	0.1730	0.0252	0.0000
9	AU	163.6076	0.1926	0.6220	0.0000
10	AG	164.8272	0.2054	0.0000	0.1098
11	AU	217.1402	0.3749	8.2828	0.0000
12	AG	218.5115	0.3251	0.0000	0.3368
13	AG	276.4295	0.6390	0.0000	0.4574
14	AU	276.9883	0.6348	6.0545	0.0000
15	AU	279.5616	0.4816	3.8852	0.0000
16	AG	280.5996	0.4738	0.0000	0.3385
17	AG	318.4309	0.6197	0.0000	0.3374
18	AU	318.9537	0.6252	4.0961	0.0000
19	AU	345.7289	1.0618	4.3932	0.0000
20	AG	346.9258	1.1218	0.0000	0.9677
21	AU	350.5972	0.7745	0.2444	0.0000
22	AG	350.9048	0.8557	0.0000	2.8712
23	AG	420.0823	0.2214	0.0000	5.3984
24	AU	429.4114	0.3424	81.6779	0.0000
25	AU	450.9988	0.1843	215.8876	0.0000
26	AG	459.3643	0.2482	0.0000	4.0228
27	AG	463.6751	1.8856	0.0000	8.2501
28	AU	463.7578	1.6781	4.9642	0.0000
29	AU	486.4823	1.9656	1.3117	0.0000
30	AG	486.8836	1.9043	0.0000	9.8972
31	AG	605.6693	2.9406	0.0000	31.4435
32	AU	605.6807	2.9613	1.9987	0.0000
33	AG	640.2762	2.7577	0.0000	0.6869
34	AU	641.8455	2.9006	10.2031	0.0000

35	AU	682.1826	3.3328	0.0882	0.0000
36	AG	682.7175	3.2822	0.0000	0.5125
37	AU	697.1631	4.3801	8.6576	0.0000
38	AG	697.5981	4.3916	0.0000	18.9503
39	AU	730.2188	3.7190	12.6405	0.0000
40	AG	731.6593	3.8048	0.0000	1.1451
41	AG	735.3392	3.0908	0.0000	0.4231
42	AU	736.0482	3.1191	9.1592	0.0000
43	AG	948.4601	3.7445	0.0000	0.6899
44	AU	954.0564	3.6951	356.9207	0.0000
45	AG	1096.9765	9.4565	0.0000	0.6325
46	AU	1106.1494	9.5699	473.6815	0.0000
47	AU	1139.6319	6.3929	57.0017	0.0000
48	AG	1144.3930	7.0854	0.0000	2.8703
49	AG	1267.6956	1.7023	0.0000	3.1099
50	AU	1271.8410	1.9618	147.3041	0.0000
51	AG	1288.3725	12.3570	0.0000	3.9916
52	AU	1288.8775	7.2972	119.4027	0.0000
53	AU	1371.7539	4.7435	61.9188	0.0000
54	AG	1373.9050	4.8265	0.0000	10.6252
55	AU	1437.6095	14.8110	49.4871	0.0000
56	AG	1438.5134	15.0729	0.0000	7.1602
57	AG	1500.3948	15.7388	0.0000	3.5103
58	AU	1507.7630	15.5510	1175.1806	0.0000
59	AG	1540.8815	14.0363	0.0000	4.0741
60	AU	1546.5097	14.6645	209.7339	0.0000
61	AU	1665.7175	15.9897	165.3433	0.0000
62	AG	1666.0789	19.5569	0.0000	12.6352
63	AG	1669.8241	14.0147	0.0000	7.0801
64	AU	1671.0554	16.9175	179.4486	0.0000
65	AU	3786.2167	9.0050	279.9388	0.0000
66	AG	3786.4738	9.0060	0.0000	106.9816

07_hb

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	12.3120	0.0015	0.0035	0.0000
2	AU	23.6330	0.0031	0.6312	0.0000
3	AU	62.6895	0.0297	4.1760	0.0000
4	AG	64.1840	0.0304	0.0000	3.8498
5	AG	84.5132	0.0620	0.0000	0.5207
6	AG	118.3583	0.1228	0.0000	0.1313
7	AU	119.2129	0.1316	0.0077	0.0000
8	AG	120.9124	0.1054	0.0000	1.0881
9	AG	200.4460	0.2839	0.0000	0.8752
10	AU	203.3436	0.3163	7.8713	0.0000
11	AG	286.8524	0.8369	0.0000	1.5329
12	AU	287.2786	0.8475	4.4884	0.0000

13	AU	297.5865	0.4412	0.5181	0.0000
14	AG	297.7982	0.4045	0.0000	3.4189
15	AU	322.8518	0.8209	17.7485	0.0000
16	AG	328.0541	0.7472	0.0000	2.2411
17	AG	380.0895	0.8427	0.0000	3.1949
18	AU	386.7530	0.7627	8.7689	0.0000
19	AG	439.1368	1.3708	0.0000	5.1023
20	AU	440.4296	1.3994	0.0081	0.0000
21	AG	454.9111	1.4654	0.0000	7.8211
22	AU	459.1412	1.6081	0.9407	0.0000
23	AU	474.4091	0.5418	0.4620	0.0000
24	AG	478.2487	0.5853	0.0000	0.0109
25	AU	522.2173	2.0545	20.5641	0.0000
26	AG	522.9538	2.0082	0.0000	19.4507
27	AG	662.3923	1.3965	0.0000	3.8332
28	AU	677.9503	1.4584	14.6755	0.0000
29	AG	696.7354	2.8692	0.0000	1.1923
30	AU	697.9694	3.0997	2.5395	0.0000
31	AG	708.7740	4.2789	0.0000	2.4645
32	AU	719.1450	4.2238	10.8738	0.0000
33	AG	725.7071	2.2178	0.0000	0.8534
34	AU	734.1210	3.0350	14.8809	0.0000
35	AU	764.3731	3.1017	25.2463	0.0000
36	AG	770.3121	3.1717	0.0000	80.6651
37	AG	831.2057	0.4500	0.0000	0.1838
38	AU	879.6024	0.4842	156.0478	0.0000
39	AU	897.8098	0.6574	67.3587	0.0000
40	AG	898.4183	0.6533	0.0000	0.3508
41	AG	914.2122	2.2154	0.0000	0.4155
42	AU	927.1123	2.6802	207.7246	0.0000
43	AU	1157.4038	2.8327	98.4204	0.0000
44	AG	1157.4802	2.9137	0.0000	9.2160
45	AG	1209.8343	1.8921	0.0000	0.2653
46	AU	1214.7633	2.1060	126.5008	0.0000
47	AU	1227.1308	3.7842	559.2520	0.0000
48	AG	1241.0765	5.8067	0.0000	2.9788
49	AG	1290.3649	6.7474	0.0000	6.0113
50	AU	1294.8499	6.8583	201.5534	0.0000
51	AG	1403.5403	3.0711	0.0000	3.0307
52	AU	1416.9381	2.2272	80.3614	0.0000
53	AU	1428.9008	11.8158	148.7560	0.0000
54	AG	1430.4281	8.2083	0.0000	47.9989
55	AG	1460.0611	7.4201	0.0000	2.6173
56	AU	1473.5818	5.2384	96.9401	0.0000
57	AU	1544.0823	13.0903	1449.5829	0.0000
58	AG	1561.1511	4.8746	0.0000	10.8117
59	AG	1639.6518	9.5155	0.0000	23.6207
60	AU	1648.4064	9.4627	8.1772	0.0000
61	AU	1688.1052	14.6631	136.5554	0.0000
62	AG	1693.7123	12.5257	0.0000	12.4371

