

Electronic Supplementary Information

Fluorescent Nano-sized Aggregates of Halogen Bonded Complexes Formed with Perfluoropropyl Iodides: a Systematic Comparison between Two Isomeric Halogen Bond Acceptors, Aniline and 4-Methyl Pyridine

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A. Optimised geometries

ALN_ic3F7I_1

6	1.206985	0.574183	0.323082
6	-0.000606	1.272364	0.403772
6	-1.207331	0.573303	0.317910
6	-1.201767	-0.809302	0.164537
6	0.001078	-1.508937	0.090883
6	1.203086	-0.808426	0.169689
1	2.145896	1.115226	0.372153
1	-2.146837	1.113662	0.362958
1	-2.144046	-1.340553	0.100664
1	0.001729	-2.584968	-0.030109
1	2.146016	-1.338990	0.109854
1	0.828304	3.070419	0.917448
1	-0.833018	3.069814	0.913891
53	0.004144	3.663402	-2.222291
7	-0.001293	2.684519	0.484184
6	0.008300	4.440307	-4.297022
6	-1.285764	4.011313	-5.029933
6	1.305808	4.012269	-5.024383
9	0.007731	5.811161	-4.267391
9	1.361811	4.526003	-6.264732
9	1.395102	2.678725	-5.123150
9	2.377711	4.462734	-4.355869
9	-1.336833	4.525008	-6.270511
9	-1.373651	2.677704	-5.129080
9	-2.360853	4.460987	-4.366017

ALN_ic3F7I_2

6	1.210374	0.552952	0.256172
6	0.018866	1.270614	0.388616
6	-1.203200	0.599909	0.293956
6	-1.228540	-0.774567	0.080958
6	-0.041687	-1.493929	-0.044154
6	1.175577	-0.821342	0.043393
1	2.160851	1.072729	0.311871
1	-2.130571	1.156140	0.379259
1	-2.182449	-1.283841	0.010993
1	-0.065108	-2.563523	-0.211214
1	2.106305	-1.367281	-0.056054
1	0.892404	3.026863	0.968300
1	-0.768104	3.059506	0.991933
53	0.036009	3.797160	-2.119241
7	0.048577	2.677602	0.531372
6	0.029875	4.561020	-4.199316
6	1.293691	5.416272	-4.458103

6	-1.295180	5.305890	-4.490973
9	0.086053	3.503227	-5.069355
9	-1.350159	5.721982	-5.767273
9	-1.439457	6.378238	-3.698998
9	-2.337440	4.486333	-4.291469
9	1.345459	5.836839	-5.733063
9	1.326167	6.496137	-3.663933
9	2.396569	4.688105	-4.231367

ALN_ic3F7I_3

6	1.207805	1.116582	0.396676
6	0.002731	1.636937	0.888056
6	-1.203703	1.119509	0.396925
6	-1.199598	0.110695	-0.559624
6	0.000054	-0.404036	-1.047320
6	1.201054	0.107782	-0.559871
1	2.149449	1.515366	0.759593
1	-2.144302	1.520576	0.760037
1	-2.143794	-0.272056	-0.929917
1	-0.000970	-1.184630	-1.797619
1	2.144241	-0.277260	-0.930360
1	0.841256	2.788856	2.354866
1	-0.832692	2.790887	2.355040
7	0.004112	2.697726	1.798460
6	0.004470	3.413948	-3.173454
6	-1.299799	2.832667	-3.788782
6	1.307202	2.829507	-3.789047
9	1.401376	3.116715	-5.094250
9	1.341021	1.498405	-3.649733
9	2.374817	3.334498	-3.159104
9	-1.393541	3.120103	-5.093966
9	-1.336817	1.501651	-3.649460
9	-2.366059	3.340245	-3.158623
9	0.004221	3.097495	-1.856256
53	0.007099	5.599756	-3.383797

ALN_ic3F7I_4

6	0.470882	0.728673	1.190945
6	-0.923840	0.737756	1.031081
6	-1.476214	0.124036	-0.104371
6	-0.655220	-0.475832	-1.049691
6	0.733512	-0.476684	-0.893480
6	1.284222	0.126626	0.240420
1	0.912309	1.206861	2.058545
1	-2.551497	0.131269	-0.245701
1	-1.100949	-0.940102	-1.921622
1	1.369873	-0.957932	-1.625415
1	2.358938	0.134867	0.379715
1	-1.350645	1.544848	2.865904
1	-2.708015	1.123454	1.962786
7	-1.736733	1.393672	1.946805
6	0.936967	4.398440	-3.396964
6	0.098372	4.375517	-4.701642
6	0.537712	5.534806	-2.419230
9	-0.731807	5.407514	-2.012399
9	0.670920	6.737475	-3.001986
9	1.336317	5.517924	-1.343926
9	-1.200299	4.169329	-4.445903
9	0.213486	5.536676	-5.366286
9	0.534887	3.402531	-5.512102
9	2.232647	4.635107	-3.766775
53	0.807212	2.452870	-2.379849

ALN_ic3F7I_5

6	0.808541	1.229606	-0.623168
6	-0.561689	1.103153	-0.418672
6	-1.144716	-0.153405	-0.250738
6	-0.356199	-1.316404	-0.298633

6	1.025319	-1.180910	-0.506413
6	1.593513	0.076024	-0.665239
1	1.259076	2.206371	-0.743456
1	-1.189801	1.985350	-0.377600
1	-2.217109	-0.240393	-0.112534
1	1.648230	-2.068018	-0.541399
1	2.663466	0.156260	-0.818341
1	-1.837087	-2.605413	0.274184
1	-0.325895	-3.317195	0.116938
7	-0.937943	-2.573117	-0.182722
6	-0.445771	-0.274372	5.121942
6	-0.598584	-1.750526	5.572045
6	0.864032	0.395613	5.613138
9	-1.480096	0.418495	5.687795
9	0.897635	1.676839	5.225411
9	1.944486	-0.228542	5.125855
9	0.939064	0.375969	6.953502
9	-1.773057	-2.240492	5.150979
9	0.384135	-2.517346	5.080207
9	-0.576196	-1.850167	6.910129
53	-0.584538	-0.138783	2.928075

ALN_ic3F7I_6

6	-0.370331	1.349240	-0.806020
6	-1.354137	0.412618	-0.505810
6	-1.013408	-0.902863	-0.188822
6	0.332968	-1.307624	-0.181170
6	1.319910	-0.357222	-0.485979
6	0.967387	0.950304	-0.792494
1	-0.637285	2.371319	-1.041849
1	-2.398729	0.701227	-0.505256
1	-1.790784	-1.629021	0.023556
1	2.363515	-0.652269	-0.479794
1	1.747225	1.668254	-1.018487
1	-0.005105	-3.169162	0.595495
1	1.617269	-2.784320	0.408026
7	0.675067	-2.628410	0.082498
6	-0.421288	0.019610	5.117060
6	1.067698	-0.118264	5.528280
6	-1.081701	1.338867	5.595294
9	-1.094320	-1.002805	5.727644
9	-2.374301	1.358357	5.245050
9	-0.477022	2.408813	5.063260
9	-1.023106	1.446988	6.932269
9	1.548660	-1.301815	5.121394
9	1.816333	0.854010	4.992214
9	1.204723	-0.064750	6.862409
53	-0.619228	-0.177087	2.932516

ALN_ic3F7I_7

6	0.001900	1.316842	-0.435391
6	-1.196766	0.619757	-0.292776
6	-1.198217	-0.739677	-0.002143
6	0.009293	-1.433693	0.155252
6	1.213072	-0.731345	0.006475
6	1.204305	0.628053	-0.284195
1	-0.000970	2.376771	-0.657120
1	-2.142136	1.138647	-0.404184
1	-2.137636	-1.271346	0.106897
1	2.155340	-1.256512	0.122239
1	2.146838	1.153467	-0.388857
1	-0.821879	-3.163423	0.847275
1	0.847431	-3.157655	0.853241
7	0.013152	-2.808475	0.404672
6	-0.009933	0.116330	4.037262
6	-1.310437	-0.725738	4.168292
6	1.295395	-0.716727	4.177595
9	2.360879	0.066482	3.984155
9	1.334391	-1.694338	3.257907

9	1.386799	-1.282756	5.387376
9	-2.379903	0.050089	3.967233
9	-1.336105	-1.703570	3.248370
9	-1.406557	-1.292418	5.377402
53	-0.020830	1.721669	5.534775
9	-0.007412	0.665266	2.799535

ALN_ic3F7I_8

6	0.389709	1.249167	-0.672769
6	-0.944720	0.953368	-0.398108
6	-1.321376	-0.322072	0.006126
6	-0.362489	-1.334215	0.147649
6	0.977464	-1.035350	-0.134409
6	1.344617	0.243197	-0.538787
1	0.679721	2.245376	-0.982631
1	-1.701424	1.723647	-0.494605
1	-2.362783	-0.539916	0.217978
1	1.729636	-1.810419	-0.034669
1	2.387541	0.454428	-0.746069
1	-1.605883	-2.687740	1.031875
1	-0.013484	-3.177246	0.948056
7	-0.741387	-2.628845	0.513598
6	0.397936	0.257290	3.803792
6	1.055105	1.242678	4.812660
6	-1.076931	-0.097267	4.146052
9	-1.563989	-0.978820	3.262794
9	-1.843487	0.999490	4.090905
9	-1.178837	-0.624177	5.372557
9	2.288533	1.556582	4.401092
9	0.343845	2.377642	4.882619
9	1.130993	0.718844	6.041125
53	1.596023	-1.579972	3.697452
9	0.395676	0.871219	2.597004

ALN_ic3F7I_trm1

6	3.810454	1.923596	-0.038953
6	3.596761	1.106449	-1.145108
6	3.368736	-0.259800	-0.983185
6	3.354245	-0.821673	0.299824
6	3.577403	-0.000977	1.409763
6	3.801506	1.359677	1.236653
1	3.982266	2.984581	-0.167361
1	3.601279	1.527739	-2.143179
1	3.223052	-0.895043	-1.850068
1	3.574905	-0.431711	2.404857
1	3.966802	1.984396	2.106234
1	2.665928	-2.654622	-0.283859
1	2.804258	-2.475769	1.363190
7	3.184129	-2.209661	0.463453
6	-2.046768	0.091575	-0.332499
6	-2.509809	-1.274188	0.240821
6	-2.531929	1.313943	0.491849
9	-2.600505	0.206418	-1.575464
9	-2.128738	2.449041	-0.092172
9	-2.052112	1.280031	1.741826
9	-3.871375	1.343077	0.557107
9	-2.091314	-2.270145	-0.552306
9	-2.023883	-1.477537	1.472944
9	-3.847448	-1.338646	0.301598
53	0.146123	0.124929	-0.502389
6	7.918943	-4.151620	0.239001
6	8.737575	-3.712805	1.478381
6	8.580684	-3.774901	-1.109714
9	7.850200	-5.519249	0.275977
9	7.837832	-4.230416	-2.128757
9	9.800085	-4.325953	-1.222804
9	8.710569	-2.447199	-1.237078
9	8.124923	-4.117560	2.600229
9	9.963586	-4.260681	1.469240

9	8.877379	-2.380812	1.525984
53	5.875126	-3.313401	0.342464

ALN_ic3F7I_trm2

6	3.874416	1.845464	0.085431
6	3.661613	1.071609	-1.051614
6	3.396661	-0.293073	-0.940479
6	3.343726	-0.897148	0.322191
6	3.566420	-0.120197	1.463268
6	3.827414	1.239384	1.340706
1	4.074698	2.905491	-0.003630
1	3.695504	1.525929	-2.034518
1	3.251711	-0.894908	-1.831002
1	3.534473	-0.583949	2.442892
1	3.991680	1.830107	2.233920
1	2.619071	-2.690473	-0.335722
1	2.729843	-2.570348	1.318401
7	3.134507	-2.284862	0.435541
6	-2.019638	0.175162	-0.379461
6	-2.524251	-1.188177	0.163768
6	-2.492084	1.395651	0.454999
9	-2.547346	0.321734	-1.630380
9	-2.052276	2.529934	-0.103634
9	-2.036567	1.331529	1.712843
9	-3.831500	1.454706	0.496165
9	-2.113966	-2.181245	-0.637275
9	-2.065961	-1.421583	1.401118
9	-3.863899	-1.222664	0.199217
53	0.176223	0.160383	-0.508671
6	7.851470	-4.266170	0.232499
6	7.985422	-5.261751	-0.946260
6	8.261181	-4.862988	1.601640
9	8.716651	-3.235261	-0.022525
9	8.164611	-3.928047	2.557616
9	9.534040	-5.290360	1.583476
9	7.479571	-5.898666	1.938000
9	7.660245	-4.656726	-2.097645
9	9.247437	-5.704479	-1.066532
9	7.185604	-6.324805	-0.782775
53	5.787666	-3.476945	0.332571

ALN_nc3F7I_trm1

6	4.659625	-0.912658	1.235238
6	4.160643	-1.340247	0.000180
6	4.709799	-0.822408	-1.177760
6	5.743146	0.105157	-1.117403
6	6.241217	0.534761	0.113586
6	5.693188	0.015189	1.287281
1	4.226495	-1.297100	2.152113
1	4.315273	-1.136321	-2.137878
1	6.155291	0.502545	-2.037226
1	7.048319	1.255309	0.157329
1	6.066177	0.342148	2.250515
1	2.958563	-2.811961	0.756010
1	3.001016	-2.758430	-0.908642
53	0.563861	-0.593307	-0.096923
7	3.061936	-2.217524	-0.055959
6	-1.255690	0.648545	-0.153151
6	-2.540169	-0.198468	0.055753
6	-3.886647	0.591976	0.035208
9	-1.193789	1.589639	0.813064
9	-1.338869	1.278986	-1.344189
9	-2.463060	-0.821942	1.253296
9	-2.611925	-1.132383	-0.919764
9	-3.919917	1.507825	1.008016
9	-4.066269	1.202416	-1.140264
9	-4.897528	-0.266724	0.226107
6	1.676666	3.806343	0.178672
6	1.892208	5.325507	-0.066999

6	0.595369	6.196566	-0.064689
9	1.079086	3.635136	1.373829
9	0.855611	3.321372	-0.773696
9	2.703969	5.813770	0.896315
9	2.485225	5.494820	-1.269082
9	-0.031173	6.118770	1.113158
9	-0.244119	5.807909	-1.028772
9	0.932440	7.474277	-0.283575
53	3.565370	2.695697	0.142018

ALN_nC3F7I_trm2

6	4.068602	1.619878	0.337628
6	3.971677	0.304242	-0.127318
6	4.042974	0.057757	-1.504303
6	4.215642	1.115180	-2.396182
6	4.319435	2.423093	-1.931407
6	4.242713	2.666256	-0.560261
1	4.007164	1.818433	1.401894
1	3.945602	-0.957137	-1.874161
1	4.273097	0.908054	-3.458059
1	4.458208	3.241675	-2.625994
1	4.322362	3.679322	-0.184441
1	4.073449	-0.581519	1.709686
1	4.049293	-1.656677	0.440677
53	0.782797	-0.886864	0.929436
7	3.736652	-0.752500	0.770875
6	-1.414225	-0.993319	1.043667
6	-2.091333	0.133144	0.216254
6	-3.652653	0.147021	0.231898
9	-1.836658	-2.190612	0.580432
9	-1.808831	-0.887456	2.331919
9	-1.707069	0.016327	-1.074743
9	-1.677810	1.330127	0.689908
9	-4.147084	-0.989305	-0.269463
9	-4.118081	0.309992	1.474421
9	-4.086102	1.166907	-0.520758
6	9.395634	-0.765633	-0.532032
6	9.789315	-0.469034	0.942409
6	11.265200	-0.803981	1.329162
9	10.194920	-0.056813	-1.353235
9	9.593083	-2.074916	-0.785985
9	9.598412	0.845153	1.188742
9	8.988553	-1.189365	1.759929
9	12.124501	-0.094934	0.591565
9	11.519204	-2.105121	1.160312
9	11.454641	-0.496591	2.618190
53	7.296028	-0.249390	-0.920449

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6	1.340814	0.550189	-0.067349
6	0.423766	1.529836	-0.464483
6	-0.930327	1.192155	-0.569558
6	-1.354513	-0.100255	-0.279007
6	-0.441635	-1.074863	0.120140
6	0.907374	-0.739411	0.222012
1	2.390153	0.806701	0.033476
1	-1.651380	1.950685	-0.854694
1	-2.407989	-0.342442	-0.356707
1	-0.776473	-2.078433	0.351105
1	1.629966	-1.484113	0.535019
7	0.840417	2.861341	-0.653837
1	1.814347	2.959792	-0.907312
1	0.250531	3.396025	-1.277590
1	0.247608	3.517574	1.374266
7	-0.169044	3.902190	2.214932
6	-0.306197	3.048090	3.308064
6	-0.387597	1.657787	3.131068
6	-0.422587	3.564279	4.608395
6	-0.576190	0.819371	4.223675

1	-0.306786	1.238954	2.136822
6	-0.611819	2.715980	5.694006
1	-0.367725	4.637557	4.762163
6	-0.690308	1.335606	5.514319
1	-0.633852	-0.251152	4.059783
1	-0.697539	3.139458	6.688771
1	-0.836873	0.677001	6.361707
1	0.180025	4.823654	2.431669

ANL2_02

6	1.150900	0.430186	0.332495
6	0.507658	1.468236	-0.350947
6	-0.793709	1.267453	-0.825044
6	-1.436135	0.051873	-0.614499
6	-0.796814	-0.980593	0.069467
6	0.500335	-0.781727	0.539134
1	2.153329	0.582097	0.718677
1	-1.308481	2.074021	-1.335971
1	-2.447224	-0.083677	-0.980324
1	-1.302353	-1.923534	0.236518
1	1.010468	-1.572667	1.076602
7	1.119380	2.730914	-0.468404
1	2.129783	2.707590	-0.436397
1	0.796926	3.276537	-1.256592
1	0.067843	3.594885	1.276028
7	-0.517080	4.082593	1.945546
6	-1.057106	3.331361	2.988263
6	-1.254380	1.947965	2.853385
6	-1.468484	3.952288	4.178252
6	-1.841343	1.217644	3.880227
1	-0.950566	1.450105	1.942171
6	-2.055304	3.211714	5.198626
1	-1.328577	5.022347	4.296493
6	-2.247845	1.837658	5.061592
1	-1.980751	0.149858	3.751381
1	-2.363371	3.714732	6.108739
1	-2.704375	1.262988	5.858238
1	-0.133043	4.975935	2.214570