63	AG	3186.3531	6.4286	0.0000	1027.5584
64	AU	3215.7263	6.6625	5.8035	0.0000
65	AG	3215.7744	6.6626	0.0000	219.1791
66	AU	3259.9145	6.7086	4623.5352	0.0000

07_p1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	22.2673	0.0037	0.0461	0.7219
2	A	33.4242	0.0065	0.1161	0.5836
3	A	38.7299	0.0124	0.0771	2.0231
4	A	42.4604	0.0129	0.1184	1.1929
5	A	52.0350	0.0178	0.2912	1.6332
6	A	82.9516	0.0416	0.1183	1.6432
7	A	120.4712	0.0898	0.4889	0.2230
8	A	121.7614	0.1127	0.9218	0.1671
9	A	206.1301	0.2563	1.3650	0.4023
10	A	214.2722	0.2904	0.6946	0.1204
11	A	282.8655	0.6573	2.4099	0.2888
12	A	284.4757	0.7178	0.9867	0.6369
13	A	303.1202	0.4356	3.0411	1.7164
14	A	304.9261	0.4713	0.9369	0.8292
15	A	305.9677	0.5818	1.1738	0.2437
16	A	309.1148	0.5907	3.5664	0.3366
17	A	354.2797	0.6610	6.8175	0.0992
18	A	357.6461	0.6789	4.8008	0.1137
19	A	422.3551	0.1638	127.8348	1.5223
20	A	430.7155	0.2009	79.4544	1.1973
21	A	455.0027	1.3858	1.3406	2.9049
22	A	455.2442	1.3899	1.5383	3.4822
23	A	463.1335	0.4840	53.8073	3.4484
24	A	465.1554	0.5458	4.5276	0.8523
25	A	487.6122	0.4938	54.6704	0.2280
26	A	504.0378	0.3491	24.4755	2.2018
27	A	518.2459	1.7973	7.9012	10.7301
28	A	518.6549	1.6573	6.5541	7.2697
29	A	651.9228	1.3304	21.2061	0.5508
30	A	652.0884	1.3282	8.0527	1.4462
31	A	695.3146	3.2450	3.1388	0.4875
32	A	696.4474	4.2259	16.5849	1.3104
33	A	696.6516	4.2226	12.5230	0.7476
34	A	698.1115	3.3149	0.5676	0.2164
35	A	733.1525	2.7977	2.8259	2.8043
36	A	734.2739	2.8015	29.3350	0.9169
37	A	760.2290	3.0480	14.6011	37.9192
38	A	760.4480	3.0526	5.7993	2.7600
39	A	898.0830	0.7107	25.2990	0.1339
40	A	898.9198	0.7415	40.9735	0.2935

41	A	902.5268	1.4410	33.4945	0.2592
42	A	903.5105	1.8367	79.6760	0.3509
43	A	1148.3472	4.0232	19.5985	1.5062
44	A	1151.9684	3.5220	12.8202	5.1894
45	A	1176.8991	1.9169	224.9192	1.6969
46	A	1180.8289	1.9474	291.9552	1.6366
47	A	1204.7749	1.7441	88.6235	0.2885
48	A	1206.5119	1.8751	44.5098	0.1877
49	A	1273.4351	3.8653	89.1495	1.6766
50	A	1278.5177	3.9812	191.7569	1.1746
51	A	1357.0280	3.6603	2.2271	0.3200
52	A	1362.7303	3.6475	13.3820	1.5488
53	A	1415.5567	13.1399	7.9261	1.8767
54	A	1421.3813	13.1692	14.6558	20.5293
55	A	1467.8274	10.0847	110.6934	0.4195
56	A	1470.1142	10.0307	50.5892	0.2000
57	A	1518.6645	9.5785	318.6226	2.0713
58	A	1528.3591	10.0172	804.3226	0.5452
59	A	1650.3198	11.8874	2.0743	3.4514
60	A	1652.7761	11.8135	1.4000	8.3071
61	A	1676.9264	15.3802	14.6299	3.3364
62	A	1678.6210	15.3693	33.7292	4.1820
63	A	3216.3534	6.6657	3.8140	73.4733
64	A	3219.7389	6.6800	3.8534	95.0542
65	A	3779.7121	8.9643	104.8061	62.8523
66	A	3785.0461	8.9899	110.5946	62.1153

07_p2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	AU	9.4658	0.0006	0.0833	0.0000
2	AG	19.1902	0.0022	0.0000	4.1009
3	AG	36.9791	0.0100	0.0000	2.5402
4	AU	40.2424	0.0130	0.3910	0.0000
5	AU	52.9205	0.0145	0.0252	0.0000
6	AG	70.7853	0.0409	0.0000	0.9818
7	AU	117.5399	0.1141	0.8320	0.0000
8	AG	120.2183	0.1118	0.0000	0.1507
9	AU	205.1680	0.2732	2.5002	0.0000
10	AG	211.5758	0.2712	0.0000	1.4491
11	AU	282.3082	0.6628	3.0302	0.0000
12	AG	282.6712	0.6548	0.0000	1.0507
13	AG	299.0818	0.4411	0.0000	2.2638
14	AU	303.1975	0.4351	3.0828	0.0000
15	AU	305.0587	0.6043	3.7488	0.0000
16	AG	305.3489	0.6121	0.0000	0.2757
17	AU	354.1194	0.6885	14.5034	0.0000
18	AG	354.4536	0.6834	0.0000	0.1171

19	AU	422.7992	0.1889	134.1839	0.0000
20	AG	425.1832	0.1840	0.0000	2.4234
21	AU	454.6602	1.4146	2.6800	0.0000
22	AG	455.2849	1.4211	0.0000	6.2885
23	AG	462.4374	0.5033	0.0000	5.0990
24	AU	463.1606	0.4676	32.7401	0.0000
25	AG	493.7808	0.3682	0.0000	1.3010
26	AU	494.8021	0.3672	99.1683	0.0000
27	AU	517.8473	1.8473	11.8851	0.0000
28	AG	517.9106	1.8187	0.0000	19.3963
29	AG	650.8285	1.3230	0.0000	1.9864
30	AU	650.8476	1.3243	36.3004	0.0000
31	AG	694.3057	3.3736	0.0000	0.7238
32	AU	694.4376	3.2620	4.9335	0.0000
33	AG	695.3523	4.0689	0.0000	1.6982
34	AU	696.5860	4.2453	27.6921	0.0000
35	AU	730.7263	2.8763	28.9356	0.0000
36	AG	731.3011	2.9096	0.0000	1.6579
37	AG	760.0231	3.0550	0.0000	38.3529
38	AU	760.0490	3.0422	21.0129	0.0000
39	AG	893.8692	0.6544	0.0000	0.2983
40	AU	894.2321	0.6549	57.6342	0.0000
41	AG	899.1228	2.0006	0.0000	0.8565
42	AU	904.0431	1.9578	108.8960	0.0000
43	AU	1147.4957	4.3484	21.8421	0.0000
44	AG	1152.5790	3.1860	0.0000	7.2412
45	AG	1174.4759	2.0489	0.0000	1.4029
46	AU	1176.8470	1.8343	624.2241	0.0000
47	AG	1205.0055	1.8192	0.0000	0.5220
48	AU	1205.2348	1.6819	95.7369	0.0000
49	AG	1273.2374	3.8949	0.0000	3.0589
50	AU	1276.9076	4.4030	290.8159	0.0000
51	AU	1358.3216	3.6860	14.4783	0.0000
52	AG	1358.4834	3.8003	0.0000	1.8734
53	AU	1415.8203	13.0409	8.8867	0.0000
54	AG	1420.7149	12.7348	0.0000	20.7654
55	AG	1466.9708	10.0122	0.0000	0.5062
56	AU	1469.1134	10.3792	152.7982	0.0000
57	AG	1519.5045	9.7621	0.0000	2.9438
58	AU	1531.7124	10.2310	1198.8505	0.0000
59	AU	1650.4192	11.8082	3.2488	0.0000
60	AG	1652.2237	11.8993	0.0000	11.7555
61	AU	1676.7693	15.4447	58.4463	0.0000
62	AG	1679.5961	15.6119	0.0000	7.5262
63	AU	3219.5893	6.6790	7.6972	0.0000
64	AG	3219.6145	6.6792	0.0000	152.1648
65	AU	3791.7877	9.0217	230.4690	0.0000
66	AG	3791.9082	9.0223	0.0000	180.2150

07_p3

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-10.8860	0.0009	0.1243	2.7971
2	A	13.7733	0.0014	0.0080	0.1605
3	A	36.8229	0.0111	0.0504	2.5859
4	A	48.2963	0.0148	0.0189	1.3624
5	A	50.0086	0.0144	0.0196	0.1341
6	A	71.9288	0.0374	0.0173	1.0981
7	A	118.5447	0.1089	0.3792	0.0014
8	A	121.0463	0.1075	0.0263	0.2960
9	A	206.7617	0.2699	3.0461	0.0595
10	A	215.8422	0.2970	0.0422	0.3984
11	A	282.8625	0.6590	0.1477	0.9298
12	A	283.8136	0.6780	3.3480	0.0859
13	A	300.3711	0.4447	2.5557	1.2152
14	A	303.5128	0.4410	0.0521	1.6486
15	A	305.8194	0.6104	1.4064	0.0772
16	A	306.4019	0.6281	1.1063	0.1057
17	A	354.7309	0.6858	13.0710	0.0540
18	A	354.7845	0.6871	0.0301	0.1727
19	A	433.8385	0.3226	73.6731	2.1925
20	A	443.0254	0.3078	0.4952	1.1743
21	A	455.2430	1.3976	2.5032	0.1007
22	A	455.5997	1.3693	0.1749	6.0447
23	A	467.9923	0.4133	0.0354	1.5202
24	A	470.3189	0.4040	36.7100	0.4972
25	A	503.0721	0.2762	0.9575	2.9182
26	A	506.8888	0.2679	188.6787	0.1396
27	A	517.6595	1.8319	0.7874	12.3254
28	A	518.0260	1.6919	14.8027	5.6601
29	A	650.6119	1.3277	22.8132	0.0115
30	A	650.9268	1.3257	6.4030	1.9155
31	A	694.0001	3.2667	5.0774	0.1474
32	A	695.8226	4.2254	13.7577	1.7131
33	A	696.2428	4.2342	13.5127	0.2742
34	A	697.0393	3.3253	0.1840	0.6914
35	A	727.9345	2.8795	28.7061	0.6729
36	A	729.7933	2.8499	0.0836	0.5690
37	A	760.1469	3.0393	16.3671	38.7463
38	A	760.5868	3.0447	4.2976	0.4964
39	A	893.5081	0.6736	6.5607	0.3245
40	A	894.3158	0.6872	63.8774	0.1557
41	A	900.4132	1.7467	38.2624	0.1401
42	A	902.5479	1.8553	71.7116	0.4088
43	A	1145.4805	4.0328	17.0317	0.0155
44	A	1151.8629	3.0739	17.8876	7.6821
45	A	1173.0656	2.0670	2.4261	1.7813
46	A	1179.5695	1.8488	555.1123	0.1556