ANL2_03

6	1.227845	0.913248	-0.099930
6	0.006287	1.597702	-0.057616
6	-1.071622	1.022629	0.625874
6	-0.922532	-0.206444	1.258919
6	0.292743	-0.887922	1.217290
6	1.364442	-0.319777	0.529463
1	2.071429	1.354640	-0.621003
1	-2.016182	1.550751	0.681578
1	-1.766300	-0.630486	1.790978
1	0.402847	-1.846439	1.709511
1	2.316262	-0.836844	0.483971
7	-0.105047	2.882181	-0.618826
1	0.473566	3.035959	-1.433231
1	-1.057025	3.179782	-0.782912
1	0.495607	3.851267	1.530356
7	0.188893	3.686737	2.482136
6	-1.198142	3.603397	2.598067
6	-2.025095	4.381157	1.772599
6	-1.800192	2.767175	3.549393
6	-3.409537	4.297991	1.878627
1	-1.570524	5.052548	1.052495
6	-3.184283	2.694996	3.652757
1	-1.174226	2.157029	4.191885
6	-4.003457	3.451568	2.814502
1	-4.029520	4.905217	1.228037
1	-3.627139	2.034813	4.390311
1	-5.081700	3.389141	2.894850
1	0.678710	2.896294	2.878004

ANL2_04

6	1.083488	0.956895	0.022817
6	0.039956	1.878292	-0.133840
6	-1.233852	1.550367	0.345358
6	-1.451234	0.329564	0.974629
6	-0.413263	-0.587618	1.130931
6	0.853880	-0.265281	0.646285
1	2.076237	1.205325	-0.338720
1	-2.044918	2.262180	0.246849
1	-2.442471	0.098364	1.347238
1	-0.588483	-1.538449	1.619172
1	1.672468	-0.967567	0.756278
7	0.292824	3.146967	-0.684982
1	1.021288	3.162611	-1.385546
1	-0.535197	3.630420	-1.004993
1	0.703263	4.014144	1.550737
7	0.211082	3.934859	2.433065
6	-1.162380	4.140404	2.308145
6	-1.658053	5.055013	1.365829
6	-2.077189	3.464497	3.128526
6	-3.027285	5.260001	1.231599
1	-0.958797	5.604464	0.745269
6	-3.443370	3.680114	2.991911
1	-1.709412	2.751568	3.858854
6	-3.933717	4.572139	2.037990
1	-3.388515	5.968682	0.494270
1	-4.132017	3.139567	3.631852
1	-4.999251	4.734041	1.931289
1	0.452782	3.068624	2.894206

ANL2_05

6	0.988868	0.973451	0.069447
6	0.208153	2.102586	-0.209852
6	-1.155650	2.080729	0.105295
6	-1.719017	0.954461	0.694984
6	-0.942678	-0.169324	0.973266
6	0.414086	-0.151526	0.651854
1	2.048678	0.983795	-0.164374
1	-1.766271	2.954629	-0.088738
1	-2.774824	0.960804	0.940087
1	-1.386944	-1.045234	1.429961
1	1.032727	-1.017587	0.858281
7	0.807082	3.269211	-0.717313
1	1.600354	3.104872	-1.321804
1	0.155526	3.919591	-1.134725
1	1.126203	4.070753	1.557317
7	0.524741	4.123860	2.371231
6	-0.740773	4.630605	2.078077
6	-0.897657	5.612325	1.087234
6	-1.878041	4.196329	2.774337
6	-2.158069	6.117366	0.785353
1	-0.021736	5.976377	0.561706
6	-3.132808	4.710982	2.470536
1	-1.773208	3.435184	3.540218
6	-3.288234	5.669247	1.468694
1	-2.256679	6.872745	0.013312
1	-3.998833	4.353646	3.016668
1	-4.268272	6.064538	1.231561
1	0.505990	3.235856	2.853444

ANL2_06

6	1.027726	0.929635	0.219384
6	0.537151	2.181491	-0.173889
6	-0.825513	2.458706	-0.012472
6	-1.672705	1.503899	0.539072
6	-1.185144	0.258130	0.930714
6	0.170468	-0.021894	0.762385
1	2.084093	0.708255	0.105119

1	-1.213693	3.429981	-0.295580
1	-2.722819	1.741291	0.664565
1	-1.849773	-0.483253	1.357071
1	0.566818	-0.986577	1.058496
7	1.418911	3.172316	-0.640795
1	2.217722	2.817760	-1.148620
1	0.966782	3.922948	-1.144663
1	1.662717	3.998977	1.634310
7	1.004883	4.215183	2.374270
6	-0.087023	4.959161	1.928753
6	0.071521	5.902979	0.901997
6	-1.356539	4.804966	2.504347
6	-1.014888	6.643815	0.448440
1	1.054449	6.051147	0.468579
6	-2.435226	5.553924	2.049267
1	-1.495544	4.076587	3.296212
6	-2.279091	6.473997	1.012347
1	-0.870416	7.364972	-0.348698
1	-3.409256	5.411252	2.504085
1	-3.123032	7.052455	0.657226
1	0.748373	3.374819	2.873693

ANL2_07

6	1.039823	0.771348	0.281378
6	0.799462	2.085719	-0.139485
6	-0.474991	2.635445	0.043069
6	-1.480815	1.885131	0.642184
6	-1.242232	0.577283	1.061293
6	0.024563	0.026048	0.872074
1	2.026810	0.339128	0.150922
1	-0.668275	3.657312	-0.261298
1	-2.458158	2.332065	0.783233
1	-2.029945	-0.003997	1.524738
1	0.227525	-0.990673	1.189048
7	1.848698	2.866536	-0.655886
1	2.545884	2.345553	-1.169895
1	1.542461	3.679506	-1.172657
1	2.315965	3.685704	1.586780
7	1.735515	4.048823	2.333944
6	0.802994	4.985471	1.889702
6	1.119060	5.851299	0.831118
6	-0.455269	5.104675	2.497417
6	0.191071	6.783556	0.378823
1	2.099380	5.787503	0.371932
6	-1.374109	6.043293	2.043181
1	-0.715512	4.439817	3.314207
6	-1.065443	6.886093	0.975225
1	0.455072	7.440103	-0.443138
1	-2.344026	6.111231	2.523385
1	-1.785802	7.613118	0.620995
1	1.329666	3.290392	2.864512

ANL2_08

6	-0.115139	1.330612	0.309451
6	-0.282016	0.012187	0.749515
6	0.573401	-0.988169	0.301017
6	1.600648	-0.699677	-0.595961
6	1.762225	0.611782	-1.041387
6	0.916969	1.621156	-0.592111
1	-1.064939	-0.221959	1.461146
1	0.433617	-2.000982	0.660895
1	2.262418	-1.483049	-0.944600
1	2.553841	0.854174	-1.741372
1	1.058898	2.641726	-0.933095
7	-0.912688	2.365337	0.829543
1	-1.068895	3.135081	0.193313
1	-1.778789	2.050039	1.244523
6	-1.152171	1.321868	4.070874
6	0.184817	0.977240	3.818184

6	-2.046244	0.375126	4.559908
1	-1.479394	2.338698	3.883973
6	0.601958	-0.331835	4.099375
6	-1.630455	-0.930187	4.821276
1	-3.075767	0.662232	4.744355
6	-0.296629	-1.269737	4.593829
1	1.631326	-0.614234	3.905571
1	-2.328872	-1.665068	5.202228
1	0.047085	-2.278219	4.795752
7	1.074298	1.929443	3.321811
1	1.897612	1.531921	2.891039
1	0.632886	2.591903	2.694648

ANL2_09

6	0.158325	1.308201	0.311534
6	-0.316459	0.071265	0.763499
6	0.242636	-1.109059	0.286095
6	1.273511	-1.082236	-0.651742
6	1.741212	0.149352	-1.108849
6	1.194276	1.335818	-0.631120
1	-1.104653	0.036818	1.506310
1	-0.132484	-2.056484	0.655575
1	1.703636	-2.004485	-1.022702
1	2.540330	0.189452	-1.840417
1	1.574049	2.290149	-0.981838
7	-0.333298	2.506871	0.858017
1	-0.315623	3.295031	0.225447
1	-1.233781	2.416643	1.308235
6	-0.703834	1.538874	4.110190
6	0.494132	0.872583	3.808387
6	-1.786876	0.842869	4.636909
1	-0.773486	2.606209	3.931599
6	0.581462	-0.500622	4.079285
6	-1.700680	-0.526283	4.887991
1	-2.704319	1.377009	4.859076
6	-0.503518	-1.186977	4.611607
1	1.499564	-1.030135	3.847743
1	-2.545564	-1.065451	5.298398
1	-0.415190	-2.250386	4.804755
7	1.573711	1.575196	3.274280
1	2.255176	0.986764	2.815144
1	1.287931	2.329151	2.660296

ANL2_10

6	0.158328	1.308201	0.311535
6	-0.316457	0.071266	0.763500
6	0.242635	-1.109058	0.286096
6	1.273509	-1.082238	-0.651743
6	1.741210	0.149350	-1.108851
6	1.194276	1.335817	-0.631121
1	-1.104650	0.036821	1.506313
1	-0.132485	-2.056483	0.655577
1	1.703632	-2.004487	-1.022704
1	2.540327	0.189449	-1.840420
1	1.574050	2.290148	-0.981841
7	-0.333293	2.506873	0.858018
1	-0.315617	3.295032	0.225448
1	-1.233776	2.416646	1.308236
6	-0.703836	1.538873	4.110190
6	0.494132	0.872584	3.808390
6	-1.786879	0.842866	4.636905
1	-0.773490	2.606209	3.931600
6	0.581463	-0.500620	4.079288
6	-1.700682	-0.526286	4.887986
1	-2.704324	1.377004	4.859069
6	-0.503518	-1.186977	4.611606
1	1.499567	-1.030131	3.847749
1	-2.545566	-1.065456	5.298389
1	-0.415188	-2.250386	4.804753

7	1.573711	1.575200	3.274287
1	2.255179	0.986769	2.815153
1	1.287929	2.329152	2.660299

ANL2_11

6	0.323918	1.596532	-0.010860
6	-1.065550	1.665428	0.140900
6	-1.857750	0.559055	-0.147245
6	-1.282243	-0.630316	-0.590999
6	0.101234	-0.697851	-0.745774
6	0.901425	0.403176	-0.459222
1	-1.521021	2.580676	0.504142
1	-2.931614	0.627370	-0.017464
1	-1.901401	-1.491419	-0.809539
1	0.565539	-1.617105	-1.083263
1	1.979351	0.333353	-0.558156
7	1.138197	2.676098	0.381364
1	2.033330	2.712676	-0.088020
1	0.678436	3.576153	0.349698
6	0.179752	-0.241252	3.183565
6	1.166907	0.477744	3.876000
6	-0.575670	-1.207599	3.837637
1	0.010475	-0.043094	2.133539
6	1.370394	0.193923	5.235741
6	-0.371548	-1.486196	5.188932
1	-1.333172	-1.747552	3.280103
6	0.609156	-0.775549	5.879643
1	2.133773	0.736694	5.784589
1	-0.963698	-2.240208	5.693050
1	0.784870	-0.975320	6.931049
7	1.965556	1.412257	3.218670
1	2.421598	2.083817	3.817796
1	1.588857	1.835732	2.377827

ANL2_12

6	0.619709	1.512347	0.045730
6	-0.708809	1.907084	0.239698
6	-1.750484	1.041346	-0.076650
6	-1.488235	-0.227338	-0.590848
6	-0.165247	-0.619152	-0.787596
6	0.882855	0.239558	-0.473308
1	-0.922487	2.885289	0.657472
1	-2.773381	1.360377	0.086430
1	-2.301392	-0.900824	-0.831277
1	0.056446	-1.604699	-1.180094
1	1.909826	-0.083508	-0.605776
7	1.677981	2.341407	0.464151
1	2.547479	2.184708	-0.028128
1	1.450049	3.326296	0.486996
6	0.085394	-0.398219	3.154882
6	1.228483	0.024449	3.851728
6	-0.871384	-1.185716	3.784741
1	-0.047530	-0.111373	2.120219
6	1.378760	-0.369582	5.190763
6	-0.719357	-1.574407	5.115564
1	-1.746108	-1.497294	3.224401
6	0.415423	-1.158186	5.810485
1	2.259727	-0.056243	5.742395
1	-1.468635	-2.187896	5.600873
1	0.554222	-1.448224	6.846270
7	2.219408	0.770828	3.215944
1	2.834343	1.280612	3.832300
1	1.943316	1.315398	2.406336

ANL2_13

6	0.684202	0.849656	0.339912
6	-0.427585	0.156686	0.834394
6	-0.745130	-1.102921	0.339692

6	0.024405	-1.692700	-0.661762
6	1.125598	-0.998864	-1.163276
6	1.457425	0.257075	-0.668045
1	-1.030371	0.598921	1.618776
1	-1.605050	-1.625247	0.743820
1	-0.230374	-2.672325	-1.047726
1	1.735227	-1.439752	-1.944265
1	2.325832	0.781929	-1.053322
7	1.055952	2.085814	0.882853
1	1.511725	2.716062	0.238778
1	0.331890	2.545401	1.415691
6	0.572449	1.274018	4.075473
6	0.831482	-0.085185	3.839970
6	-0.701329	1.696285	4.439352
1	1.371839	1.995236	3.948669
6	-0.215035	-1.005392	4.007129
6	-1.743616	0.780914	4.586504
1	-0.879771	2.751818	4.614504
6	-1.483117	-0.573187	4.374073
1	-0.032958	-2.057613	3.816814
1	-2.734283	1.114086	4.869838
1	-2.277974	-1.301750	4.488838
7	2.071706	-0.500613	3.385525
1	2.313252	-1.471129	3.500892
1	2.842708	0.139628	3.480602

ANL2_14

6	0.107241	1.436693	0.351795
6	-0.814279	0.418822	0.629589
6	-0.449312	-0.914366	0.501768
6	0.834032	-1.265630	0.085948
6	1.751450	-0.256154	-0.196394
6	1.397365	1.083152	-0.063508
1	-1.805616	0.678023	0.984068
1	-1.166391	-1.687164	0.750826
1	1.114369	-2.307794	-0.002474
1	2.755285	-0.509032	-0.519967
1	2.124496	1.861662	-0.271651
7	-0.229317	2.779462	0.558603
1	0.283265	3.442655	-0.004191
1	-1.219590	2.975112	0.561510
6	1.067862	-0.374672	3.463535
6	0.146355	-1.392552	3.741330
6	0.702880	0.958512	3.591352
1	2.059204	-0.633862	3.109062
6	-1.143775	-1.039025	4.156628
6	-0.580470	1.309763	4.007166
1	1.419948	1.731316	3.342284
6	-1.497877	0.300277	4.289508
1	-1.870896	-1.817543	4.364779
1	-0.860822	2.351924	4.095579
1	-2.501715	0.553146	4.613077
7	0.482931	-2.735317	3.534534
1	-0.029646	-3.398515	4.097324
1	1.473206	-2.930955	3.531624

ANL2_15

6	-0.327498	1.365807	0.352927
6	-1.483670	0.698739	-0.071544
6	-1.486944	-0.686252	-0.207790
6	-0.346070	-1.431823	0.080213
6	0.804114	-0.768673	0.505153
6	0.819494	0.613162	0.636407
1	-2.382555	1.268744	-0.284195
1	-2.392161	-1.183805	-0.538479
1	-0.353371	-2.510788	-0.010853
1	1.691561	-1.335790	0.758651
1	1.710822	1.113594	0.997918
7	-0.342541	2.749541	0.562974

1	0.566111	3.189065	0.572892
1	-1.002380	3.263043	-0.002915
6	1.483663	-0.722573	4.164668
6	0.327476	-1.389617	3.740197
6	1.486969	0.662418	4.300909
1	2.382533	-1.292599	4.377328
6	-0.819499	-0.636946	3.456715
6	0.346112	1.408014	4.012903
1	2.392195	1.159950	4.631603
6	-0.804086	0.744889	3.587965
1	-1.710835	-1.137360	3.095198
1	0.353438	2.486980	4.103968
1	-1.691522	1.312025	3.334465
7	0.342486	-2.773351	3.530152
1	-0.566174	-3.212859	3.520249
1	1.002330	-3.286866	4.096022

ANL2_16

6	-0.354648	1.024028	1.067193
6	-0.745495	-0.177900	0.462973
6	0.036810	-1.319993	0.599969
6	1.214620	-1.288022	1.345740
6	1.603063	-0.091730	1.946602
6	0.832345	1.057419	1.808602
1	-1.668048	-0.215461	-0.107519
1	-0.279421	-2.240817	0.123031
1	1.820039	-2.179625	1.453786
1	2.513831	-0.047683	2.532609
1	1.135886	1.976271	2.296231
7	-1.189468	2.153603	1.001053
1	-0.724008	3.024108	1.218588
1	-1.728318	2.227939	0.149109
1	-2.247401	1.468563	3.082011
7	-1.891493	1.154285	3.977325
1	-1.676664	0.167292	3.943762
6	-0.842437	1.941640	4.450407
6	-0.818188	3.320212	4.187519
6	0.195038	1.388968	5.215229
6	0.228672	4.110240	4.650960
1	-1.629635	3.763775	3.621165
6	1.233877	2.186910	5.679667
1	0.192115	0.324270	5.423354
6	1.267156	3.552444	5.396246
1	0.229195	5.172695	4.432882
1	2.029520	1.735526	6.262036
1	2.080785	4.170187	5.755918

ANL2_17

6	-0.110095	1.045212	1.134967
6	-0.860405	0.001724	0.577615
6	-0.371403	-1.300514	0.591593
6	0.866145	-1.587605	1.166475
6	1.612318	-0.548849	1.720775
6	1.136042	0.757475	1.704269
1	-1.831018	0.213849	0.140705
1	-0.964215	-2.095267	0.153037
1	1.242945	-2.602996	1.179212
1	2.575256	-0.752535	2.174764
1	1.717596	1.552901	2.155158
7	-0.643233	2.344823	1.198317
1	0.046239	3.066391	1.358693
1	-1.255084	2.585353	0.430541
1	-1.552275	1.842912	3.398459
7	-1.169269	1.412047	4.231940
1	-1.209705	0.404926	4.157735
6	0.094020	1.900531	4.563203
6	0.420995	3.242777	4.314968
6	1.055776	1.079774	5.169946
6	1.681555	3.734816	4.637028

1	-0.324244	3.894242	3.872065
6	2.310709	1.581377	5.494196
1	0.819098	0.039083	5.364504
6	2.640440	2.909726	5.224228
1	1.914062	4.774359	4.432923
1	3.040970	0.925429	5.955065
1	3.621005	3.295778	5.474065

ANL2_18

6	0.078061	1.013703	1.242665
6	-0.907068	0.204533	0.661943
6	-0.664285	-1.146834	0.438319
6	0.557154	-1.716906	0.795441
6	1.537040	-0.911205	1.373116
6	1.307148	0.442447	1.593045
1	-1.865847	0.636799	0.393863
1	-1.437031	-1.757481	-0.014853
1	0.742282	-2.770150	0.623496
1	2.491772	-1.336598	1.660120
1	2.070403	1.053713	2.059956
7	-0.199628	2.357928	1.547928
1	0.623004	2.923895	1.705124
1	-0.839941	2.809674	0.909477
1	-0.931694	1.681677	3.767311
7	-0.542151	1.071838	4.476806
1	-0.772913	0.108204	4.277829
6	0.817932	1.290629	4.692578
6	1.353267	2.583215	4.579457
6	1.676590	0.240680	5.049044
6	2.710296	2.807323	4.787028
1	0.693787	3.407722	4.332019
6	3.030105	0.474696	5.260788
1	1.278210	-0.764582	5.136494
6	3.563167	1.756604	5.124132
1	3.103320	3.813606	4.690625
1	3.676155	-0.354472	5.527337
1	4.619295	1.934259	5.285355

ANL2_19

6	0.257479	0.819054	1.314535
6	-0.901553	0.320965	0.705417
6	-0.985276	-1.020203	0.345688
6	0.077247	-1.888777	0.592785
6	1.230306	-1.392532	1.198782
6	1.327012	-0.051739	1.554472
1	-1.738865	0.986790	0.522213
1	-1.888771	-1.387845	-0.127518
1	0.008064	-2.933369	0.314932
1	2.065699	-2.052693	1.401636
1	2.221723	0.317290	2.041833
7	0.307388	2.153048	1.756364
1	1.242492	2.495997	1.928757
1	-0.223882	2.802134	1.192331
1	-0.513323	1.441547	3.933292
7	-0.261234	0.689792	4.564440
1	-0.714564	-0.169742	4.286725
6	1.116769	0.567145	4.738559
6	1.936053	1.706745	4.722987
6	1.714617	-0.682608	4.956381
6	3.312147	1.590778	4.889579
1	1.481684	2.681457	4.583579
6	3.089696	-0.788601	5.128208
1	1.094896	-1.572966	4.967162
6	3.903767	0.343572	5.088331
1	3.926705	2.484261	4.870226
1	3.530343	-1.766677	5.286784
1	4.975482	0.256488	5.217967

ANL2_20

6	0.178162	0.503595	1.382220
6	-1.165098	0.530920	0.985512
6	-1.864243	-0.655759	0.790230
6	-1.242661	-1.887264	0.993858
6	0.093986	-1.913796	1.388459
6	0.803893	-0.733268	1.578140
1	-1.660917	1.485130	0.838461
1	-2.902383	-0.615819	0.480295
1	-1.790366	-2.809701	0.844563
1	0.593692	-2.861199	1.554492
1	1.837094	-0.767518	1.902994
7	0.857531	1.702159	1.663537
1	1.864320	1.612830	1.675704
1	0.565406	2.491504	1.103812
1	0.181017	1.515293	3.992988
7	0.191915	0.757658	4.665966
1	-0.620242	0.168314	4.545519
6	1.397672	0.057424	4.674606
6	2.606430	0.726974	4.428099
6	1.439435	-1.316827	4.951083
6	3.812073	0.033244	4.428831
1	2.589455	1.794987	4.240983
6	2.649235	-2.000907	4.956000
1	0.512994	-1.848839	5.139703
6	3.846240	-1.336867	4.687031
1	4.733828	0.569926	4.232083
1	2.655681	-3.065136	5.164143
1	4.786551	-1.874246	4.687136

ANL2_21

6	-0.076000	0.471894	1.564855
6	-0.174997	-0.915847	1.720192
6	0.426125	-1.767089	0.799522
6	1.126369	-1.257239	-0.292609
6	1.218202	0.124920	-0.452722
6	0.627490	0.984903	0.467406
1	-0.700587	-1.324934	2.574951
1	0.346141	-2.838519	0.942643
1	1.590282	-1.924584	-1.008566
1	1.756268	0.539398	-1.297755
1	0.716064	2.059414	0.342679
7	-0.597275	1.340455	2.540105
1	-0.901094	2.236612	2.184730
1	-1.301930	0.921626	3.131540
1	2.668429	0.087028	3.318823
7	2.054055	0.357507	4.074349
1	1.476982	1.142699	3.795976
6	1.313428	-0.699602	4.601835
6	1.715675	-2.031074	4.422583
6	0.153151	-0.446529	5.350080
6	0.966722	-3.073984	4.954571
1	2.608154	-2.242671	3.843261
6	-0.593834	-1.496665	5.873591
1	-0.152195	0.580163	5.519250
6	-0.199003	-2.819799	5.677476
1	1.293002	-4.095868	4.795690
1	-1.489177	-1.278275	6.445462
1	-0.782569	-3.635330	6.086526

ANL2_22

6	-0.256573	0.531508	1.637043
6	-0.696660	-0.796524	1.686131
6	-0.271345	-1.709904	0.727780
6	0.588584	-1.320058	-0.297686
6	1.020632	0.004628	-0.352207
6	0.607547	0.923947	0.606626
1	-1.350361	-1.116869	2.488790
1	-0.615793	-2.735814	0.788664

1	0.914590	-2.034682	-1.043471
1	1.687208	0.326520	-1.144325
1	0.960088	1.949582	0.564616
7	-0.603240	1.438658	2.653970
1	-0.661746	2.402353	2.354696
1	-1.418769	1.169246	3.186963
1	2.215734	-0.623276	3.456519
7	1.645799	-0.258210	4.207074
1	1.291605	0.660312	3.966465
6	0.644329	-1.132332	4.628049
6	0.721281	-2.507896	4.366029
6	-0.458314	-0.649817	5.350210
6	-0.285058	-3.366522	4.792230
1	1.565532	-2.895192	3.805539
6	-1.464044	-1.515386	5.767503
1	-0.514623	0.407756	5.583275
6	-1.391362	-2.880011	5.489019
1	-0.207850	-4.425219	4.570534
1	-2.309027	-1.120351	6.320964
1	-2.175893	-3.551515	5.815446

ANL-iC3H7I_1

6	3.946650	-1.206122	-0.074539
6	3.654500	-0.000030	-0.723678
6	3.946629	1.206122	-0.074643
6	4.523933	1.201075	1.190278
6	4.819060	0.000090	1.833382
6	4.523954	-1.200957	1.190381
1	3.709255	-2.146141	-0.561232
1	3.709217	2.146094	-0.561417
1	4.743358	2.144846	1.676422
1	5.268501	0.000136	2.818630
1	4.743395	-2.144682	1.676607
1	3.126696	-0.837763	-2.517051
1	3.126686	0.837536	-2.517126
53	-0.072721	-0.000027	-0.956031
7	3.009992	-0.000090	-1.965850
6	-2.150950	0.000029	-0.154037
6	-2.385075	1.270624	0.645687
6	-2.385212	-1.270650	0.645513
1	-2.747764	0.000124	-1.064614
1	-2.217429	2.165015	0.044662
1	-3.421959	1.286119	1.002848
1	-1.726583	1.314029	1.516136
1	-2.217661	-2.164976	0.044365
1	-3.422098	-1.286083	1.002670
1	-1.726726	-1.314244	1.515957

ANL-iC3H7I_2

6	-4.097939	0.976387	0.536319
6	-3.689163	0.513120	-0.720536
6	-3.884168	-0.836186	-1.040943
6	-4.481000	-1.696189	-0.125747
6	-4.892236	-1.232947	1.122968
6	-4.693873	0.108754	1.444786
1	-3.935966	2.015788	0.801304
1	-3.556424	-1.209290	-2.005454
1	-4.624172	-2.737203	-0.392178
1	-5.356497	-1.905755	1.833254
1	-5.004138	0.485986	2.412576
1	-3.209085	2.351012	-1.487402
1	-3.056173	1.091268	-2.581116
53	0.012131	0.923582	-0.556945
7	-3.025878	1.365858	-1.610134
6	2.050783	0.552124	0.260155
6	2.831567	-0.327795	-0.701502
6	1.935944	-0.031250	1.658489
1	2.469979	1.556415	0.292685
1	1.377586	0.624702	2.327158

1	2.941060	-0.171489	2.074487
1	1.438608	-1.003577	1.639249
1	2.902873	0.119073	-1.693709
1	3.848034	-0.470890	-0.315206
1	2.366162	-1.311092	-0.800580

ANL-nC3F7I_d_1

6	4.119420	-1.153726	-0.208074
6	3.697497	0.048913	-0.781575
6	3.986628	1.255432	-0.138094
6	4.697426	1.255117	1.057615
6	5.124164	0.057558	1.628166
6	4.829594	-1.144588	0.988008
1	3.883047	-2.093876	-0.694925
1	3.646460	2.190480	-0.570192
1	4.915877	2.197574	1.545833
1	5.675656	0.060912	2.560010
1	5.151890	-2.084011	1.421517
1	3.052934	-0.769519	-2.542275
1	2.966372	0.890282	-2.497083
53	0.167801	-0.114866	-0.922116
7	2.906432	0.039540	-1.952210
6	-1.876213	-0.261084	-0.120551
6	-2.097127	0.389979	1.277237
6	-1.396797	-0.278266	2.499576
9	-2.722387	0.366585	-0.971033
9	-2.254694	-1.558523	-0.054284
9	-1.696170	1.680516	1.224638
9	-3.428104	0.370434	1.538839
9	-1.738097	0.393033	3.607487
9	-1.784216	-1.550252	2.638161
9	-0.065771	-0.244416	2.381118

ANL-nC3F7I_d_2

6	3.541305	-0.788798	0.952683
6	3.584898	-0.783671	-0.444220
6	3.941811	0.388798	-1.115997
6	4.260050	1.535650	-0.395993
6	4.222932	1.531099	0.996984
6	3.860992	0.362746	1.664576
1	3.248699	-1.691467	1.478372
1	3.960455	0.402905	-2.200520
1	4.536101	2.437848	-0.929038
1	4.469478	2.426191	1.554220
1	3.824316	0.345059	2.747471
1	3.305587	-2.797347	-0.673254
1	3.586990	-1.987909	-2.098069
53	0.302586	-1.523877	-1.532234
7	3.182551	-1.925628	-1.172440
6	-1.863311	-1.210244	-1.761143
6	-2.323230	0.276728	-1.823507
6	-2.173266	1.129878	-0.527062
9	-2.527769	-1.823085	-0.754212
9	-2.264974	-1.782057	-2.920882
9	-3.641724	0.290637	-2.142407
9	-1.643338	0.901620	-2.811572
9	-2.861047	0.590465	0.484489
9	-2.657448	2.356281	-0.763917
9	-0.892596	1.247010	-0.162409

ANL-nC3F7I_s_1

6	-4.090837	0.373509	-1.197488
6	-3.855007	-0.337406	-0.017400
6	-4.124788	0.266775	1.213779
6	-4.633515	1.560661	1.259161
6	-4.875402	2.268810	0.083615
6	-4.599669	1.666997	-1.142622
1	-3.867575	-0.084525	-2.155162

1	-3.927851	-0.274592	2.132963
1	-4.839556	2.016889	2.220298
1	-5.269967	3.276430	0.122669
1	-4.779142	2.206679	-2.065034
1	-3.451579	-2.126556	-0.923109
1	-3.474682	-2.200014	0.737743
53	-0.373985	-1.144704	-0.014694
7	-3.267346	-1.621009	-0.065966
6	1.805039	-0.813938	0.024542
6	2.164714	0.695696	-0.023555
6	3.688211	1.036897	0.000063
9	2.379802	-1.433283	-1.031584
9	2.328050	-1.351374	1.150080
9	1.655601	1.229206	-1.156981
9	1.603117	1.311516	1.041251
9	3.837518	2.367660	-0.045439
9	4.264188	0.584760	1.118653
9	4.315581	0.505020	-1.054036

ANL-nc3F7I_s_2

6	-4.414795	-0.193666	-1.231372
6	-3.989756	-0.696693	0.001466
6	-4.450443	-0.104005	1.180575
6	-5.332693	0.969838	1.122914
6	-5.762971	1.468601	-0.105159
6	-5.297240	0.880694	-1.279553
1	-4.047694	-0.639505	-2.149619
1	-4.110893	-0.480338	2.139658
1	-5.683618	1.419067	2.044529
1	-6.448997	2.305362	-0.146278
1	-5.620187	1.259836	-2.241987
1	-3.046030	-2.345841	-0.755265
1	-3.071627	-2.284901	0.905674
53	-0.405972	-0.447072	0.045183
7	-3.037605	-1.738664	0.054347
6	1.518838	0.628380	0.041548
6	2.728352	-0.342336	-0.029660
6	4.140648	0.323394	-0.038143
9	1.570572	1.467146	-1.017790
9	1.625694	1.375885	1.163492
9	2.630432	-1.079924	-1.159161
9	2.686564	-1.171033	1.038524
9	4.286510	1.125939	-1.097201
9	4.342279	1.035597	1.074968
9	5.073837	-0.636294	-0.102022

ANL-nc3H7I_d_1

6	3.649457	-1.169594	-0.122413
6	3.495730	0.027041	-0.834236
6	3.438067	1.232185	-0.122411
6	3.540035	1.236298	1.264122
6	3.698249	0.045000	1.970231
6	3.750444	-1.155741	1.264168
1	3.673553	-2.111464	-0.660039
1	3.296712	2.163498	-0.660259
1	3.491265	2.179643	1.796107
1	3.773628	0.051453	3.050445
1	3.866331	-2.093036	1.796355
1	3.688768	-0.796312	-2.697964
1	3.537947	0.872759	-2.697433
53	-0.069844	-0.152991	-1.471176
7	3.317055	0.011295	-2.220253
6	-1.679896	-0.127899	0.034699
6	-1.224967	0.458812	1.360865
1	-1.985391	-1.168632	0.123386
1	-0.886349	1.487607	1.207743
1	-2.119628	0.516907	1.996225
1	-2.475359	0.450754	-0.427260
6	-0.143540	-0.349549	2.076046

1	0.783135	-0.369578	1.500720
1	0.080771	0.084584	3.053157
1	-0.466900	-1.383268	2.233081

ANL-nC3H7I_d_2

6	3.114886	0.019500	-1.285294
6	2.545285	0.838518	-0.302571
6	2.904257	0.639826	1.036336
6	3.817876	-0.350901	1.378654
6	4.388423	-1.162162	0.399223
6	4.027565	-0.968683	-0.933176
1	2.831182	0.154084	-2.323698
1	2.456198	1.257707	1.807260
1	4.083913	-0.489470	2.420363
1	5.099313	-1.932993	0.669687
1	4.458427	-1.592581	-1.707930
1	1.604624	2.114854	-1.598974
1	1.460746	2.546896	0.012075
53	-1.095699	-0.006067	-0.364540
7	1.574424	1.787992	-0.644139
6	-2.874920	-1.298560	-0.173241
6	-4.185899	-0.554246	-0.368647
1	-2.791228	-1.735003	0.820488
1	-4.196097	-0.083460	-1.355984
1	-4.980011	-1.313272	-0.378957
1	-2.722694	-2.070562	-0.923224
6	-4.491494	0.480959	0.712676
1	-3.739165	1.272485	0.719897
1	-5.468008	0.941848	0.546383
1	-4.501386	0.019501	1.704783

ANL-nC3H7I_s_1

6	3.942061	-1.201798	-0.071891
6	3.639391	0.005150	-0.714243
6	3.927005	1.210404	-0.061870
6	4.510715	1.203724	1.200138
6	4.816401	0.001899	1.836642
6	4.525708	-1.198318	1.190159
1	3.708010	-2.141221	-0.561337
1	3.681220	2.150866	-0.543505
1	4.726634	2.146780	1.689196
1	5.270819	0.000652	2.819602
1	4.753408	-2.142637	1.671375
1	3.110465	-0.827875	-2.509031
1	3.100012	0.846392	-2.502074
53	-0.070155	-0.017123	-0.937278
7	2.987497	0.006229	-1.953489
6	-2.118460	-0.033288	-0.132801
6	-2.141398	-0.039666	1.386964
1	-2.580766	-0.922444	-0.557061
1	-1.599377	-0.914248	1.756811
1	-1.610388	0.838595	1.764000
1	-2.591922	0.853438	-0.549778
6	-3.579254	-0.050885	1.920259
1	-3.587184	-0.055418	3.013178
1	-4.133563	0.830843	1.585802
1	-4.122460	-0.936733	1.578550

ANL-nC3H7I_s_2

6	3.971294	-1.212095	-0.039103
6	3.679950	-0.008433	-0.692749
6	3.990195	1.200088	-0.057012
6	4.585129	1.199671	1.199781
6	4.879784	0.001025	1.847365
6	4.566311	-1.202340	1.217612
1	3.719854	-2.153675	-0.515626
1	3.753503	2.138316	-0.547497
1	4.818533	2.145116	1.676001