47	A	1204.8349	1.7885	1.0967	0.0406
48	A	1208.8795	1.8029	95.3109	0.3371
49	A	1268.3452	3.8231	11.0760	0.3682
50	A	1277.9755	4.0684	251.7252	2.1161
51	A	1356.1882	3.9003	5.3313	0.0156
52	A	1358.2928	3.7932	3.9440	1.0997
53	A	1417.1360	13.0521	7.3902	2.1954
54	A	1421.2379	13.1990	13.5870	19.4315
55	A	1468.7773	10.6019	13.9939	0.3297
56	A	1470.3189	9.6907	118.9333	0.1759
57	A	1522.8425	9.4370	496.0298	2.3383
58	A	1525.1979	9.9249	657.5104	0.0584
59	A	1651.0087	12.1462	0.3543	0.0002
60	A	1654.7778	12.0184	0.2890	12.1385
61	A	1675.4860	15.4948	28.8867	6.4401
62	A	1676.3124	15.2469	23.2425	0.1682
63	A	3221.0685	6.6857	4.6237	60.1083
64	A	3221.0876	6.6859	4.6317	100.6611
65	A	3782.4018	8.9778	147.2071	18.2791
66	A	3782.5469	8.9781	67.2746	113.8156

Table S1. Topological properties computed at the ring Atom (ACP), Bond (BCP) and Ring Critical Points (RCP), *viz.* the total electron density (ρ), the Lagrangian kinetic energy (G), the Hamiltonian kinetic energy (K), the potential energy (V), the energy density (H), the Laplacian of the total electron density ($\Delta\rho$), the Electron Localisation Function (ELF), the Source Function (SF), the total Electrostatic Potential (EPS), the ellipticity of the total electron density (ϵ), and the eta index (η).

		ρ	G	K	V	H	$\Delta\rho$	ELF	SF	EPS	ϵ	η
0	ACP1	1.195E+02	7.776E+00	1.360E+05	-1.361E+05	-1.360E+05	-5.442E+05	1.000E+00	1.542E+04	6.984E+05	0.000010	-1.000018
	ACP2	1.195E+02	7.914E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.800E+04	6.864E+05	0.000017	-1.000021
	ACP3	1.196E+02	7.808E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.444E+05	1.000E+00	2.043E+04	6.635E+05	0.000011	-1.000022
	ACP4	1.195E+02	7.914E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.800E+04	6.864E+05	0.000017	-1.000021
	ACP5	1.195E+02	7.776E+00	1.360E+05	-1.361E+05	-1.360E+05	-5.442E+05	1.000E+00	1.542E+04	6.984E+05	0.000010	-1.000018
	ACP6	4.266E+02	1.682E+02	1.155E+06	-1.155E+06	-1.155E+06	-4.620E+06	1.000E+00	6.926E+04	1.213E+06	0.000039	-1.000045
	BCP1	3.602E-01	2.677E-01	5.309E-01	-7.986E-01	-5.309E-01	-1.053E+00	7.928E-01	3.176E-02	1.662E+00	0.251966	1.843804
	BCP2	3.182E-01	1.038E-01	3.302E-01	-4.340E-01	-3.302E-01	-9.055E-01	9.439E-01	3.136E-02	9.950E-01	0.382206	2.151574
	BCP3	3.172E-01	1.012E-01	3.284E-01	-4.295E-01	-3.284E-01	-9.089E-01	9.460E-01	3.836E-02	9.946E-01	0.375144	2.161915
	BCP4	3.172E-01	1.012E-01	3.284E-01	-4.295E-01	-3.284E-01	-9.089E-01	9.460E-01	3.836E-02	9.946E-01	0.375144	2.161915
	BCP5	3.182E-01	1.038E-01	3.302E-01	-4.340E-01	-3.302E-01	-9.055E-01	9.439E-01	3.136E-02	9.950E-01	0.382206	2.151574
	BCP6	3.602E-01	2.677E-01	5.309E-01	-7.986E-01	-5.309E-01	-1.053E+00	7.928E-01	3.176E-02	1.662E+00	0.251966	1.843804
	RCP	2.311E-02	3.325E-02	-7.856E-03	-2.539E-02	7.856E-03	1.644E-01	2.553E-02	-3.295E-02	2.971E-01	-1.197354	0.183200
1	ACP1	1.195E+02	7.767E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.531E+04	6.732E+05	0.000010	-1.000018
	ACP2	1.195E+02	7.934E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.835E+04	6.539E+05	0.000022	-1.000023
	ACP3	1.195E+02	7.980E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	2.016E+04	1.720E+06	0.000007	-1.000014
	ACP4	1.195E+02	7.934E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.835E+04	6.539E+05	0.000022	-1.000023
	ACP5	1.195E+02	7.767E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.531E+04	6.732E+05	0.000010	-1.000018
	ACP6	1.943E+02	2.576E+01	3.034E+05	-3.034E+05	-3.034E+05	-1.213E+06	1.000E+00	3.059E+04	6.179E+05	0.000004	-1.000029
	BCP1	3.593E-01	2.541E-01	5.231E-01	-7.771E-01	-5.231E-01	-1.076E+00	8.082E-01	3.193E-02	1.598E+00	0.244623	1.946738
	BCP2	3.215E-01	1.082E-01	3.374E-01	-4.456E-01	-3.374E-01	-9.169E-01	9.413E-01	3.186E-02	9.862E-01	0.420470	2.230390
	BCP3	3.091E-01	9.656E-02	3.125E-01	-4.091E-01	-3.125E-01	-8.638E-01	9.464E-01	3.702E-02	9.462E-01	0.305632	2.028859
	BCP4	3.091E-01	9.656E-02	3.125E-01	-4.091E-01	-3.125E-01	-8.638E-01	9.464E-01	3.702E-02	9.462E-01	0.305632	2.028859
	BCP5	3.215E-01	1.082E-01	3.374E-01	-4.456E-01	-3.374E-01	-9.169E-01	9.413E-01	3.186E-02	9.862E-01	0.420470	2.230390
	BCP6	3.593E-01	2.541E-01	5.231E-01	-7.771E-01	-5.231E-01	-1.076E+00	8.082E-01	3.193E-02	1.598E+00	0.244623	1.946738