1	5.342832	0.004664	2.826275
1	4.784926	-2.144151	1.707844
1	3.126466	-0.854390	-2.473880
1	3.139466	0.819594	-2.486256
53	-0.051823	0.017257	-0.961900
7	3.018591	-0.012422	-1.927091
6	-2.136702	0.037428	-0.257587
6	-3.137905	0.033092	-1.401035
1	-2.215574	0.931591	0.357704
1	-2.965085	0.902687	-2.041030
1	-2.976435	-0.850618	-2.024444
1	-2.227072	-0.843835	0.374506
6	-4.579393	0.047373	-0.877604
1	-5.292825	0.044160	-1.705628
1	-4.784536	-0.829251	-0.256383
1	-4.773097	0.938173	-0.273099

pyCH3-iC3H7I

6	-3.584088	1.140730	-0.007423
6	-4.971874	1.190608	0.080211
6	-5.700717	-0.000005	0.125346
6	-4.971484	-1.190504	0.083583
6	-3.583715	-1.140420	-0.004193
7	-2.891361	0.000206	-0.049970
1	-2.999578	2.055325	-0.042455
1	-5.477218	2.149263	0.115506
1	-5.476515	-2.149220	0.121593
1	-2.998903	-2.054917	-0.036636
6	-7.204180	-0.000160	0.190183
1	-7.629595	-0.001652	-0.818656
1	-7.579393	-0.885542	0.706936
1	-7.579683	0.886554	0.704436
6	2.437771	-0.000431	-0.400129
6	2.991651	-1.269845	0.226705
6	2.991899	1.270040	0.224344
53	0.216595	-0.000078	-0.255718
1	2.600960	-0.001449	-1.476938
1	2.761994	1.315537	1.291504
1	4.082878	1.285747	0.111442
1	2.586753	2.164699	-0.250133
1	4.082627	-1.285978	0.113828
1	2.586327	-2.165308	-0.246101
1	2.761744	-1.313310	1.293950

pyCH3_nC3F7I_d

6	3.822021	-0.548696	0.928918
6	5.201778	-0.633113	1.072231
6	6.030151	0.071431	0.195006
6	5.404791	0.830300	-0.797552
6	4.017062	0.857441	-0.867479
7	3.233081	0.182498	-0.021810
1	3.159189	-1.087997	1.598035
1	5.624466	-1.245489	1.860216
1	5.990808	1.394836	-1.513430
1	3.509860	1.439286	-1.630412
6	7.527663	0.034370	0.328527
1	7.869034	0.835822	0.991616
1	7.865208	-0.912020	0.754565
1	8.016202	0.175181	-0.637192
6	-1.766754	0.382997	-0.462798
6	-2.595179	0.493379	0.850487
6	-2.616920	-0.750738	1.789172
9	-3.130765	-1.815863	1.166685
9	-3.381107	-0.472616	2.854281
9	-1.389432	-1.059444	2.224472
9	-2.138346	1.544681	1.569185
9	-3.887235	0.740969	0.516234
9	-2.205422	-0.700611	-1.150349
9	-2.077086	1.479970	-1.198292

53	0.422496	0.293461	-0.220706
pyCH3_nC3F7I_s			
6	-4.115983	-1.126671	-0.241065
6	-5.490154	-1.155125	-0.446872
6	-6.210083	0.042219	-0.459123
6	-5.487148	1.220025	-0.253702
6	-4.113088	1.155226	-0.055472
7	-3.432715	0.005317	-0.048680
1	-3.536596	-2.044279	-0.226835
1	-5.992799	-2.104024	-0.593706
1	-5.987372	2.181441	-0.245172
1	-3.531399	2.057015	0.106737
6	-7.693284	0.064230	-0.706979
1	-7.897211	0.150826	-1.779110
1	-8.168646	-0.852653	-0.354162
1	-8.166218	0.914133	-0.211891
6	1.535816	-0.065363	0.740156
6	2.373996	0.049145	-0.560595
6	3.924954	0.033867	-0.384875
9	4.502351	0.139508	-1.590485
9	4.334396	-1.107073	0.179481
9	4.334221	1.059401	0.369222
9	2.058562	-0.983738	-1.376041
9	2.058363	1.208462	-1.183236
9	1.870718	-1.218045	1.369463
9	1.871171	0.959288	1.561439
53	-0.635298	-0.030263	0.346957

pyCH3-nC3H7I_d			
6	3.468308	1.215244	0.296184
6	4.816277	1.560154	0.286431
6	5.771237	0.591143	-0.029494
6	5.299992	-0.691921	-0.316917
6	3.931821	-0.942408	-0.281993
7	3.022264	-0.011945	0.017550
1	2.710825	1.953998	0.540651
1	5.116515	2.574104	0.525916
1	5.989744	-1.491388	-0.563300
1	3.545811	-1.933532	-0.501033
6	7.238657	0.920363	-0.082641
1	7.521091	1.242516	-1.090203
1	7.489126	1.730753	0.604514
1	7.849966	0.051459	0.168459
6	-2.159965	-1.159796	0.098633
6	-2.920250	-0.616138	-1.101516
6	-2.534753	-1.256808	-2.434173
53	-0.002950	-0.691058	0.056687
1	-2.209691	-2.245991	0.157775
1	-2.511042	-0.731116	1.034231
1	-2.791763	0.469042	-1.154676
1	-3.987459	-0.792946	-0.909931
1	-2.675002	-2.341638	-2.401548
1	-3.147626	-0.862969	-3.248577
1	-1.487008	-1.062585	-2.672905

pyCH3-nC3H7I_s			
6	3.862942	-1.120421	0.213632
6	5.241638	-1.142632	0.399645
6	5.965023	0.049545	0.320512
6	5.240858	1.212515	0.048627
6	3.862196	1.136135	-0.122692
7	3.174531	-0.005556	-0.042995
1	3.282960	-2.036782	0.269993
1	5.744755	-2.081668	0.601321
1	5.743348	2.169874	-0.032342
1	3.281615	2.028729	-0.335944
6	7.452919	0.083209	0.543077

1	7.676593	0.241283	1.603131
1	7.920555	-0.856967	0.244618
1	7.919977	0.895786	-0.016628
6	-2.078535	-0.104038	-0.691110
6	-2.826759	0.093193	0.617841
6	-4.345215	0.060981	0.405726
53	0.106718	-0.064150	-0.428748
1	-2.294053	0.684876	-1.409647
1	-2.293785	-1.069798	-1.145100
1	-2.533290	-0.686182	1.326711
1	-2.533555	1.047009	1.065404
1	-4.666591	0.851358	-0.278935
1	-4.666324	-0.896218	-0.015458
1	-4.873799	0.203552	1.351901

pyNR2-iC3F7I_dimlam

6	0.835725	-1.560272	1.131529
6	-0.426952	-2.136580	1.193497
6	-1.103611	-2.438271	0.000430
6	-0.427544	-2.137979	-1.193317
6	0.835168	-1.561596	-1.132644
7	1.480455	-1.266548	-0.000891
1	1.357628	-1.325093	2.054484
1	-0.860965	-2.336158	2.161679
1	-0.862028	-2.338701	-2.161053
1	1.356614	-1.327501	-2.056133
7	-2.404489	-2.965065	0.001038
6	-2.863885	-3.621849	-1.224837
1	-2.836998	-2.929314	-2.064583
1	-2.259125	-4.504221	-1.470047
1	-3.899592	-3.927405	-1.085663
6	-2.863245	-3.620740	1.227751
1	-2.258325	-4.502863	1.473466
1	-2.835975	-2.927450	2.066858
1	-3.899009	-3.926464	1.089378
53	-3.976667	-0.507073	0.000356
6	-5.164857	1.356505	-0.000248
6	-6.006572	1.449824	-1.297502
6	-6.006188	1.450915	1.297163
9	-4.318165	2.431526	-0.000822
9	-6.688929	2.604567	-1.349892
9	-5.203867	1.406847	-2.370062
9	-6.886587	0.441986	-1.383404
9	-6.886234	0.443193	1.384119
9	-5.203197	1.408762	2.369548
9	-6.688468	2.605735	1.348836

pyNR2-iC3F7I_dim2am

6	0.678880	1.688420	-1.132811
6	-0.574996	2.283732	-1.193813
6	-1.246529	2.594670	-0.000233
6	-0.574552	2.283358	1.192990
6	0.679306	1.688067	1.131336
7	1.319571	1.384117	-0.000903
1	1.196766	1.446002	-2.056149
1	-1.006345	2.490575	-2.161664
1	-1.005554	2.489900	2.161065
1	1.197530	1.445357	2.054408
7	-2.539531	3.140348	0.000147
6	-2.989204	3.802183	1.226853
1	-2.972072	3.108281	2.065743
1	-2.371859	4.675515	1.473059
1	-4.020495	4.122665	1.088419
6	-2.989802	3.802707	-1.226064
1	-2.372602	4.676167	-1.472177
1	-2.973059	3.109181	-2.065268
1	-4.021039	4.123096	-1.087006
53	-4.132199	0.695604	-0.000023
6	-5.441524	-1.084424	-0.000152

6	-5.225148	-1.903082	-1.297417
6	-5.226250	-1.902438	1.297708
9	-6.750511	-0.682124	-0.000789
9	-6.056555	-2.955969	-1.349301
9	-5.477549	-1.138008	-2.369553
9	-3.968701	-2.358540	-1.384485
9	-3.969890	-2.357906	1.386043
9	-5.479471	-1.136764	2.369223
9	-6.057763	-2.955251	1.349435

pyNR2-iC3F7I_trm1

6	-0.797901	1.523628	1.140695
6	0.441892	2.139102	1.197200
6	1.110050	2.460018	0.000545
6	0.441899	2.139688	-1.196271
6	-0.797894	1.524186	-1.140075
7	-1.421636	1.212887	0.000232
1	-1.320142	1.269552	2.057299
1	0.869458	2.355850	2.164047
1	0.869471	2.356907	-2.163010
1	-1.320129	1.270559	-2.056806
7	2.384125	3.022203	0.000686
6	2.855441	3.658012	-1.231300
1	2.852930	2.946892	-2.056200
1	2.243976	4.526531	-1.505768
1	3.883993	3.980931	-1.081619
6	2.855447	3.657381	1.232994
1	2.243983	4.525759	1.507911
1	2.852938	2.945837	2.057529
1	3.883998	3.980377	1.083475
6	-5.912274	-0.961022	-0.000320
6	-6.687131	-0.617937	-1.293171
6	-6.686907	-0.619053	1.292960
9	-5.735241	-2.323945	-0.000924
9	-5.976510	-0.988701	-2.369364
9	-6.936020	0.697350	-1.382586
9	-7.864259	-1.265677	-1.350355
9	-6.935780	0.696157	1.383554
9	-7.864026	-1.266841	1.349788
9	-5.976101	-0.990747	2.368710
53	-3.928043	0.037579	-0.000060
53	3.975274	0.499616	0.000032
6	5.147444	-1.367936	-0.000497
6	5.989223	-1.464124	-1.299413
6	5.987945	-1.465663	1.299131
9	4.293642	-2.434382	-0.001550
9	6.663691	-2.621975	-1.349503
9	5.185644	-1.415810	-2.370527
9	6.873402	-0.460458	-1.383453
9	6.872042	-0.462098	1.385226
9	5.183315	-1.418615	2.369510
9	6.662363	-2.623573	1.348512

pyNR2-iC3F7I_trm2

6	0.818807	-1.524899	1.140702
6	-0.424941	-2.132322	1.197206
6	-1.095105	-2.448975	0.000544
6	-0.424921	-2.132954	-1.196274
6	0.818826	-1.525501	-1.140070
7	1.444543	-1.218205	0.000240
1	1.342584	-1.274001	2.057303
1	-0.853935	-2.346286	2.164043
1	-0.853899	-2.347429	-2.163005
1	1.342618	-1.275088	-2.056795
7	-2.372890	-3.002540	0.000679
6	-2.848939	-3.634325	-1.231515
1	-2.842145	-2.922564	-2.055864
1	-2.243366	-4.506636	-1.507004
1	-3.879549	-3.950576	-1.081737

6	-2.848961	-3.633675	1.233198
1	-2.243393	-4.505840	1.509158
1	-2.842182	-2.921480	2.057172
1	-3.879568	-3.950005	1.083569
6	5.941811	0.941783	-0.000312
6	6.715669	0.596488	-1.293169
6	6.715467	0.597576	1.292955
9	5.768707	2.305216	-0.000900
9	6.006104	0.969287	-2.369358
9	6.960801	-0.719504	-1.382594
9	7.894649	1.240859	-1.350368
9	6.960584	-0.718341	1.383526
9	7.894439	1.241994	1.349796
9	6.005735	0.971282	2.368719
53	3.954721	-0.051128	-0.000049
53	-3.929331	-0.458224	-0.000004
6	-5.177892	1.358603	-0.000489
6	-4.932786	2.168966	1.298844
6	-4.932750	2.168297	-1.300233
9	-6.496762	0.998563	-0.000415
9	-5.727805	3.247921	1.348059
9	-5.211670	1.411242	2.369124
9	-3.661467	2.579516	1.385208
9	-3.661429	2.578802	-1.386773
9	-5.211605	1.410022	-2.370131
9	-5.727768	3.247226	-1.350026

pyNR2-iC3F7I_trm3

6	0.791167	1.747800	-1.141754
6	-0.478905	2.298123	-1.197863
6	-1.162564	2.583624	-0.000991
6	-0.478421	2.298177	1.195616
6	0.791634	1.747864	1.139018
7	1.430464	1.469675	-0.001491
1	1.325739	1.521477	-2.058521
1	-0.917371	2.492579	-2.164571
1	-0.916495	2.492681	2.162492
1	1.326584	1.521599	2.055579
7	-2.464110	3.078940	-0.000736
6	-2.967455	3.689125	1.231543
1	-2.928090	2.978761	2.056164
1	-2.401605	4.587951	1.506261
1	-4.011329	3.958562	1.082122
6	-2.967908	3.689214	-1.232788
1	-2.402152	4.588053	-1.507656
1	-2.928864	2.978910	-2.057477
1	-4.011724	3.958650	-1.082956
6	6.089836	-0.312740	-0.002458
6	6.372619	-1.118521	-1.290973
6	6.379588	-1.101119	1.295242
9	6.954958	0.755517	-0.011983
9	6.148698	-0.354410	-2.371327
9	5.591725	-2.205964	-1.371894
9	7.653503	-1.524264	-1.348692
9	5.599088	-2.187284	1.395052
9	7.660745	-1.506202	1.351465
9	6.161567	-0.322507	2.366412
53	3.998811	0.436584	-0.001824
53	-3.922965	0.477755	-0.000547
6	-4.997960	-1.447399	-0.000223
6	-5.833124	-1.587009	1.299017
6	-5.832947	-1.587545	-1.299518
9	-4.090676	-2.468735	0.000046
9	-6.447404	-2.777890	1.348979
9	-5.032594	-1.497979	2.369803
9	-6.767489	-0.629953	1.383796
9	-6.767273	-0.630498	-1.384838
9	-5.032268	-1.499002	-2.370231
9	-6.447259	-2.778428	-1.349050

pyNR2-iC3F7I_trm4

6	0.617939	1.867111	-1.141535
6	-0.645285	2.433070	-1.196412
6	-1.325246	2.724602	0.001109
6	-0.644503	2.428551	1.197074
6	0.618695	1.862827	1.139235
7	1.253896	1.578940	-0.001897
1	1.149495	1.635780	-2.058805
1	-1.081485	2.634721	-2.162672
1	-1.080067	2.626562	2.164373
1	1.150865	1.628070	2.055278
7	-2.620822	3.235142	0.002500
6	-3.117391	3.847772	1.236261
1	-3.086755	3.134599	2.058856
1	-2.541116	4.739064	1.513823
1	-4.157975	4.129942	1.087372
6	-3.118117	3.852667	-1.228527
1	-2.542025	4.745077	-1.502859
1	-3.087933	3.142791	-2.053984
1	-4.158625	4.134208	-1.077918
6	5.883017	-0.280449	-0.008276
6	6.141560	-1.113972	-1.284171
6	6.170143	-1.050158	1.301157
9	6.765909	0.772612	-0.044053
9	5.921522	-0.365756	-2.376387
9	5.341933	-2.189351	-1.339102
9	7.414954	-1.542269	-1.344750
9	5.372230	-2.120886	1.426883
9	7.444681	-1.475980	1.354511
9	5.974196	-0.248795	2.359738
53	3.804964	0.504147	-0.004532
53	-4.090880	0.639865	-0.002102
6	-5.277006	-1.218318	-0.004938
6	-5.008902	-2.014704	-1.308365
6	-5.000018	-2.024346	1.290686
9	-6.607344	-0.903358	0.000779
9	-5.766795	-3.119973	-1.359313
9	-5.317203	-1.262713	-2.374613
9	-3.724619	-2.381262	-1.400651
9	-3.715198	-2.391746	1.371341
9	-5.300785	-1.280218	2.364573
9	-5.757752	-3.129855	1.338710

pyNR2-iC3H7I_dimlam

6	3.465600	-1.468016	-1.152454
6	2.751195	-0.279564	-1.203253
6	2.360148	0.344715	-0.002055
6	2.760198	-0.299006	1.185791
6	3.474144	-1.486448	1.110272
7	3.835757	-2.089110	-0.027448
1	3.760896	-1.947899	-2.081477
1	2.504784	0.141570	-2.166690
1	2.521059	0.106325	2.157805
1	3.776336	-1.981416	2.029099
7	1.607479	1.503447	0.010154
6	1.462346	2.240352	1.257193
1	1.030950	1.603980	2.031140
1	2.418494	2.640305	1.621782
1	0.773840	3.068059	1.096069
6	1.452869	2.260372	-1.223687
1	2.406180	2.666430	-1.588931
1	1.015813	1.636380	-2.004519
1	0.765444	3.085156	-1.044013
53	-1.291542	0.031823	0.012201
6	-3.310666	-0.911352	0.013309
6	-4.087586	-0.446369	1.232698
6	-4.008557	-0.616937	-1.303113
1	-3.059450	-1.967561	0.092117
1	-3.428757	-0.967119	-2.157587