	RCP	2.337E-02	3.353E-02	-7.750E-03	-2.578E-02	7.750E-03	1.651E-01	2.606E-02	-2.935E-02	2.669E-01	-1.190110	0.189768
2	ACP1	1.195E+02	7.717E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	1.643E+04	6.683E+05	0.000009	-1.000018
	ACP2	1.195E+02	7.935E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	2.374E+04	9.368E+05	0.000017	-1.000018
	ACP3	1.196E+02	7.933E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.444E+05	1.000E+00	2.185E+04	1.734E+06	0.000008	-1.000014
	ACP4	1.195E+02	7.947E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.544E+04	6.515E+05	0.000022	-1.000023
	ACP5	1.195E+02	7.762E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.281E+04	6.655E+05	0.000010	-1.000018
	ACP6	1.943E+02	2.576E+01	3.034E+05	-3.034E+05	-3.034E+05	-1.213E+06	1.000E+00	2.811E+04	6.148E+05	0.000005	-1.000029
	BCP1	3.604E-01	2.547E-01	5.256E-01	-7.803E-01	-5.256E-01	-1.084E+00	8.089E-01	3.205E-02	1.600E+00	0.237567	1.947979
	BCP2	3.147E-01	1.075E-01	3.252E-01	-4.327E-01	-3.252E-01	-8.706E-01	9.379E-01	3.708E-02	9.732E-01	0.369573	2.111912
	BCP3	3.006E-01	9.514E-02	2.973E-01	-3.924E-01	-2.973E-01	-8.085E-01	9.431E-01	4.636E-02	9.300E-01	0.266793	1.907108
	BCP4	2.513E-01	3.720E-01	3.293E-01	-7.013E-01	-3.293E-01	1.709E-01	3.736E-01	-3.756E-03	1.974E+00	0.094155	0.438130
	BCP5	3.233E-01	1.095E-01	3.414E-01	-4.510E-01	-3.414E-01	-9.276E-01	9.409E-01	2.586E-02	9.920E-01	0.423670	2.261854
	BCP6	3.594E-01	2.473E-01	5.203E-01	-7.676E-01	-5.203E-01	-1.092E+00	8.165E-01	2.748E-02	1.579E+00	0.231845	1.991470
	RCP	2.352E-02	3.366E-02	-7.715E-03	-2.595E-02	7.715E-03	1.655E-01	2.637E-02	-1.523E-02	2.600E-01	-1.196144	0.191973
3	ACP1	1.195E+02	7.713E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	1.388E+04	6.601E+05	0.000008	-1.000019
	ACP2	1.195E+02	7.945E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.891E+04	9.333E+05	0.000017	-1.000019
	ACP3	1.196E+02	7.881E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.444E+05	1.000E+00	2.513E+04	1.767E+06	0.000009	-1.000015
	ACP4	1.195E+02	7.945E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.891E+04	9.333E+05	0.000017	-1.000019
	ACP5	1.195E+02	7.713E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	1.388E+04	6.601E+05	0.000008	-1.000019
	ACP6	1.943E+02	2.576E+01	3.034E+05	-3.034E+05	-3.034E+05	-1.213E+06	1.000E+00	2.689E+04	6.118E+05	0.000005	-1.000029
	BCP1	3.606E-01	2.484E-01	5.233E-01	-7.717E-01	-5.233E-01	-1.100E+00	8.168E-01	2.859E-02	1.583E+00	0.224951	1.990031
	BCP2	3.165E-01	1.090E-01	3.292E-01	-4.382E-01	-3.292E-01	-8.811E-01	9.375E-01	2.894E-02	9.795E-01	0.372734	2.142376
	BCP3	2.992E-01	9.407E-02	2.943E-01	-3.883E-01	-2.943E-01	-8.008E-01	9.434E-01	4.092E-02	9.235E-01	0.262579	1.883518
	BCP4	2.992E-01	9.407E-02	2.943E-01	-3.883E-01	-2.943E-01	-8.008E-01	9.434E-01	4.092E-02	9.235E-01	0.262579	1.883518
	BCP5	3.165E-01	1.090E-01	3.292E-01	-4.382E-01	-3.292E-01	-8.811E-01	9.375E-01	2.894E-02	9.795E-01	0.372734	2.142376
	BCP6	3.606E-01	2.484E-01	5.233E-01	-7.717E-01	-5.233E-01	-1.100E+00	8.168E-01	2.859E-02	1.583E+00	0.224951	1.990031
	RCP	2.363E-02	3.375E-02	-7.664E-03	-2.609E-02	7.664E-03	1.657E-01	2.666E-02	-1.498E-02	2.531E-01	-1.202658	0.194047
4	ACP1	1.195E+02	7.776E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.724E+04	6.525E+05	0.000011	-1.000019
	ACP2	1.195E+02	7.880E+00	1.360E+05	-1.361E+05	-1.360E+05	-5.441E+05	1.000E+00	1.635E+04	6.445E+05	0.000018	-1.000023
	ACP3	1.196E+02	8.137E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.445E+05	1.000E+00	1.614E+04	2.130E+07	0.000011	-1.000013
	ACP4	1.195E+02	7.846E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	1.697E+04	6.133E+05	0.000019	-1.000024