1	-4.187952	0.453755	-1.423545
1	-4.979155	-1.127121	-1.315005
1	-3.563324	-0.676546	2.160657
1	-5.059157	-0.954460	1.252570
1	-4.269705	0.630046	1.197388

pyNR2-iC3H7I_dim1py

6	1.612624	-1.127976	-0.033257
6	2.996550	-1.193366	0.013228
6	3.745151	0.001579	0.089717
6	2.998888	1.200371	0.090658
6	1.614790	1.140799	0.040176
7	0.908252	0.007811	-0.018845
1	1.033829	-2.045562	-0.089155
1	3.476548	-2.160744	-0.011116
1	3.480646	2.166427	0.129019
1	1.037871	2.061232	0.043833
7	5.116698	-0.002096	0.162670
6	5.846122	1.251198	0.058080
1	5.700685	1.738979	-0.915053
1	5.538086	1.948656	0.841287
1	6.908706	1.054819	0.188735
6	5.843934	-1.247354	-0.022047
1	5.533876	-1.993344	0.714222
1	5.698603	-1.671045	-1.024766
1	6.906747	-1.061841	0.121975
6	-4.391141	-0.016086	-0.238242
6	-4.935020	1.292253	0.313366
6	-4.928095	-1.241041	0.485030
53	-2.167326	-0.003690	-0.147403
1	-4.582387	-0.089027	-1.308094
1	-6.021614	-1.266030	0.400615
1	-4.531995	-2.165883	0.063577
1	-4.671821	-1.213213	1.546867
1	-6.028620	1.299644	0.226881
1	-4.543856	2.153952	-0.229179
1	-4.678939	1.409437	1.369155

pyNR2-iC3H7I_dim2am

6	-4.053437	1.995609	-0.894354
6	-3.624014	0.689378	-1.080673
6	-3.405017	-0.133921	0.041738
6	-3.671687	0.450233	1.296022
6	-4.098617	1.769101	1.356643
7	-4.294539	2.558069	0.294747
1	-4.216428	2.627875	-1.762835
1	-3.461386	0.330887	-2.086323
1	-3.547636	-0.101970	2.215788
1	-4.298492	2.216404	2.326462
7	-2.931628	-1.426278	-0.078841
6	-2.976332	-2.308139	1.078530
1	-2.428012	-1.872096	1.914759
1	-4.003835	-2.521928	1.403503
1	-2.486394	-3.246005	0.822653
6	-2.925694	-2.059196	-1.389756
1	-3.938223	-2.199089	-1.792608
1	-2.345191	-1.467506	-2.099008
1	-2.443270	-3.031518	-1.306383
53	0.221407	-0.646123	0.065780
6	2.393378	-0.154103	0.161681
6	2.928879	0.043132	-1.245883
6	2.595548	1.050042	1.065099
1	2.807852	-1.053770	0.613046
1	2.206749	0.875387	2.068702
1	2.105541	1.936358	0.656417
1	3.668757	1.260891	1.144383
1	2.773562	-0.839147	-1.867581
1	2.451729	0.896337	-1.732934
1	4.006188	0.241050	-1.193773

pyNR2-iC3H7I_trm1			
6	0.744316	-1.623810	1.135273
6	-0.479744	-2.271776	1.196979
6	-1.145484	-2.609378	0.000793
6	-0.479776	-2.272766	-1.195689
6	0.744285	-1.624750	-1.134553
7	1.366719	-1.292389	0.000214
1	1.257780	-1.357741	2.054782
1	-0.902367	-2.500453	2.163964
1	-0.902424	-2.502244	-2.162474
1	1.257725	-1.359442	-2.054296
7	-2.387720	-3.209879	0.001059
6	-2.912762	-3.758598	-1.240943
1	-2.961713	-2.987376	-2.011139
1	-2.308915	-4.595437	-1.617349
1	-3.928432	-4.109136	-1.066625
6	-2.912722	-3.757577	1.243530
1	-2.308850	-4.594092	1.620615
1	-2.961669	-2.985718	2.013087
1	-3.928389	-4.108280	1.069526
6	6.107267	1.072554	-0.000944
6	6.861406	0.706853	-1.269660
6	6.860338	0.710269	1.269385
53	4.112641	0.085319	-0.000453
53	-4.054782	-0.403932	-0.000076
6	-5.242219	1.482008	-0.000833
6	-6.069705	1.559720	-1.271929
6	-6.068281	1.561629	1.271071
1	-4.456248	2.235029	-0.001837
1	-5.445290	1.508105	2.164313
1	-6.608656	2.515673	1.286567
1	-6.804060	0.755564	1.314695
1	-5.447714	1.504853	-2.165787
1	-6.610096	2.513740	-1.288253
1	-6.805532	0.753592	-1.313519
1	5.846636	2.130209	-0.002476
1	6.303999	0.992779	2.164141
1	7.824736	1.232992	1.285408
1	7.057379	-0.363533	1.315698
1	6.305819	0.986953	-2.165641
1	7.825816	1.229533	-1.286280
1	7.058484	-0.367069	-1.312918

pyNR2-iC3H7I_trm2			
6	0.544929	1.771192	-1.135078
6	-0.663466	2.447924	-1.196035
6	-1.321439	2.799152	0.000575
6	-0.663480	2.446196	1.196685
6	0.544914	1.769552	1.134765
7	1.159220	1.423587	-0.000403
1	1.052031	1.494204	-2.054903
1	-1.080630	2.687575	-2.162735
1	-1.080656	2.684450	2.163725
1	1.052005	1.491234	2.054194
7	-2.550040	3.426566	0.001021
6	-3.064902	3.982702	1.243946
1	-3.130571	3.210584	2.012036
1	-2.444288	4.805861	1.623186
1	-4.072945	4.354647	1.069709
6	-3.064882	3.984509	-1.241103
1	-2.444264	4.808221	-1.619133
1	-3.130534	3.213509	-2.010316
1	-4.072929	4.356195	-1.066343
6	5.823150	-1.088059	-0.002081
6	6.587166	-0.750176	1.268439
6	6.588578	-0.745884	-1.270601
53	3.860714	-0.038209	-0.001396
53	-4.259342	0.644399	-0.001049

6	-5.439229	-1.247039	-0.002496
6	-5.136644	-2.026318	-1.270526
6	-5.149417	-2.020341	1.272158
1	-6.461930	-0.874384	-0.008504
1	-4.087399	-2.326930	-1.307512
1	-5.360293	-1.447297	-2.167014
1	-5.751070	-2.934443	-1.286262
1	-4.100611	-2.320783	1.321068
1	-5.382027	-1.437110	2.163624
1	-5.764009	-2.928385	1.286001
1	5.529263	-2.136961	-0.004016
1	6.022113	-1.015299	2.163057
1	7.534586	-1.303073	1.284352
1	6.817994	0.316854	1.315153
1	7.536016	-1.298727	-1.287329
1	6.819455	0.321297	-1.313451
1	6.024521	-1.007981	-2.166738

pyNR2-iC3H7I_trm3

6	0.710543	1.922790	-1.071918
6	-0.542969	2.533210	-1.015272
6	-1.200939	2.668242	0.237581
6	-0.497801	2.178764	1.371966
6	0.753665	1.585228	1.202367
7	1.372006	1.443943	0.007077
1	1.213546	1.814113	-2.030705
1	-0.992197	2.887553	-1.930885
1	-0.910877	2.249326	2.367005
1	1.291063	1.205589	2.069065
7	-2.469664	3.222506	0.343694
6	-2.989461	3.565626	1.660180
1	-2.998808	2.689436	2.309975
1	-2.406495	4.359486	2.146627
1	-4.019243	3.901765	1.553130
6	-3.036391	3.927895	-0.797491
1	-2.466204	4.830155	-1.057274
1	-3.077070	3.275541	-1.670935
1	-4.058678	4.215561	-0.558620
6	6.172486	-0.738080	-0.503205
6	6.149463	-2.167252	0.015548
6	7.208350	0.134082	0.188511
53	4.154095	0.174157	-0.286387
53	-4.044766	0.389920	-0.041696
6	-5.169957	-1.516321	-0.300664
6	-6.239794	-1.624599	0.771762
6	-5.714622	-1.593975	-1.716214
1	-4.386390	-2.255561	-0.144647
1	-4.922216	-1.517465	-2.461229
1	-6.441903	-0.800781	-1.903126
1	-6.220709	-2.557296	-1.851523
1	-5.816600	-1.570271	1.775183
1	-6.984051	-0.831954	0.667888
1	-6.753169	-2.587969	0.667802
1	6.321357	-0.725517	-1.582230
1	7.019608	0.189525	1.263389
1	7.212223	1.150003	-0.208590
1	8.206727	-0.296258	0.041511
1	5.923531	-2.192918	1.084365
1	5.406491	-2.774236	-0.503466
1	7.134219	-2.627163	-0.133753

pyNR2-iC3H7I_trm4

6	0.527523	1.997381	-1.074664
6	-0.709019	2.624094	-1.079773
6	-1.376267	2.849146	0.141801
6	-0.698776	2.429433	1.304977
6	0.537338	1.812806	1.187662
7	1.160986	1.586158	0.027755
1	1.042080	1.817356	-2.014222

1	-1.140226	2.922705	-2.023627
1	-1.121712	2.570684	2.288412
1	1.059695	1.483317	2.081265
7	-2.630606	3.421045	0.193740
6	-3.163429	3.853153	1.477732
1	-3.192493	3.019927	2.181523
1	-2.577117	4.669360	1.921151
1	-4.187293	4.193943	1.334835
6	-3.174210	4.053903	-0.999253
1	-2.590397	4.930459	-1.311303
1	-3.211130	3.344500	-1.827436
1	-4.196046	4.367861	-0.794004
6	5.909334	-0.742574	-0.275872
6	5.815794	-2.174357	0.227557
6	6.938744	0.089800	0.472221
53	3.913387	0.233359	-0.145708
53	-4.216234	0.575711	-0.027217
6	-5.307870	-1.362340	-0.174814
6	-5.665070	-1.630784	-1.626359
6	-4.469721	-2.458378	0.460003
1	-6.200453	-1.162506	0.415283
1	-3.531523	-2.600735	-0.080470
1	-4.235237	-2.239287	1.502041
1	-5.029116	-3.400882	0.424591
1	-4.767692	-1.747399	-2.237835
1	-6.269830	-0.829234	-2.051562
1	-6.239607	-2.562887	-1.685860
1	6.109558	-0.726170	-1.346510
1	7.928622	-0.371643	0.368372
1	6.994129	1.108199	0.085452
1	6.701123	0.142728	1.537494
1	6.791262	-2.664876	0.120625
1	5.079254	-2.752682	-0.331791
1	5.538530	-2.201204	1.284192

pyNR2-nC3F7I_d_1_dimam

6	4.132975	-1.175251	-0.192534
6	3.692763	0.018603	-0.788249
6	3.987903	1.205428	-0.096615
6	4.665877	1.136293	1.113869
6	4.803684	-1.121610	1.022836
1	3.961931	-2.137814	-0.650689
1	3.698656	2.173686	-0.476747
1	4.890610	2.054139	1.649282
1	5.141067	-2.045355	1.483833
53	0.235181	-0.170607	-0.829610
7	2.956109	0.021953	-1.979401
6	-1.817251	-0.346271	-0.060888
6	-2.091510	0.397546	1.280856
6	-1.403119	-0.161404	2.563608
9	-2.665103	0.180825	-0.973173
9	-2.139823	-1.649432	0.092297
9	-1.725714	1.691803	1.142127
9	-3.427085	0.356064	1.509733
9	-1.775870	0.587213	3.608799
9	-1.772575	-1.425434	2.791823
9	-0.070895	-0.113368	2.463523
7	5.079017	0.003302	1.688692
6	3.024231	-1.172776	-2.821303
1	2.679947	-2.048682	-2.273104
1	2.357382	-1.035829	-3.671065
1	4.040664	-1.361020	-3.190595
6	2.883230	1.277688	-2.727084
1	2.441727	2.063515	-2.115761
1	3.870102	1.609415	-3.074822
1	2.234102	1.130305	-3.588736

pyNR2-nC3F7I_d_1_dimpy

6	-3.095920	1.156276	-0.444426
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6	-4.470249	1.143560	-0.288271
6	-5.119507	-0.062309	0.064565
6	-4.286043	-1.193482	0.225618
6	-2.920784	-1.064508	0.044480
7	-2.313687	0.082083	-0.284322
1	-2.590494	2.078426	-0.713843
1	-5.022636	2.058949	-0.440484
1	-4.690109	-2.160168	0.487302
1	-2.274670	-1.927993	0.168192
7	-6.472245	-0.130328	0.240142
6	-7.104836	-1.404904	0.543765
1	-6.956698	-2.135061	-0.260437
1	-6.713973	-1.830846	1.473135
1	-8.174060	-1.249652	0.669622
6	-7.298049	1.044052	0.003907
1	-7.006647	1.872462	0.657174
1	-7.233801	1.384686	-1.036112
1	-8.335666	0.797389	0.217658
6	2.618164	0.293659	-0.944213
6	3.429490	1.239268	-0.012657
53	0.434756	0.237045	-0.616276
6	3.228568	2.773188	-0.200825
9	2.890953	0.634485	-2.230207
9	3.120869	-0.952325	-0.743984
9	4.752251	1.002633	-0.210616
9	3.139191	0.940970	1.275167
9	3.574488	3.158157	-1.433410
9	4.006911	3.420662	0.678185
9	1.959296	3.134605	0.020303

pyNR2-nC3F7I_d_2_dimam

6	3.534506	-0.418926	0.460889
6	3.453173	0.077123	-0.851084
6	3.529142	1.472658	-0.995050
6	3.660389	2.266820	0.137108
6	3.665700	0.472795	1.517995
1	3.494276	-1.476597	0.673964
1	3.483971	1.949160	-1.962828
1	3.715715	3.345690	0.024896
1	3.725654	0.088373	2.532035
53	0.296080	-0.780814	-1.986426
7	3.255986	-0.768771	-1.949762
6	-1.899345	-0.871828	-2.064498
6	-2.634435	0.447038	-1.678499
6	-2.556570	0.901011	-0.188664
9	-2.345970	-1.866406	-1.266319
9	-2.273214	-1.164095	-3.330891
9	-3.949579	0.285026	-1.964882
9	-2.154688	1.451713	-2.445715
9	-3.073343	-0.027986	0.621438
9	-3.262846	2.029463	-0.048789
9	-1.295491	1.143335	0.182958
7	3.729559	1.800732	1.387208
6	3.571565	-2.187105	-1.777844
1	2.976926	-2.617779	-0.973364
1	3.311066	-2.713235	-2.694832
1	4.635117	-2.350774	-1.561011
6	3.575429	-0.241083	-3.276681
1	2.982255	0.647133	-3.489711
1	4.639506	0.009168	-3.376665
1	3.316107	-0.993305	-4.019947

pyNR2-nC3F7I_d_2_dimpy

6	-2.947616	0.860718	0.477698
6	-4.326197	0.972174	0.498143
6	-5.117421	-0.082917	-0.012639
6	-4.412848	-1.196451	-0.526225
6	-3.029951	-1.200396	-0.495239
7	-2.288722	-0.199598	-0.005007

1	-2.333819	1.665927	0.869225
1	-4.772787	1.867338	0.904929
1	-4.929252	-2.047763	-0.944344
1	-2.482491	-2.052435	-0.885998
7	-6.482170	-0.029861	-0.009527
6	-7.255178	-1.111672	-0.600328
1	-7.048079	-1.222831	-1.671110
1	-7.044467	-2.065720	-0.107057
1	-8.314878	-0.898296	-0.479115
6	-7.164361	1.161637	0.472008
1	-6.907630	1.372134	1.514941
1	-6.917060	2.043907	-0.129863
1	-8.238959	1.002365	0.416738
6	2.686884	-0.410347	-0.054087
6	3.424298	-0.336187	1.313738
53	0.481788	-0.308835	0.018357
6	3.380289	1.021855	2.076939
9	3.050036	-1.594220	-0.612522
9	3.176258	0.575442	-0.849758
9	2.920912	-1.286629	2.135323
9	4.737879	-0.612847	1.106750
9	3.937271	1.999800	1.355479
9	4.068652	0.895821	3.220604
9	2.126165	1.375419	2.381506

pyNR2-nC3F7I_s_1_dimam

6	3.927883	-1.191064	0.003314
6	3.576153	0.001625	-0.650950
6	3.912845	1.195910	0.008297
6	4.543797	1.135737	1.244409
6	4.558058	-1.128108	1.239683
1	3.719185	-2.159538	-0.425859
1	3.691951	2.163461	-0.416835
1	4.801063	2.059596	1.754255
1	4.826958	-2.050773	1.745675
53	0.097763	-0.019877	-0.850062
7	2.885601	-0.000182	-1.869009
6	-2.012751	-0.034505	-0.221901
6	-2.152414	-0.038363	1.325038
6	-3.613518	-0.048708	1.876222
9	-2.626516	-1.128846	-0.721860
9	-2.640399	1.053850	-0.717671
9	-1.533244	-1.135495	1.814464
9	-1.547231	1.064668	1.818688
9	-3.573418	-0.051029	3.214448
9	-4.284423	1.035304	1.473545
9	-4.270602	-1.139602	1.469359
7	4.872996	0.004524	1.874282
6	2.921691	-1.226444	-2.666280
1	2.510875	-2.062978	-2.102691
1	2.295479	-1.086028	-3.545872
1	3.939918	-1.480190	-2.988525
6	2.906228	1.229751	-2.661159
1	2.484925	2.058688	-2.094098
1	3.921170	1.497639	-2.982315
1	2.281811	1.085130	-3.541345

pyNR2-nC3F7I_s_1_dimpy

6	-2.917546	1.169087	0.633149
6	-4.300692	1.148442	0.626998
6	-4.977755	0.046891	0.054130
6	-4.160481	-0.979667	-0.473363
6	-2.784308	-0.853174	-0.412481
7	-2.151356	0.195780	0.126326
1	-2.391053	2.012089	1.069677
1	-4.838325	1.977803	1.062159
1	-4.585191	-1.864224	-0.924400
1	-2.150671	-1.636391	-0.816805
7	-6.341329	-0.021317	0.012294

6	-6.995820	-1.202370	-0.529512
1	-6.708330	-1.372667	-1.571737
1	-6.754433	-2.102860	0.047331
1	-8.073368	-1.056998	-0.498401
6	-7.142759	1.027853	0.623644
1	-6.965426	1.099502	1.703143
1	-6.930712	2.002693	0.173526
1	-8.196221	0.807647	0.465724
6	2.827777	0.422281	0.322752
6	3.473907	1.103154	-0.911869
53	0.622501	0.344445	0.192269
6	5.031264	1.205161	-0.910707
9	3.201589	1.105296	1.434315
9	3.329364	-0.834051	0.431665
9	2.996986	2.365968	-1.014877
9	3.125581	0.414176	-2.023958
9	5.467298	1.921465	0.131039
9	5.594358	-0.007018	-0.865991
9	5.431422	1.813961	-2.037268

pyNR2-nC3F7I_s_2_dimam

6	3.724557	-1.292534	-0.115914
6	3.541364	-0.015149	-0.671969
6	3.984916	1.070203	0.102387
6	4.550860	0.830488	1.348213
6	4.303713	-1.410325	1.141162
1	3.424050	-2.189243	-0.636786
1	3.896414	2.089746	-0.241704
1	4.891189	1.670481	1.946770
1	4.442162	-2.398093	1.571039
53	0.084918	0.370946	-1.018569
7	2.909786	0.168386	-1.907926
6	-2.011338	0.577035	-0.375751
6	-2.962115	-0.317397	-1.217424
6	-4.475464	-0.248390	-0.838600
9	-2.122855	0.234169	0.924888
9	-2.397751	1.865396	-0.499136
9	-2.576621	-1.606716	-1.087285
9	-2.859697	0.040567	-2.517492
9	-4.671074	-0.638966	0.424274
9	-4.949409	0.992667	-0.986653
9	-5.162973	-1.065059	-1.647646
7	4.719712	-0.381247	1.884741
6	2.846159	-0.979499	-2.813190
1	2.320445	-1.809969	-2.344081
1	2.279611	-0.691935	-3.697395
1	3.843747	-1.318218	-3.121447
6	3.101842	1.452283	-2.582732
1	2.750165	2.271307	-1.956817
1	4.153521	1.629360	-2.842840
1	2.505137	1.457303	-3.493445

pyNR2-nC3F7I_s_2_dimpy

6	-2.847063	1.146244	-0.036017
6	-4.227808	1.202438	0.026794
6	-4.971989	0.000654	0.070565
6	-4.221330	-1.197391	0.035864
6	-2.840908	-1.134222	-0.027398
7	-2.143892	0.007785	-0.062543
1	-2.269195	2.064630	-0.068243
1	-4.712115	2.167581	0.040912
1	-4.700421	-2.165001	0.057285
1	-2.258089	-2.049691	-0.052695
7	-6.336001	-0.002755	0.142656
6	-7.063917	-1.262317	0.121717
1	-6.897873	-1.813566	-0.811263
1	-6.771170	-1.904029	0.958610
1	-8.128645	-1.058716	0.211792
6	-7.070706	1.252664	0.112196

1	-6.781464	1.902255	0.944215
1	-6.907600	1.797732	-0.824924
1	-8.134323	1.044004	0.203803
6	2.834459	0.020062	-0.374837
6	3.549275	0.027094	1.001517
53	0.631904	0.014813	-0.187627
6	5.109678	0.031192	0.971616
9	3.242671	-1.074876	-1.064976
9	3.236769	1.112039	-1.073086
9	3.171961	-1.071845	1.696306
9	3.166025	1.129103	1.688145
9	5.583519	-1.057167	0.355663
9	5.577652	1.117495	0.347598
9	5.572130	0.037111	2.230984

pyNR2-nC3F7I_s_trm1

6	-2.942307	1.137925	-0.098092
6	-4.322045	1.194210	0.014556
6	-5.061952	-0.002904	0.060997
6	-4.320845	-1.199039	0.008828
6	-2.941164	-1.140832	-0.103544
7	-2.245500	-0.000965	-0.158969
1	-2.364382	2.055709	-0.137496
1	-4.799967	2.160757	0.060994
1	-4.797797	-2.166277	0.050634
1	-2.362318	-2.057837	-0.147343
7	-6.451420	-0.003725	0.112140
6	-7.128196	-1.238341	0.509678
1	-6.861189	-2.055635	-0.159239
1	-6.887256	-1.527674	1.540341
1	-8.202722	-1.086212	0.426303
6	-7.129437	1.228318	0.515503
1	-6.888796	1.513017	1.547525
1	-6.863243	2.049032	-0.149540
1	-8.203809	1.075507	0.431395
6	2.760307	0.002433	-0.525714
6	3.482655	-0.000678	0.847362
53	0.562514	0.000828	-0.321167
6	5.042989	0.000198	0.806492
9	3.158731	-1.088672	-1.224770
9	3.157647	1.097451	-1.219247
9	3.106513	-1.102965	1.536804
9	3.105424	1.097739	1.542363
9	5.509139	-1.085373	0.180302
9	5.508061	1.089376	0.185787
9	5.513179	-0.002737	2.062515
6	-7.365631	0.008192	-5.034874
6	-8.888248	0.002821	-5.344813
6	-9.272320	0.005969	-6.858701
9	-6.806342	1.103192	-5.587759
9	-6.797249	-1.078605	-5.594615
9	-9.449516	1.098519	-4.786658
9	-9.440351	-1.100992	-4.793553
9	-8.800422	1.097409	-7.468206
9	-8.791346	-1.077645	-7.475034
9	-10.606753	0.000740	-6.966447
53	-6.981848	0.002993	-2.867829

pyNR2-nC3F7I_s_trm2

6	-2.940358	1.138581	-0.039906
6	-4.320409	1.195617	0.068501
6	-5.060852	-0.001090	0.114591
6	-4.320209	-1.197607	0.066801
6	-2.940167	-1.140185	-0.041524
7	-2.243936	-0.000704	-0.096919
1	-2.361932	2.056036	-0.079364
1	-4.798069	2.162450	0.111534
1	-4.797705	-2.164580	0.108463
1	-2.361586	-2.057485	-0.082282

7	-6.450703	-0.001238	0.159268
6	-7.129810	-1.235137	0.554719
1	-6.860315	-2.052985	-0.112584
1	-6.893468	-1.524190	1.586534
1	-8.203934	-1.082562	0.466824
6	-7.130014	1.231981	0.556491
1	-6.893706	1.519597	1.588714
1	-6.860665	2.050828	-0.109645
1	-8.204112	1.079350	0.468392
6	2.762513	-0.000088	-0.452959
6	3.481559	-0.000476	0.921857
53	0.564263	-0.000370	-0.253627
6	5.041987	-0.000306	0.884785
9	3.162248	-1.092889	-1.148617
9	3.162036	1.093253	-1.147889
9	3.103358	-1.101103	1.612842
9	3.103136	1.099613	1.613579
9	5.509270	-1.087426	0.262140
9	5.509051	1.087328	0.262874
9	5.509116	-0.000683	2.141985
6	-7.399673	0.002373	-4.979074
6	-6.108119	0.002683	-5.843219
6	-6.328020	0.003750	-7.389597
9	-8.133959	-1.088090	-5.280172
9	-8.133518	1.093530	-5.278728
9	-5.384469	-1.097598	-5.541494
9	-5.384023	1.102269	-5.540039
9	-7.003096	-1.083398	-7.775829
9	-7.002653	1.091683	-7.774391
9	-5.136018	0.003910	-7.997085
53	-6.931192	0.000855	-2.829099

pyNR2-nC3H7I_d_1_dimam

6	4.040150	-1.109074	-0.090336
6	3.699490	0.057231	-0.803771
6	3.982206	1.278346	-0.160221
6	4.539337	1.265875	1.110581
6	4.594167	-0.995402	1.176730
1	3.875379	-2.093534	-0.502577
1	3.770882	2.227928	-0.629172
1	4.750773	2.210096	1.604856
1	4.850300	-1.897752	1.725104
53	0.079821	-0.051429	-0.863051
7	3.096215	0.006116	-2.045969
6	-1.961332	-0.080023	-0.024209
6	-2.017434	0.410311	1.413064
1	-2.281021	-1.115647	-0.122961
1	-1.636456	1.434158	1.466315
1	-3.081567	0.461103	1.681295
1	-2.535742	0.547252	-0.700822
6	-1.284063	-0.479354	2.415469
1	-0.213230	-0.510245	2.204250
1	-1.416418	-0.107182	3.433808
1	-1.663451	-1.505049	2.379900
7	4.850218	0.161273	1.797309
6	3.070701	-1.257027	-2.769537
1	2.580430	-2.029667	-2.175546
1	2.487249	-1.127197	-3.679403
1	4.076669	-1.605681	-3.040444
6	3.005389	1.223058	-2.839937
1	2.475713	2.001764	-2.289256
1	3.991908	1.607507	-3.133120
1	2.429580	1.011717	-3.739334

pyNR2-nC3H7I_d_1_dimpy

6	-3.156518	0.977664	1.064862
6	-4.540239	0.897813	1.043050
6	-5.166619	-0.064034	0.220413
6	-4.304784	-0.874077	-0.551145

6	-2.933358	-0.701709	-0.446354
7	-2.342747	0.200886	0.343043
1	-2.671651	1.714388	1.699013
1	-5.113939	1.575918	1.657742
1	-4.688320	-1.626988	-1.224069
1	-2.267659	-1.325403	-1.036162
7	-6.531827	-0.205721	0.176241
6	-7.132741	-1.085083	-0.813402
1	-6.935127	-0.753243	-1.841418
1	-6.760567	-2.107098	-0.704875
1	-8.210151	-1.106963	-0.660472
6	-7.378574	0.764747	0.850758
1	-7.148114	0.808764	1.918354
1	-7.271010	1.774493	0.432630
1	-8.418327	0.459499	0.748697
6	2.901261	0.716714	0.541744
6	3.429753	1.865900	-0.303904
53	0.706171	0.493961	0.448431
1	3.296894	-0.244864	0.217707
1	2.960242	2.800915	0.016163
1	4.500751	1.963961	-0.079467
1	3.115381	0.855763	1.598868
6	3.246184	1.675378	-1.809018
1	3.686753	2.506639	-2.364989
1	3.726243	0.751939	-2.147447
1	2.187250	1.615729	-2.068977

pyNR2-nC3H7I_d_2_dimam

6	3.449825	-0.461527	0.375309
6	3.473588	0.078803	-0.925761
6	3.556290	1.482890	-1.008860
6	3.583343	2.234119	0.157506
6	3.482472	0.392407	1.468490
1	3.400628	-1.526864	0.545278
1	3.593733	1.992732	-1.960143
1	3.641956	3.316861	0.088209
1	3.458611	-0.028773	2.469785
53	0.151897	-0.649818	-2.171885
7	3.389491	-0.718147	-2.051554
6	-2.053049	-0.574770	-2.229833
6	-2.627204	0.580469	-1.426654
1	-2.367882	-1.543908	-1.847573
1	-2.239102	1.526135	-1.815673
1	-3.708387	0.585466	-1.621396
1	-2.289010	-0.503756	-3.288372
6	-2.383885	0.488604	0.078838
1	-1.317220	0.531307	0.308302
1	-2.874715	1.312236	0.602059
1	-2.777383	-0.449040	0.482857
7	3.545772	1.726209	1.394035
6	3.572257	-2.156240	-1.916586
1	2.849792	-2.570395	-1.211830
1	3.389421	-2.624224	-2.882345
1	4.584203	-2.420795	-1.580584
6	3.677298	-0.136056	-3.354596
1	3.021602	0.714083	-3.548282
1	4.720726	0.195749	-3.444833
1	3.478467	-0.881756	-4.122407

pyNR2-nC3H7I_d_2_dimpy

6	-3.042041	1.073837	0.173468
6	-4.426412	1.131800	0.214281
6	-5.175117	-0.056000	0.063344
6	-4.428115	-1.236238	-0.144615
6	-3.043650	-1.170696	-0.166993
7	-2.337167	-0.046845	-0.010562
1	-2.463201	1.985383	0.292004
1	-4.906673	2.088230	0.360536
1	-4.909761	-2.192354	-0.288355

1	-2.466184	-2.077274	-0.324002
7	-6.547255	-0.063457	0.119101
6	-7.274827	-1.276160	-0.218235
1	-7.117649	-1.580666	-1.261578
1	-6.975770	-2.103950	0.429926
1	-8.338963	-1.104766	-0.066827
6	-7.273025	1.195773	0.156663
1	-6.972902	1.793739	1.021040
1	-7.115210	1.795709	-0.749518
1	-8.337434	0.988706	0.250698
6	2.932577	-0.015653	-0.197653
6	3.589979	-0.412908	1.115768
53	0.725903	-0.018327	-0.111823
1	3.202387	0.995107	-0.500513
1	3.243526	-1.407751	1.411381
1	4.667297	-0.504874	0.920948
1	3.173950	-0.708110	-1.000734
6	3.367507	0.580015	2.255930
1	3.901560	0.267260	3.156576
1	3.725559	1.577062	1.981284
1	2.306540	0.662136	2.501038

pyNR2-nC3H7I_s_1_dimam

6	3.956896	-1.193522	-0.024435
6	3.633640	0.000888	-0.698164
6	3.943559	1.195397	-0.018372
6	4.509953	1.132274	1.246854
6	4.522586	-1.130502	1.241110
1	3.771153	-2.161258	-0.466279
1	3.747011	2.163230	-0.455303
1	4.742899	2.056232	1.768938
1	4.765847	-2.054440	1.758506
53	-0.012867	-0.019161	-0.832104
7	3.023244	0.000629	-1.938770
6	-2.092297	-0.032612	-0.112438
6	-2.174628	-0.036639	1.404844
1	-2.534685	-0.922531	-0.555379
1	-1.649327	-0.911204	1.797641
1	-1.659245	0.841959	1.801757
1	-2.544737	0.854315	-0.551209
6	-3.633733	-0.046003	1.877153
1	-3.685696	-0.048859	2.968661
1	-4.172878	0.835814	1.519282
1	-4.162875	-0.932174	1.515132
7	4.805725	0.000849	1.895445
6	2.978128	-1.237450	-2.703951
1	2.481863	-2.023404	-2.133191
1	2.390620	-1.070046	-3.605045
1	3.978268	-1.588803	-2.992608
6	2.964269	1.242000	-2.697648
1	2.459258	2.019443	-2.122916
1	3.960411	1.605978	-2.984481
1	2.378650	1.072620	-3.599602

pyNR2-nC3H7I_s_1_dimpy

6	-3.072471	1.225341	-0.658571
6	-4.447469	1.200971	-0.484766
6	-5.054734	0.059517	0.083180
6	-4.185786	-1.002493	0.416817
6	-2.824420	-0.863341	0.196048
7	-2.250934	0.223561	-0.329693
1	-2.601993	2.103030	-1.092497
1	-5.029308	2.058597	-0.789279
1	-4.556280	-1.924474	0.840460
1	-2.153042	-1.677308	0.454288
7	-6.408642	-0.012015	0.301324
6	-7.004710	-1.269852	0.721293
1	-6.883519	-2.060819	-0.030810
1	-6.563485	-1.617121	1.659120

1	-8.068898	-1.118201	0.892118
6	-7.277885	1.030378	-0.219887
1	-6.994146	2.009190	0.175353
1	-7.256727	1.081756	-1.316649
1	-8.300232	0.829707	0.095095
6	2.940139	0.518407	-1.115844
6	3.676951	1.095519	0.082819
53	0.765761	0.393015	-0.791173
1	3.062662	1.133257	-2.006035
1	3.285889	2.092351	0.305598
1	3.477253	0.479731	0.964386
1	3.256387	-0.499251	-1.339124
6	5.187781	1.172077	-0.168641
1	5.707292	1.588053	0.698703
1	5.607244	0.181084	-0.365773
1	5.414271	1.807268	-1.030100

pyNR2-nC3H7I_s_2_dimam

6	2.893104	-0.278673	-1.180510
6	2.470754	0.344878	0.010163
6	2.869535	-0.279875	1.208295
6	3.613030	-1.450254	1.151944
6	3.635340	-1.449067	-1.110754
1	2.650137	0.128983	-2.150576
1	2.607501	0.126798	2.173792
1	3.914386	-1.930709	2.078703
1	3.955007	-1.928617	-2.031810
53	-1.167915	-0.025006	-0.026478
7	1.688949	1.485561	0.003041
6	-3.155571	-0.968176	-0.043685
6	-4.281593	0.043503	0.086785
1	-3.133046	-1.674111	0.783944
1	-4.159928	0.608667	1.014813
1	-4.220513	0.766458	-0.731175
1	-3.194137	-1.514085	-0.984071
6	-5.649872	-0.649328	0.071727
1	-6.455136	0.083447	0.165893
1	-5.805954	-1.199521	-0.860545
1	-5.744835	-1.358439	0.898969
7	4.004899	-2.052256	0.024082
6	1.543849	2.234480	-1.237342
1	1.138992	1.597757	-2.024971
1	0.833074	3.043148	-1.075973
1	2.495164	2.661813	-1.582988
6	1.518782	2.232658	1.241307
1	1.098777	1.594538	2.019818
1	2.462768	2.660095	1.606408
1	0.810834	3.041115	1.066962

pyNR2-nC3H7I_s_2_dimpy

6	-2.924226	1.141113	0.005016
6	-4.307509	1.199780	0.072151
6	-5.051202	0.000211	0.119118
6	-4.301150	-1.195328	0.070569
6	-2.918198	-1.129229	0.003518
7	-2.216228	0.007835	-0.027622
1	-2.349142	2.062062	-0.028325
1	-4.790840	2.165688	0.086329
1	-4.779345	-2.163807	0.083471
1	-2.338231	-2.047066	-0.031035
7	-6.421406	-0.003487	0.210223
6	-7.148404	-1.255485	0.076808
1	-7.014774	-1.712291	-0.912861
1	-6.827594	-1.975840	0.833752
1	-8.209685	-1.066917	0.227808
6	-7.155043	1.244808	0.078460
1	-6.838054	1.965858	0.836351
1	-7.023849	1.703621	-0.910607
1	-8.215306	1.050409	0.229215

6	3.034006	0.021571	-0.322690
6	3.692471	0.025937	1.048129
53	0.835153	0.015832	-0.204082
1	3.288146	0.908217	-0.901280
1	3.357755	0.902331	1.610387
1	3.362505	-0.850133	1.613687
1	3.292954	-0.865859	-0.897936
6	5.222020	0.029876	0.937825
1	5.684821	0.032997	1.928288
1	5.582875	-0.853765	0.403186
1	5.578085	0.913439	0.399855