	ACP5	1.195E+02	7.895E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.708E+04	1.766E+06	0.000005	-1.000010
	ACP6	1.943E+02	2.573E+01	3.033E+05	-3.034E+05	-3.033E+05	-1.213E+06	1.000E+00	3.769E+04	6.199E+05	0.000003	-1.000030
	BCP1	3.626E-01	2.620E-01	5.321E-01	-7.941E-01	-5.321E-01	-1.080E+00	8.032E-01	3.893E-02	1.606E+00	0.254322	1.909218
	BCP2	3.192E-01	1.048E-01	3.326E-01	-4.374E-01	-3.326E-01	-9.114E-01	9.435E-01	3.193E-02	9.618E-01	0.386780	2.174213
	BCP3	3.133E-01	1.039E-01	3.249E-01	-4.288E-01	-3.249E-01	-8.842E-01	9.411E-01	3.006E-02	9.509E-01	0.277156	2.111323
	BCP4	3.194E-01	1.101E-01	3.382E-01	-4.483E-01	-3.382E-01	-9.123E-01	9.380E-01	3.167E-02	9.763E-01	0.300139	2.221402
	BCP5	3.107E-01	9.639E-02	3.142E-01	-4.106E-01	-3.142E-01	-8.712E-01	9.474E-01	3.144E-02	9.264E-01	0.308093	2.011520
	BCP6	3.396E-01	2.284E-01	4.769E-01	-7.054E-01	-4.769E-01	-9.941E-01	8.119E-01	3.589E-02	1.511E+00	0.154080	1.906473
	RCP	2.370E-02	3.394E-02	-7.862E-03	-2.608E-02	7.862E-03	1.672E-01	2.663E-02	-1.423E-01	2.415E-01	-1.218632	0.189928
5	ACP1	1.195E+02	7.774E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.360E+04	6.661E+05	0.000010	-1.000019
	ACP2	1.195E+02	7.921E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.440E+05	1.000E+00	1.870E+04	6.714E+05	0.000019	-1.000021
	ACP3	1.196E+02	7.816E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.445E+05	1.000E+00	2.684E+04	9.201E+05	0.000007	-1.000017
	ACP4	1.195E+02	7.893E+00	1.360E+05	-1.361E+05	-1.360E+05	-5.442E+05	1.000E+00	1.950E+04	6.386E+05	0.000020	-1.000023
	ACP5	1.195E+02	7.892E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.343E+04	1.915E+06	0.000005	-1.000010
	ACP6	1.943E+02	2.573E+01	3.033E+05	-3.034E+05	-3.033E+05	-1.213E+06	1.000E+00	2.657E+04	6.132E+05	0.000004	-1.000030
	BCP1	3.639E-01	2.603E-01	5.334E-01	-7.937E-01	-5.334E-01	-1.092E+00	8.071E-01	2.788E-02	1.608E+00	0.250602	1.932790
	BCP2	3.190E-01	1.058E-01	3.324E-01	-4.383E-01	-3.324E-01	-9.064E-01	9.423E-01	2.898E-02	9.733E-01	0.395247	2.175890
	BCP3	3.099E-01	1.002E-01	3.148E-01	-4.150E-01	-3.148E-01	-8.582E-01	9.429E-01	4.455E-02	9.541E-01	0.329237	2.040988
	BCP4	3.158E-01	1.058E-01	3.271E-01	-4.328E-01	-3.271E-01	-8.852E-01	9.405E-01	4.802E-02	9.769E-01	0.357135	2.139718
	BCP5	3.105E-01	9.771E-02	3.144E-01	-4.121E-01	-3.144E-01	-8.669E-01	9.459E-01	2.802E-02	9.397E-01	0.315128	2.017687
	BCP6	3.399E-01	2.239E-01	4.752E-01	-6.991E-01	-4.752E-01	-1.005E+00	8.184E-01	2.556E-02	1.504E+00	0.150948	1.938668
	RCP	2.313E-02	3.314E-02	-7.710E-03	-2.543E-02	7.710E-03	1.634E-01	2.577E-02	-1.362E-02	2.567E-01	-1.206140	0.186895
6	ACP1	1.195E+02	7.777E+00	1.360E+05	-1.361E+05	-1.360E+05	-5.441E+05	1.000E+00	1.537E+04	6.868E+05	0.000010	-1.000018
	ACP2	1.195E+02	7.937E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.839E+04	6.410E+05	0.000021	-1.000023
	ACP3	1.196E+02	7.897E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.444E+05	1.000E+00	2.021E+04	9.967E+05	0.000001	-1.000014
	ACP4	1.195E+02	7.918E+00	1.360E+05	-1.360E+05	-1.360E+05	-5.441E+05	1.000E+00	1.802E+04	6.904E+05	0.000018	-1.000021
	ACP5	1.195E+02	7.766E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.537E+04	6.843E+05	0.000010	-1.000018
	ACP6	1.943E+02	2.575E+01	3.034E+05	-3.034E+05	-3.034E+05	-1.213E+06	1.000E+00	3.094E+04	6.183E+05	0.000003	-1.000029
	BCP1	3.607E-01	2.618E-01	5.290E-01	-7.908E-01	-5.290E-01	-1.069E+00	8.007E-01	3.198E-02	1.632E+00	0.249345	1.898758
	BCP2	3.205E-01	1.068E-01	3.353E-01	-4.421E-01	-3.353E-01	-9.141E-01	9.421E-01	3.186E-02	9.975E-01	0.403447	2.205778
	BCP3	3.134E-01	1.002E-01	3.209E-01	-4.211E-01	-3.209E-01	-8.826E-01	9.449E-01	3.784E-02	9.711E-01	0.337475	2.083242

	BCP4	3.135E-01	9.768E-02	3.206E-01	-4.182E-01	-3.206E-01	-8.916E-01	9.476E-01	3.755E-02	9.667E-01	0.339070	2.096501
	BCP5	3.193E-01	1.053E-01	3.327E-01	-4.379E-01	-3.327E-01	-9.095E-01	9.430E-01	3.146E-02	9.856E-01	0.398485	2.180733
	BCP6	3.590E-01	2.599E-01	5.254E-01	-7.854E-01	-5.254E-01	-1.062E+00	8.005E-01	3.178E-02	1.629E+00	0.247084	1.893503
	RCP	2.325E-02	3.340E-02	-7.784E-03	-2.562E-02	7.784E-03	1.647E-01	2.581E-02	-3.116E-02	2.817E-01	-1.194561	0.185736
7	ACP1	1.195E+02	7.785E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.734E+04	6.616E+05	0.000011	-1.000019
	ACP2	1.195E+02	7.861E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.655E+04	6.461E+05	0.000016	-1.000023
	ACP3	1.196E+02	8.134E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.445E+05	1.000E+00	1.619E+04	1.317E+07	0.000011	-1.000013
	ACP4	1.195E+02	7.837E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.443E+05	1.000E+00	1.666E+04	6.487E+05	0.000016	-1.000023
	ACP5	1.195E+02	7.841E+00	1.361E+05	-1.361E+05	-1.361E+05	-5.442E+05	1.000E+00	1.708E+04	1.054E+06	0.000001	-1.000010
	ACP6	1.943E+02	2.577E+01	3.033E+05	-3.034E+05	-3.033E+05	-1.213E+06	1.000E+00	3.782E+04	6.432E+05	0.000002	-1.000029
	BCP1	3.590E-01	2.630E-01	5.266E-01	-7.897E-01	-5.266E-01	-1.055E+00	7.968E-01	3.820E-02	1.627E+00	0.259836	1.869221
	BCP2	3.198E-01	1.048E-01	3.336E-01	-4.384E-01	-3.336E-01	-9.155E-01	9.438E-01	3.248E-02	9.752E-01	0.386056	2.180567
	BCP3	3.141E-01	1.044E-01	3.266E-01	-4.310E-01	-3.266E-01	-8.889E-01	9.409E-01	3.055E-02	9.647E-01	0.272678	2.121309
	BCP4	3.179E-01	1.079E-01	3.346E-01	-4.425E-01	-3.346E-01	-9.066E-01	9.395E-01	3.125E-02	9.765E-01	0.289642	2.184443
	BCP5	3.137E-01	9.713E-02	3.198E-01	-4.170E-01	-3.198E-01	-8.909E-01	9.483E-01	3.164E-02	9.467E-01	0.334649	2.065827
	BCP6	3.478E-01	2.496E-01	5.007E-01	-7.503E-01	-5.007E-01	-1.005E+00	7.965E-01	3.614E-02	1.587E+00	0.195558	1.844895
	RCP	2.374E-02	3.398E-02	-7.925E-03	-2.606E-02	7.925E-03	1.676E-01	2.670E-02	-1.476E-01	2.554E-01	-1.220614	0.189299