B. IR and Raman spectra

ALN_ic3F7I_1

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.7331	0.0000	0.2058	0.2578
2	A	15.7764	0.0012	0.0133	3.8696
3	A	20.9709	0.0011	0.0793	5.0073
4	A	40.2705	0.0178	0.0230	0.0161
5	A	51.7480	0.0176	0.0603	2.4584
6	A	54.8210	0.0097	0.6752	1.9241
7	A	78.7183	0.0765	0.0633	0.0925
8	A	112.8542	0.0424	12.2681	12.4592
9	A	133.1500	0.2078	0.0026	0.1820
10	A	142.4731	0.2433	10.6673	7.0847
11	A	178.1400	0.3582	3.7015	3.7619
12	A	233.4011	0.4165	12.6502	68.3988
13	A	254.7346	0.6996	0.7715	0.1129
14	A	255.2479	0.1695	1.4541	0.2252
15	A	279.8898	0.8675	0.7289	5.4760
16	A	298.9389	0.9462	0.3509	0.7464
17	A	324.9830	1.1391	0.0797	2.2296
18	A	343.1476	1.1889	0.0301	1.3807
19	A	353.8823	0.1079	6.9161	0.1134
20	A	411.8999	0.2855	0.0564	0.1227
21	A	432.4760	0.1946	2.9893	0.2060
22	A	462.6668	2.2511	1.7100	2.5025
23	A	508.6767	0.4024	22.2186	6.7213
24	A	529.8960	2.9697	3.2474	0.4703
25	A	532.4554	2.9600	3.5625	20.4290
26	A	541.2730	1.0873	1.6205	7.7740
27	A	556.6094	3.2794	0.2044	0.0377
28	A	606.6569	3.8923	3.2889	1.9507
29	A	636.6191	1.5229	0.0958	4.3216
30	A	698.9859	0.5899	35.1062	3.4611
31	A	701.6432	4.7482	38.9126	0.0942
32	A	739.2472	1.3267	39.7526	83.5269
33	A	743.1321	0.6455	37.7828	12.3802
34	A	792.5969	0.7241	297.7245	101.7696
35	A	828.1803	0.5083	0.1750	0.2939
36	A	837.3304	1.0516	30.2838	60.4553
37	A	882.9553	4.7082	81.2727	110.1575
38	A	897.0193	0.7273	15.4377	1.5745
39	A	948.3717	7.5400	106.2810	0.1625
40	A	968.2634	0.7485	0.0738	0.0263
41	A	988.1368	0.7332	0.0948	1.0073
42	A	1017.8601	3.6858	0.3559	39.2597
43	A	1049.5419	1.3815	4.2133	18.4752
44	A	1076.1012	1.0755	2.6073	0.0380
45	A	1095.0104	9.4724	103.7203	15.5954
46	A	1126.3191	9.7750	37.9395	1.9601
47	A	1140.6325	0.9575	5.1126	1.3767
48	A	1158.3211	10.3306	11.3223	0.4011
49	A	1183.0154	0.9127	0.6776	4.8075
50	A	1193.4433	10.8889	342.0536	19.6166
51	A	1201.6216	0.9593	7.0136	7.0283
52	A	1208.6118	11.1521	340.3804	12.9669
53	A	1254.9530	9.4114	451.4969	89.5144
54	A	1264.3173	11.5888	255.8182	0.9239
55	A	1277.0867	3.4396	62.6610	92.8065
56	A	1349.4338	5.4953	1.5614	4.2252
57	A	1370.1871	1.4355	0.0472	0.0907
58	A	1502.9860	3.0421	3.4915	2.2814
59	A	1530.8884	3.1887	58.8123	3.2586
60	A	1637.3211	9.1218	4.1178	4.8513
61	A	1645.3898	4.4237	31.7200	62.8765
62	A	1658.1394	2.2831	98.6806	31.9516
63	A	3158.2027	6.3889	13.6991	16.3071
64	A	3159.0995	6.4002	1.9836	79.4969

65	A	3173.9015	6.4671	3.0360	122.8597
66	A	3181.0400	6.5206	19.8473	44.7103
67	A	3194.9539	6.6016	10.4905	271.7451
68	A	3534.7133	7.7178	20.7749	177.1918
69	A	3625.4439	8.4983	19.9842	44.0233

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.6306	0.0000	0.1228	0.3261
2	A	17.0517	0.0015	0.0153	4.1574
3	A	21.0043	0.0011	0.0694	4.9908
4	A	40.2064	0.0177	0.0259	0.0177
5	A	49.9028	0.0159	0.1413	2.6251
6	A	54.7852	0.0097	0.6792	1.8525
7	A	78.4287	0.0755	0.0299	0.2503
8	A	113.5791	0.0423	13.6329	14.2385
9	A	133.1864	0.2085	0.0052	0.1846
10	A	142.9292	0.2615	10.0865	6.2411
11	A	178.7001	0.3668	2.2335	4.1186
12	A	235.4988	0.7072	13.2158	69.9499
13	A	250.2897	0.1475	2.3981	6.4783
14	A	254.6542	0.6976	0.7595	0.1128
15	A	281.0840	0.7671	2.6179	2.5044
16	A	299.0563	0.9471	0.3361	0.7704
17	A	325.1891	1.1305	0.1400	2.3639
18	A	343.1611	1.2126	0.0251	1.2102
19	A	354.2691	0.1089	6.8701	0.1206
20	A	411.9220	0.2864	0.0512	0.1164
21	A	433.6899	0.1935	3.1013	0.2131
22	A	462.5485	2.2537	3.1887	3.6785
23	A	508.4010	0.4042	23.4754	10.0226
24	A	529.8688	2.9693	3.3629	0.4530
25	A	532.5875	2.8045	4.1592	17.8682
26	A	541.4244	1.0964	0.9933	5.6604
27	A	556.6674	3.2801	0.1977	0.0410
28	A	606.4598	3.8758	4.3612	1.7841
29	A	636.6247	1.5229	0.0960	4.3759
30	A	698.7326	0.5914	34.8210	3.8644
31	A	701.5443	4.7450	39.3839	0.0144
32	A	739.0240	1.3619	63.3194	86.8081
33	A	743.6968	0.6422	19.0785	14.8629
34	A	793.3418	0.7346	300.1560	113.3390
35	A	828.1875	0.5083	0.1773	0.2998
36	A	837.6333	1.0386	33.2197	64.2163
37	A	883.8376	4.3477	74.2673	90.3715
38	A	896.9197	0.7300	14.7053	1.9452
39	A	948.5043	7.5409	105.9850	0.1486
40	A	968.2100	0.7484	0.0752	0.0298
41	A	987.5330	0.7317	0.0966	1.1145
42	A	1017.8874	3.6846	0.3659	39.8917
43	A	1049.5423	1.3815	4.0801	19.0011
44	A	1076.2048	1.0759	2.6234	0.0259
45	A	1095.6735	9.5064	89.7919	25.2429
46	A	1127.2834	9.8002	37.5110	2.0917
47	A	1140.7181	0.9577	4.7680	1.3869
48	A	1156.4828	10.2621	9.5122	0.3234
49	A	1183.0177	0.9127	0.6997	4.8883
50	A	1193.4901	10.8896	371.6156	24.8806
51	A	1201.6327	0.9594	6.7765	7.1341
52	A	1208.4719	11.0965	240.1777	12.5642
53	A	1255.7309	9.7393	608.0263	72.0877
54	A	1264.8456	11.5987	257.3927	0.4956
55	A	1276.6663	3.4025	14.6181	87.8646
56	A	1349.4190	5.4888	1.5561	4.3573
57	A	1370.2022	1.4356	0.0456	0.0863
58	A	1502.9673	3.0416	3.4828	2.3467
59	A	1530.8750	3.1880	59.5173	3.0912
60	A	1637.3126	9.1200	4.1306	4.8848

61	A	1645.3544	4.4093	32.2930	64.9686
62	A	1658.0512	2.2862	99.2735	32.4144
63	A	3158.2476	6.3891	13.9665	16.1757
64	A	3159.1430	6.4003	1.9701	80.1162
65	A	3173.9008	6.4671	3.0625	123.1219
66	A	3181.0528	6.5207	19.8879	45.5545
67	A	3194.9353	6.6016	10.6369	275.3034
68	A	3534.3848	7.7166	20.0962	175.5476
69	A	3624.9133	8.4955	19.8881	43.0879

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	5.5182	0.0001	0.1325	0.2539
2	A	14.0884	0.0013	0.0163	0.1981
3	A	17.6356	0.0020	0.0839	1.4110
4	A	28.9256	0.0027	0.3595	4.4485
5	A	40.5473	0.0071	0.0226	2.2744
6	A	51.0739	0.0079	0.2476	4.6126
7	A	52.9878	0.0123	0.1018	1.3544
8	A	74.9504	0.0633	0.0243	0.1532
9	A	128.3047	0.2180	0.1042	0.2929
10	A	143.4940	0.2792	0.6152	0.3132
11	A	175.5685	0.3497	0.7184	0.5267
12	A	222.3064	0.1056	5.9290	0.7063
13	A	250.5705	0.8464	0.5727	10.7644
14	A	254.7332	0.7036	0.1909	0.0537
15	A	282.2966	0.8842	2.8396	0.5723
16	A	287.1472	0.0503	16.5274	0.0980
17	A	295.7815	0.9352	0.5394	0.4753
18	A	323.2377	1.1282	0.0608	1.7156
19	A	343.4962	1.2920	0.0137	1.1805
20	A	383.5293	0.2549	0.1671	0.6272
21	A	416.4437	0.3001	0.2534	0.0013
22	A	463.9360	2.2709	3.0553	1.7688
23	A	502.2989	0.3269	77.4626	0.6629
24	A	530.5894	2.9750	2.8352	0.3357
25	A	534.8536	2.9313	6.6190	2.9493
26	A	538.1004	1.0851	7.6317	3.3890
27	A	556.3882	3.2874	0.0795	0.1150
28	A	587.3530	0.2896	189.4525	7.0595
29	A	608.6465	3.8461	3.2671	3.8756
30	A	636.8527	1.5187	0.2929	3.0034
31	A	697.8123	0.5684	32.6100	0.1295
32	A	703.6609	4.7731	35.6057	0.0944
33	A	742.0051	5.4294	37.9797	15.1145
34	A	759.2395	0.6120	87.3103	2.0452
35	A	823.8137	0.5052	0.5284	0.5055
36	A	833.5978	1.8120	3.2368	21.1353
37	A	879.8935	3.2092	116.1784	8.2763
38	A	882.2939	0.7698	39.2443	1.1912
39	A	948.8179	7.3745	83.8689	0.0811
40	A	966.9843	0.7454	0.2106	0.0367
41	A	980.6911	0.7098	0.0263	0.2645
42	A	1013.9365	3.6005	2.4558	27.7992
43	A	1049.5117	1.3790	2.6784	17.0095
44	A	1066.4473	1.0576	2.7590	0.0412
45	A	1123.6020	10.0469	112.8611	3.6389
46	A	1135.8376	0.9741	6.8929	2.2470
47	A	1142.1616	8.7915	40.0131	0.5775
48	A	1161.5057	10.2381	0.2306	0.5076
49	A	1180.3661	0.9055	2.2139	3.4960
50	A	1198.9022	1.3947	109.0146	4.4068
51	A	1203.1132	2.4303	259.2714	9.8266
52	A	1214.8189	10.4388	301.7174	0.1577
53	A	1255.9054	11.4748	235.4289	0.6655
54	A	1264.3584	11.8454	289.4866	10.5406
55	A	1299.7400	3.2452	69.0162	14.8578
56	A	1349.4577	5.8845	6.4273	1.4334

57	A	1367.8374	1.4245	0.0007	0.2072
58	A	1501.3260	3.0885	1.6208	1.2635
59	A	1531.6032	3.2596	60.4839	1.2197
60	A	1629.0987	8.9333	4.4919	3.2250
61	A	1645.9306	4.3365	21.9907	14.0062
62	A	1663.2959	2.3692	142.5308	26.2959
63	A	3151.6659	6.3587	15.9255	22.1208
64	A	3152.5014	6.3702	4.4271	89.9895
65	A	3169.1690	6.4479	2.3974	139.5850
66	A	3174.7107	6.4940	28.2873	26.0970
67	A	3192.2860	6.5875	10.4293	211.4574
68	A	3567.6375	7.8546	17.0075	195.9748
69	A	3665.2202	8.6976	15.1196	54.4229

ALN_ic3F7I_4

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.6502	0.0000	0.1005	0.3140
2	A	15.0932	0.0011	0.3900	3.4566
3	A	21.4946	0.0027	0.0076	0.0816
4	A	37.6063	0.0075	0.6061	8.9246
5	A	40.0050	0.0171	0.0371	0.4741
6	A	49.5031	0.0051	0.2158	6.4867
7	A	75.3508	0.0637	0.5499	1.0832
8	A	78.7436	0.0236	6.0771	16.9323
9	A	130.5536	0.2334	0.0576	0.4369
10	A	142.6951	0.2807	3.6709	6.7937
11	A	177.5574	0.3607	1.9498	4.7617
12	A	220.9553	0.1037	3.8470	33.3402
13	A	244.5127	0.7289	4.3620	55.3525
14	A	255.1079	0.7129	0.6849	0.0779
15	A	282.1291	0.8818	1.3735	5.2230
16	A	298.2815	0.9580	0.4031	0.6339
17	A	318.7761	0.0617	14.3279	0.1460
18	A	324.5278	1.1352	0.0752	2.3825
19	A	342.9830	1.2888	0.1166	1.2331
20	A	385.0463	0.2520	0.1505	0.6553
21	A	413.6663	0.2988	0.2422	0.0549
22	A	462.5105	2.2590	1.5657	2.6266
23	A	485.1394	0.2016	218.8401	9.5555
24	A	520.9491	0.4268	49.5998	14.5877
25	A	529.9324	2.9653	3.8296	0.4710
26	A	533.5350	2.9117	4.7932	20.0475
27	A	541.8693	0.6980	16.7157	6.4367
28	A	556.7558	3.2934	0.2911	0.1029
29	A	606.7432	3.8949	3.1282	2.0884
30	A	635.3882	1.5101	0.3531	3.2765
31	A	699.0251	0.6453	21.3893	1.1489
32	A	702.2919	4.6788	41.6432	0.1897
33	A	741.3086	5.4604	34.4900	28.0780
34	A	766.5316	0.5678	118.4617	12.5659
35	A	825.7293	0.5069	0.4576	0.2190
36	A	835.4279	1.8801	3.9444	19.7739
37	A	879.6806	0.7123	6.2664	43.4545
38	A	884.1034	4.4094	110.0395	85.0214
39	A	947.6698	7.3793	105.5055	0.6166
40	A	967.1883	0.7437	0.4743	0.1650
41	A	976.9593	0.6959	2.7744	8.5572
42	A	1012.6564	3.5856	6.4480	38.5528
43	A	1045.3141	1.3776	8.4993	37.5626
44	A	1060.6926	1.0409	1.4421	0.0772
45	A	1097.6897	9.5413	105.5523	12.0933
46	A	1130.5417	9.4119	30.8073	2.0218
47	A	1133.5394	0.9729	3.8950	2.6595
48	A	1161.5709	10.4021	10.8429	0.3853
49	A	1181.4859	0.9030	1.7884	3.2067
50	A	1196.6031	10.2877	338.6072	11.5312
51	A	1202.0896	0.9743	39.7494	28.1605
52	A	1213.1667	10.7336	288.6881	14.0373

53	A	1257.2415	11.3169	409.7796	139.2389
54	A	1259.6923	11.5413	264.8488	2.3057
55	A	1312.8655	3.2204	80.4652	17.0061
56	A	1353.6202	6.0706	5.4076	2.7716
57	A	1368.3187	1.4266	0.0949	0.3250
58	A	1502.1043	3.1181	2.4960	2.0010
59	A	1530.6366	3.2543	67.5031	15.2125
60	A	1619.6008	8.6789	4.9811	2.4664
61	A	1643.0727	4.8913	50.3477	102.6166
62	A	1664.3298	2.2488	193.7761	60.7350
63	A	3158.5311	6.3874	13.6676	23.3878
64	A	3159.7156	6.4002	3.2942	95.9055
65	A	3173.6685	6.4681	2.9897	128.8982
66	A	3179.8317	6.5162	18.2824	22.1368
67	A	3194.0125	6.5952	4.3933	195.1298
68	A	3580.9084	7.9100	34.2779	259.4281
69	A	3682.7748	8.7922	20.8066	59.6764

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.4012	0.0000	0.0828	0.3035
2	A	20.5569	0.0020	0.2510	2.1532
3	A	22.0776	0.0037	0.0655	0.4909
4	A	40.1108	0.0174	0.0334	0.0782
5	A	44.4923	0.0056	0.7699	5.1549
6	A	48.7328	0.0086	0.1911	7.9303
7	A	75.4871	0.0619	0.2809	0.4708
8	A	79.4651	0.0193	4.3525	12.6774
9	A	131.2555	0.2379	0.2612	1.0478
10	A	142.4170	0.2786	3.6669	4.9065
11	A	177.5396	0.3601	1.6857	3.3540
12	A	223.2305	0.1090	26.1771	31.1414
13	A	242.7720	0.6998	2.5682	59.0945
14	A	255.0189	0.7116	0.6834	0.1063
15	A	281.5123	0.8787	1.4757	4.6123
16	A	298.3573	0.9526	0.4395	0.7057
17	A	307.8538	0.0579	18.5891	0.1853
18	A	324.4436	1.1355	0.0770	2.3167
19	A	343.0432	1.2885	0.1119	1.2953
20	A	385.8950	0.2558	0.4023	0.7793
21	A	413.6565	0.3029	3.2263	5.2279
22	A	462.4586	2.2660	1.8990	3.1990
23	A	503.1834	0.3083	145.8369	4.8846
24	A	529.9294	2.9698	3.5721	0.4369
25	A	533.3087	2.9539	6.2330	21.0174
26	A	537.9879	1.0276	14.8211	3.9707
27	A	556.7594	3.2933	0.2864	0.0634
28	A	567.1983	0.2910	257.8567	5.6289
29	A	606.7477	3.8820	2.5458	2.4279
30	A	635.6518	1.5117	0.7046	6.5347
31	A	700.7725	0.6581	23.9854	0.4052
32	A	702.3343	3.5878	40.8123	0.2294
33	A	741.1922	5.4323	33.3107	30.5976
34	A	756.0318	0.5720	88.6437	1.8638
35	A	829.3888	0.5405	3.5406	10.2959
36	A	835.6878	1.5130	7.9790	26.1519
37	A	878.8212	0.6586	26.4638	15.0190
38	A	883.3168	6.1066	110.3198	112.0206
39	A	948.1081	7.3179	104.3919	0.4050
40	A	964.4635	0.7329	2.0197	5.7484
41	A	979.4251	0.7154	0.3115	1.2332
42	A	1013.2381	3.5460	2.4373	44.6604
43	A	1049.0507	1.3823	2.0180	14.9090
44	A	1063.9066	1.0610	4.2013	4.3380
45	A	1099.5832	9.5769	105.0905	15.3662
46	A	1131.8444	9.9384	31.9892	1.8992
47	A	1135.3504	0.9681	3.3793	2.0228
48	A	1160.5523	10.3808	9.9233	0.3798