Table S2. In-ring electron density transfer from donor (D) to acceptor orbitals (A), along with the orbital's occupancy and the delocalisation energy, $E^{(2)}$.

molecule	D		occ.(D)		A		occ.(A)		$E^{(2)}$ (kcal/mol)							
1	BD	C	5	-	N	6	1.98203	→	RY*	C	1	0.00365	2.25			
	CR	N	6				1.99924	→	RY*	C	1	0.00813	2.37			
	BD	C	1	-	N	6	1.98203	→	BD*	C	1	-	C	2	0.03586	2.86
	BD	C	1	-	C	2	1.98607	→	BD*	C	1	-	N	6	0.01901	2.95
	BD	C	1	-	N	6	1.75483	→	RY*	C	5		0.00269	3.21		
	BD	C	1	-	N	6	1.98203	→	RY*	C	5		0.00366	3.42		
	LP	N	6				1.89920	→	RY*	C	1		0.00813	5.08		
	LP	N	6				1.89920	→	BD*	C	1	-	C	2	0.03586	10.50
	BD	C	1	-	N	6	1.75483	→	BD*	C	2	-	C	3	0.42334	16.41
	BD	C	4	-	C	5	1.70352	→	BD*	C	1	-	N	6	0.46216	22.98
	BD	C	1	-	N	6	1.75483	→	BD*	C	4	-	C	5	0.35481	61.62
	BD	C	2	-	C	3	1.62535	→	BD*	C	1	-	N	6	0.46216	81.79
2	CR	N	6				1.99923	→	RY*	C	1	0.00823	2.33			
	CR	N	6				1.99923	→	RY*	C	5	0.00876	2.66			
	BD	C	4	-	Cl	13	1.98956	→	BD*	C	5	-	N	6	0.02120	2.76
	BD	C	1	-	N	6	1.98181	→	BD*	C	1	-	C	2	0.03578	2.89
	BD	C	1	-	C	2	1.98563	→	BD*	C	1	-	N	6	0.01920	2.94
	BD	C	1	-	N	6	1.98181	→	RY*	C	5	0.00341	3.05			
	BD	C	5	-	N	6	1.75774	→	RY*	C	1	0.00275	3.31			
	BD	C	5	-	N	6	1.98089	→	RY*	C	1	0.00365	3.43			
	BD	C	4	-	C	5	1.98490	→	BD*	C	5	-	N	6	0.02120	4.10
	BD	C	5	-	N	6	1.98089	→	BD*	C	4	-	C	5	0.03745	4.16
	LP	N	6				1.89916	→	RY*	C	1	0.00823	5.00			
	LP	N	6				1.89916	→	RY*	C	5	0.00876	5.23			
	LP	N	6				1.89916	→	BD*	C	1	-	C	2	0.03578	10.42
	LP	N	6				1.89916	→	BD*	C	4	-	C	5	0.03745	10.85
	BD	C	5	-	N	6	1.75774	→	BD*	C	3	-	C	4	0.44550	13.90
	BD	C	1	-	C	2	1.71214	→	BD*	C	5	-	N	6	0.42798	20.41
	BD	C	5	-	N	6	1.75774	→	BD*	C	1	-	C	2	0.34336	62.92
	BD	C	3	-	C	4	1.65786	→	BD*	C	5	-	N	6	0.42798	79.21
3	BD	C	1	-	N	6	1.98089	→	RY*	C	5	0.00937	2.02			
	BD	C	5	-	N	6	1.98089	→	RY*	C	1	0.00937	2.02			
	BD	C	5	-	N	6	1.74693	→	RY*	C	1	0.00262	2.40			
	CR	N	6				1.99922	→	RY*	C	1	0.00937	2.46			
	CR	N	6				1.99922	→	RY*	C	5	0.00937	2.46			
	BD	C	1	-	N	6	1.98089	→	RY*	C	5	0.00328	2.51			
	BD	C	5	-	N	6	1.98089	→	RY*	C	1	0.00328	2.51			
	BD	C	2	-	Cl	13	1.98902	→	BD*	C	1	-	N	6	0.02143	2.90
	BD	C	4	-	Cl	12	1.98902	→	BD*	C	5	-	N	6	0.02143	2.90
	BD	C	1	-	C	2	1.98453	→	BD*	C	1	-	N	6	0.02143	4.11
	BD	C	4	-	C	5	1.98453	→	BD*	C	5	-	N	6	0.02143	4.11
	BD	C	1	-	N	6	1.98089	→	BD*	C	1	-	C	2	0.03725	4.21
	BD	C	5	-	N	6	1.98089	→	BD*	C	4	-	C	5	0.03725	4.21
	LP	N	6				1.89783	→	RY*	C	1	0.00937	5.32			
	LP	N	6				1.89783	→	RY*	C	5	0.00937	5.32			
	LP	N	6				1.89783	→	BD*	C	1	-	C	2	0.03725	10.57
	LP	N	6				1.89783	→	BD*	C	4	-	C	5	0.03725	10.57
	BD	C	5	-	N	6	1.74693	→	BD*	C	3	-	C	4	0.43849	12.70
	BD	C	1	-	C	2	1.73507	→	BD*	C	5	-	N	6	0.43337	16.82
	BD	C	5	-	N	6	1.74693	→	BD*	C	1	-	C	2	0.36610	70.92
BD	C	3	-	C	4	1.64556	→	BD*	C	5	-	N	6	0.43337	85.30	
4	BD	C	5	-	N	10	1.99194	→	BD*	C	1	-	N	6	0.01864	2.10

	BD	C	4	-	C	5	1.98101	→	BD*	C	5	-	N	6	0.01516	2.11
	BD	C	5	-	N	6	1.97955	→	BD*	C	4	-	C	5	0.03478	2.18
	BD	C	1	-	N	6	1.98509	→	RY*	C	5				0.00509	2.39
	CR	N	6				1.99928	→	RY*	C	1				0.00784	2.54
	BD	C	1	-	N	6	1.98509	→	RY*	C	5				0.00727	2.86
	BD	C	5	-	N	6	1.72228	→	RY*	C	1				0.00255	3.01
	CR	N	6				1.99928	→	RY*	C	5				0.00727	3.07
	BD	C	1	-	N	6	1.98509	→	BD*	C	1	-	C	2	0.03857	3.09
	BD	C	5	-	N	6	1.97955	→	RY*	C	1				0.00356	3.25
	BD	C	1	-	C	2	1.98557	→	BD*	C	1	-	N	6	0.01864	3.29
	LP	N	6				1.91356	→	RY*	C	5				0.00727	3.90
	LP	N	6				1.91356	→	RY*	C	1				0.00784	5.11
	LP	N	6				1.91356	→	BD*	C	1	-	C	2	0.03857	10.79
	LP	N	6				1.91356	→	BD*	C	4	-	C	5	0.03478	10.89
	BD	C	5	-	N	6	1.72228	→	BD*	C	3	-	C	4	0.34602	19.71
	BD	C	1	-	C	2	1.65954	→	BD*	C	5	-	N	6	0.44748	27.18
	BD	C	3	-	C	4	1.71700	→	BD*	C	5	-	N	6	0.44748	55.33
	BD	C	5	-	N	6	1.72228	→	BD*	C	1	-	C	2	0.36183	64.43
5	BD	C	5	-	N	6	1.97933	→	BD*	C	4	-	C	5	0.03472	2.04
	BD	C	4	-	C	5	1.97800	→	BD*	C	5	-	N	6	0.01498	2.05
	BD	C	5	-	N	6	1.71990	→	RY*	C	1				0.00284	2.06
	BD	C	5	-	N	10	1.99163	→	BD*	C	1	-	N	6	0.01839	2.07
	BD	C	1	-	N	6	1.98502	→	RY*	C	5				0.00512	2.20
	CR	N	6				1.99928	→	RY*	C	1				0.00752	2.72
	BD	C	1	-	N	6	1.98502	→	BD*	C	1	-	C	2	0.03885	2.96
	CR	N	6				1.99928	→	RY*	C	5				0.00717	2.99
	BD	C	1	-	N	6	1.98502	→	RY*	C	5				0.00717	3.01
	BD	C	5	-	N	6	1.97933	→	RY*	C	1				0.00362	3.11
	BD	C	1	-	C	2	1.98252	→	BD*	C	1	-	N	6	0.01839	3.24
	LP	N	6				1.91350	→	RY*	C	5				0.00717	3.56
	LP	N	6				1.91350	→	RY*	C	1				0.00752	5.13
	LP	N	6				1.91350	→	BD*	C	1	-	C	2	0.03885	11.05
	LP	N	6				1.91350	→	BD*	C	4	-	C	5	0.03472	11.06
	BD	C	5	-	N	6	1.71990	→	BD*	C	3	-	C	4	0.40740	19.83
	BD	C	1	-	C	2	1.66060	→	BD*	C	5	-	N	6	0.45139	25.49
	BD	C	3	-	C	4	1.72735	→	BD*	C	5	-	N	6	0.45139	52.61
	BD	C	5	-	N	6	1.71990	→	BD*	C	1	-	C	2	0.36081	67.16
6	CR	N	6				1.99924	→	RY*	C	1				0.00795	2.34
	CR	N	6				1.99924	→	RY*	C	5				0.00808	2.41
	BD	C	1	-	N	6	1.98258	→	BD*	C	1	-	C	2	0.03670	2.62
	BD	C	1	-	C	2	1.98654	→	BD*	C	1	-	N	6	0.01922	2.80
	BD	C	5	-	N	6	1.98240	→	BD*	C	4	-	C	5	0.03702	2.80
	BD	C	4	-	C	5	1.98602	→	BD*	C	5	-	N	6	0.01918	2.90
	BD	C	5	-	N	6	1.75127	→	RY*	C	1				0.00248	2.99
	BD	C	5	-	N	6	1.98240	→	RY*	C	1				0.00363	3.37
	BD	C	1	-	N	6	1.98258	→	RY*	C	5				0.00370	3.39
	LP	N	6				1.89893	→	RY*	C	1				0.00795	4.85
	LP	N	6				1.89893	→	RY*	C	5				0.00808	5.03
	LP	N	6				1.89893	→	BD*	C	4	-	C	5	0.03702	10.74
	LP	N	6				1.89893	→	BD*	C	1	-	C	2	0.03670	10.77
	BD	C	5	-	N	6	1.75127	→	BD*	C	3	-	C	4	0.40233	18.58
	BD	C	1	-	C	2	1.66859	→	BD*	C	5	-	N	6	0.44521	27.47
	BD	C	5	-	N	6	1.75127	→	BD*	C	1	-	C	2	0.35257	58.87
	BD	C	3	-	C	4	1.65118	→	BD*	C	5	-	N	6	0.44521	72.68
7	BD	C	4	-	C	5	1.98199	→	BD*	C	5	-	N	6	0.01931	2.37
	BD	C	5	-	N	6	1.98211	→	BD*	C	4	-	C	5	0.03763	2.54

CR	N	6		1.99927	→	RY*	C	1		0.00782	2.62	
BD	C	5	- N	6	1.74256	→	RY*	C	1	0.00234	2.82	
BD	C	1	- N	6	1.98458	→	BD*	C	1 - C	2	0.03822	2.98
BD	C	1	- N	6	1.98458	→	RY*	C	5	0.00349	3.03	
BD	C	5	- N	6	1.98211	→	RY*	C	1	0.00360	3.05	
CR	N	6		1.99927	→	RY*	C	5		0.00746	3.12	
BD	C	1	- C	2	1.98593	→	BD*	C	1 - N	6	0.02021	3.19
LP	N	6		1.91029	→	RY*	C	5		0.00746	4.19	
LP	N	6		1.91029	→	RY*	C	1		0.00782	5.00	
LP	N	6		1.91029	→	BD*	C	1 - C	2	0.03822	10.30	
LP	N	6		1.91029	→	BD*	C	4 - C	5	0.03763	10.93	
BD	C	5	- N	6	1.74256	→	BD*	C	3 - C	4	0.34018	19.92
BD	C	1	- C	2	1.65507	→	BD*	C	5 - N	6	0.43118	30.22
BD	C	5	- N	6	1.74256	→	BD*	C	1 - C	2	0.35355	57.51
BD	C	3	- C	4	1.69462	→	BD*	C	5 - N	6	0.43118	57.74