49	A	1182.2488	0.9090	3.3688	11.0672
50	A	1197.4199	10.8948	334.7880	13.1435
51	A	1201.8914	0.9631	10.9459	3.0530
52	A	1212.0871	11.1041	301.1120	16.0748
53	A	1257.0403	11.5012	446.8373	139.6470
54	A	1260.1413	11.5239	245.0329	3.5481
55	A	1310.0248	3.2672	59.5849	53.8877
56	A	1350.8558	5.8993	10.4746	12.0338
57	A	1369.0278	1.4282	0.1552	0.6050
58	A	1498.4566	3.0302	6.3574	21.4022
59	A	1531.5230	3.2617	68.0984	33.9795
60	A	1622.7073	8.6269	13.4616	56.5774
61	A	1643.9806	5.4094	36.0759	16.5599
62	A	1666.9646	2.1546	126.8920	20.4202
63	A	3157.0680	6.3859	7.6730	34.8610
64	A	3159.5880	6.3970	5.1660	70.2029
65	A	3174.4541	6.4719	2.0565	139.8601
66	A	3179.4016	6.5136	18.9084	41.5499
67	A	3196.8962	6.6062	9.0327	221.0204
68	A	3573.4630	7.8797	23.7245	150.0875
69	A	3671.8164	8.7342	19.0614	39.2370

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.0906	0.0000	0.1003	0.3294
2	A	21.0914	0.0029	0.0525	1.1764
3	A	21.4308	0.0024	0.2640	1.7252
4	A	40.2168	0.0178	0.0238	0.0275
5	A	43.9267	0.0054	0.7870	5.0971
6	A	49.4598	0.0091	0.1806	7.5260
7	A	76.1946	0.0708	0.0592	0.0923
8	A	79.1904	0.0184	4.5432	12.8144
9	A	130.2333	0.2320	0.1996	0.7558
10	A	142.4549	0.2800	4.2545	6.1691
11	A	177.3777	0.3614	2.2324	4.9234
12	A	223.3700	0.1076	25.1361	27.4723
13	A	243.1185	0.7525	2.8978	60.2614
14	A	255.1059	0.7117	0.7089	0.1209
15	A	281.8516	0.8782	1.3884	5.1065
16	A	298.3619	0.9480	0.3438	0.7418
17	A	307.1841	0.0576	18.2240	0.1660
18	A	324.5202	1.1345	0.0911	2.5709
19	A	343.1289	1.2894	0.1356	1.3112
20	A	385.9234	0.2559	0.3976	0.7898
21	A	413.8680	0.3028	3.2358	5.3198
22	A	462.5907	2.2683	1.8895	2.6343
23	A	503.0732	0.3069	147.9060	5.4235
24	A	530.0052	2.9712	3.4346	0.4311
25	A	533.3419	2.9497	7.0886	21.2298
26	A	538.0155	1.0261	14.7561	4.0100
27	A	556.7424	3.2929	0.3345	0.0465
28	A	566.7168	0.2913	258.3359	5.6585
29	A	606.8806	3.8872	2.5779	1.9243
30	A	635.6448	1.5117	0.7238	6.6919
31	A	700.7001	0.6324	23.0098	0.5148
32	A	702.2603	4.7587	41.0538	0.0772
33	A	741.2521	5.4105	33.7222	30.9288
34	A	756.1753	0.5707	88.6400	1.8802
35	A	829.4511	0.5420	3.5649	10.0705
36	A	835.7321	1.5038	7.7159	26.9028
37	A	879.3873	0.6610	21.0671	20.3461
38	A	883.4949	5.9108	113.7373	110.7350
39	A	947.9276	7.4772	103.8800	0.1263
40	A	965.1760	0.7337	2.0780	5.7002
41	A	980.5639	0.7174	0.4105	1.3007
42	A	1013.2432	3.5455	2.3185	44.7740
43	A	1049.0323	1.3820	2.0333	14.8939
44	A	1063.8239	1.0604	3.3868	4.3610

45	A	1098.8666	9.5624	104.0901	14.6535
46	A	1131.0140	9.7353	31.9108	2.1122
47	A	1135.2758	0.9700	4.2700	2.0278
48	A	1162.1938	10.4115	9.1670	0.3555
49	A	1182.2344	0.9094	3.7727	11.5754
50	A	1197.4918	10.8704	311.5393	12.2423
51	A	1201.8849	0.9625	9.8508	3.3395
52	A	1211.9847	11.1311	320.3922	21.4366
53	A	1257.4730	11.5326	464.2202	141.9274
54	A	1259.7637	11.5220	245.3376	1.6846
55	A	1310.0436	3.2639	56.1895	55.9478
56	A	1350.8608	5.9045	9.5695	12.4357
57	A	1369.0103	1.4282	0.1519	0.6123
58	A	1498.4625	3.0306	6.3618	21.4366
59	A	1531.5225	3.2620	68.6256	34.9924
60	A	1622.6594	8.6271	13.6704	57.9046
61	A	1643.9630	5.4018	35.9812	16.3311
62	A	1666.9391	2.1561	128.0791	20.9548
63	A	3156.9904	6.3857	7.6725	36.1187
64	A	3159.5732	6.3969	5.3055	69.9620
65	A	3174.4639	6.4718	2.0953	139.2522
66	A	3179.4395	6.5137	18.8497	41.0102
67	A	3196.9012	6.6063	8.9242	219.2756
68	A	3573.6626	7.8806	24.0421	151.9744
69	A	3672.0746	8.7355	19.1977	39.9519

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	13.0389	0.0007	0.0986	0.2689
2	A	17.5502	0.0014	0.0563	0.4344
3	A	25.5506	0.0055	0.0786	0.1901
4	A	40.5694	0.0049	0.9265	4.7423
5	A	40.6155	0.0053	0.6115	3.3898
6	A	50.6651	0.0098	0.2306	3.3383
7	A	54.5652	0.0122	0.3279	1.7983
8	A	75.3633	0.0642	0.1311	0.0678
9	A	128.2042	0.2175	0.1232	0.2605
10	A	144.5553	0.2831	0.8114	0.3400
11	A	175.4565	0.3518	1.0425	0.5864
12	A	223.9274	0.1064	8.2599	1.0662
13	A	250.9174	0.8625	0.4265	11.3509
14	A	254.7051	0.7097	0.2796	0.0554
15	A	275.6727	0.0468	21.5255	0.0255
16	A	282.6028	0.8783	2.6377	0.9443
17	A	295.3290	0.8420	0.1086	0.4756
18	A	323.5816	1.1303	0.0435	1.6869
19	A	343.5251	1.2905	0.0050	1.1445
20	A	384.1662	0.2558	0.1365	0.6265
21	A	415.8663	0.3010	0.1758	0.0356
22	A	463.6183	2.2692	3.3013	1.2889
23	A	503.4911	0.3415	85.0519	0.6810
24	A	530.2830	2.9703	3.0038	0.3046
25	A	535.6221	3.0115	9.2561	3.1257
26	A	538.4060	1.1039	5.7338	3.4293
27	A	556.1953	3.2873	0.0595	0.1465
28	A	608.2556	3.7617	0.4375	2.4864
29	A	612.4676	0.3087	329.6139	8.5766
30	A	636.7146	1.5177	0.1965	2.9203
31	A	697.2072	0.5781	28.0847	0.1719
32	A	703.5473	4.7679	35.1974	0.1201
33	A	742.2526	5.4798	28.6606	13.8471
34	A	756.7495	0.6073	93.3623	2.3093
35	A	825.0265	0.5061	1.1468	0.4273
36	A	834.2590	1.7996	5.6996	21.6981
37	A	878.1898	1.9877	152.5188	5.4724
38	A	881.8829	0.8819	9.7799	2.0035
39	A	948.4607	7.4146	77.6023	0.0703
40	A	966.1685	0.7444	0.1770	0.0416

41	A	981.1787	0.7118	0.1270	0.3434
42	A	1014.0200	3.6071	1.0205	27.8250
43	A	1048.7657	1.3770	2.5857	18.3539
44	A	1068.6249	1.0713	2.6493	0.0204
45	A	1124.4653	9.9858	84.6107	8.3314
46	A	1133.4524	4.5751	42.3870	0.2280
47	A	1138.5098	1.0845	0.7365	2.3101
48	A	1163.7715	9.9256	3.3873	0.3820
49	A	1179.5384	0.9038	1.4474	3.8715
50	A	1195.6474	10.8686	447.9143	15.7554
51	A	1200.2735	0.9578	12.1711	2.8349
52	A	1220.5477	11.2188	242.0356	0.3011
53	A	1257.2077	11.4951	240.3331	0.6811
54	A	1262.8555	11.7969	253.9687	8.6867
55	A	1301.8056	3.2431	78.0069	12.0681
56	A	1350.4976	5.7959	6.5881	1.0523
57	A	1368.1352	1.4267	0.0149	0.1687
58	A	1501.3665	3.0866	1.7973	1.2638
59	A	1531.7386	3.2705	58.5483	1.3864
60	A	1628.7128	8.9042	4.0771	3.4822
61	A	1646.4521	4.8653	31.7363	18.3590
62	A	1666.0596	2.2419	121.2892	18.8729
63	A	3152.4769	6.3589	14.1838	12.9551
64	A	3153.9179	6.3744	2.4106	94.6919
65	A	3168.5029	6.4477	4.0684	143.5936
66	A	3173.8034	6.4918	30.5725	22.2533
67	A	3190.7720	6.5816	11.3826	220.4410
68	A	3566.7490	7.8523	15.3232	153.5804
69	A	3661.6264	8.6760	14.0480	42.1222

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	18.2754	0.0011	0.0312	0.6756
2	A	26.9373	0.0052	0.0124	0.0397
3	A	27.9866	0.0058	0.1417	0.4970
4	A	37.5952	0.0104	0.1654	0.5501
5	A	44.0220	0.0062	0.6898	3.6464
6	A	51.9703	0.0062	0.9930	5.8973
7	A	59.6945	0.0135	0.5561	3.0224
8	A	77.5024	0.0604	0.1345	0.1375
9	A	129.7654	0.2240	0.1655	0.3383
10	A	141.9031	0.2732	0.7514	0.3784
11	A	178.9146	0.3612	0.5516	0.5218
12	A	225.2592	0.1078	8.8155	2.4801
13	A	247.8701	0.8315	0.2045	6.6171
14	A	254.4615	0.6938	0.4092	0.1581
15	A	267.0276	0.0439	22.0480	0.0975
16	A	285.2704	0.8964	1.6613	1.0704
17	A	298.1133	0.9527	0.4047	0.5251
18	A	323.0536	1.1176	0.1160	1.4731
19	A	343.6624	1.2920	0.0718	1.4004
20	A	384.1456	0.2556	0.1211	0.6034
21	A	416.3995	0.3020	0.2416	0.3067
22	A	463.4160	2.2703	3.0007	1.4673
23	A	503.5872	0.3447	80.9536	1.0657
24	A	530.5501	2.9743	3.2446	0.4168
25	A	534.6433	3.0001	8.2789	2.2141
26	A	538.4826	1.1049	5.7066	3.7343
27	A	556.8380	3.2924	0.2140	0.0784
28	A	608.2718	3.4388	7.1134	2.7794
29	A	615.8768	0.3140	314.2076	6.0979
30	A	636.7593	1.5180	0.1450	2.8020
31	A	697.8118	0.5794	28.8984	0.2414
32	A	703.5488	4.7102	34.2782	0.0771
33	A	742.1302	5.4692	32.5384	13.5055
34	A	756.4212	0.6083	88.4959	2.0216
35	A	824.7550	0.5062	2.6288	0.6274
36	A	834.2742	1.7889	5.2185	19.9608

37	A	879.6856	0.9617	65.0862	1.1155
38	A	882.2160	1.6323	65.6538	5.9054
39	A	947.6031	7.4395	87.2621	0.3322
40	A	965.8200	0.7435	0.0536	0.1905
41	A	982.8376	0.7170	0.0885	0.2758
42	A	1014.4451	3.6049	0.7199	28.7455
43	A	1049.0561	1.3777	2.5726	17.7156
44	A	1069.2516	1.0719	3.5641	0.2070
45	A	1124.2000	10.0096	117.5681	4.4380
46	A	1137.0155	1.8506	13.6325	1.9731
47	A	1139.3087	1.6683	21.5777	1.3946
48	A	1165.2362	10.2479	4.8984	0.3017
49	A	1179.8625	0.9036	1.3397	3.8268
50	A	1200.5117	0.9572	8.7038	2.7885
51	A	1202.3548	11.0345	231.3829	6.3864
52	A	1216.2410	11.2288	361.5739	1.3342
53	A	1254.2354	11.4138	246.2140	0.7588
54	A	1263.4638	11.8487	298.6327	4.9702
55	A	1300.6770	3.2480	62.0709	19.2191
56	A	1350.9242	5.7545	6.6798	1.0134
57	A	1368.3967	1.4302	0.1195	0.1394
58	A	1501.4669	3.0834	2.0649	1.4173
59	A	1531.7876	3.2667	53.5272	1.6042
60	A	1628.9261	8.8965	4.2805	6.3398
61	A	1646.4223	4.9513	29.8306	18.9470
62	A	1665.8428	2.2213	108.5365	18.5794
63	A	3153.7496	6.3639	13.5338	11.1482
64	A	3155.4107	6.3795	2.2699	85.6170
65	A	3169.5154	6.4525	4.5801	132.4502
66	A	3174.6741	6.4958	29.0929	25.3647
67	A	3191.3909	6.5845	11.3248	228.6581
68	A	3565.1541	7.8451	12.8803	142.9220
69	A	3659.6845	8.6653	12.2388	38.9946

ALN_iC3F7I_trml

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	0.9312	0.0000	0.0074	0.1723
2	A	2.7409	0.0001	0.0319	0.0906
3	A	6.4770	0.0003	0.4581	0.1529
4	A	7.6410	0.0005	0.4238	0.2983
5	A	15.6097	0.0024	0.0116	1.1326
6	A	19.0154	0.0030	0.0160	0.8273
7	A	24.9837	0.0064	0.1141	0.3357
8	A	40.2306	0.0180	0.0100	0.0096
9	A	40.3111	0.0176	0.0414	0.0018
10	A	46.7841	0.0074	0.5880	3.4306
11	A	50.7968	0.0139	0.2835	1.2421
12	A	52.1299	0.0106	0.5587	0.7685
13	A	70.1763	0.0130	1.0015	13.3211
14	A	75.3876	0.0652	0.0424	0.5701
15	A	78.2603	0.0756	0.1210	0.0635
16	A	119.2269	0.0491	20.0215	16.3852
17	A	131.1259	0.2361	0.3720	1.1939
18	A	133.0933	0.2115	0.0110	0.2198
19	A	142.3103	0.2695	1.0751	6.9222
20	A	143.3222	0.2382	19.1237	4.5015
21	A	177.5096	0.3601	1.7343	3.4080
22	A	178.3060	0.3609	4.9612	2.7243
23	A	236.3850	0.4748	7.0623	99.3503
24	A	244.2912	0.8120	4.0258	71.9609
25	A	254.7436	0.6666	0.8763	0.1921
26	A	254.8936	0.6173	0.8166	0.1852
27	A	256.4621	0.1726	0.5919	4.4454
28	A	280.4606	0.8701	1.0140	6.3505
29	A	281.9710	0.8813	1.8059	4.3800
30	A	298.2383	0.9575	0.4085	0.6887
31	A	298.8130	0.9457	0.3318	0.7339
32	A	324.2525	1.1346	0.1035	2.1441

33	A	324.8572	1.1377	0.0830	2.2988
34	A	343.0466	1.2854	0.1104	1.0110
35	A	343.1218	1.2101	0.0341	1.6209
36	A	356.5384	0.1041	7.5309	0.3195
37	A	409.7592	0.2771	1.8656	3.3148
38	A	426.2686	0.2041	3.2874	2.0016
39	A	462.4909	2.2656	1.9322	3.3238
40	A	462.7453	2.2534	1.7535	2.8873
41	A	511.5030	0.4147	36.3203	12.2393
42	A	529.9344	2.9701	3.2247	0.4517
43	A	529.9946	2.9701	3.3875	0.4414
44	A	532.8248	2.9663	4.7184	21.7727
45	A	533.7306	2.9859	7.1878	20.8027
46	A	541.5595	1.0925	1.5771	9.5409
47	A	556.7117	3.2834	0.2108	0.0477
48	A	556.9062	3.2948	0.3148	0.0773
49	A	606.7935	3.8950	5.5204	2.3010
50	A	606.9689	3.8940	1.7935	2.0000
51	A	635.9740	1.5182	0.5317	5.8082
52	A	700.8027	0.6902	37.0028	3.3752
53	A	701.9742	4.7541	38.8771	0.0848
54	A	702.8171	3.6962	45.8553	0.1356
55	A	736.7482	0.5491	109.3934	92.4972
56	A	741.4772	4.4606	6.0888	47.9158
57	A	741.9330	1.5084	59.0068	4.4582
58	A	783.1385	0.6742	389.0755	93.5643
59	A	834.5653	0.5315	1.4857	7.4538
60	A	837.0800	1.1625	33.6249	47.0939
61	A	883.8085	4.4218	211.0067	41.7012
62	A	884.5287	6.0435	27.4156	214.8264
63	A	895.2555	0.7067	22.3542	16.5473
64	A	948.7358	7.5469	101.9187	0.1904
65	A	948.8887	7.4555	106.7736	0.3259
66	A	969.8808	0.7465	1.3164	5.4097
67	A	987.7373	0.7347	0.3499	2.3835
68	A	1018.2636	3.6294	0.3463	45.6436
69	A	1049.9293	1.3837	2.2601	13.9848
70	A	1075.8802	1.0869	3.6016	3.9589
71	A	1097.4570	9.5242	103.7337	19.0656
72	A	1103.5918	9.6535	107.0471	16.4823
73	A	1129.0377	9.8137	37.0902	2.0123
74	A	1135.7576	10.0208	33.2877	1.9003
75	A	1141.8149	0.9630	3.7039	1.3235
76	A	1158.9387	10.3428	9.9940	0.4395
77	A	1161.6435	10.3957	7.4430	0.5529
78	A	1184.5372	0.9157	1.9231	10.7636
79	A	1195.4036	10.9258	363.0749	17.7735
80	A	1200.3440	10.8525	293.8345	11.2146
81	A	1202.5775	0.9647	8.0627	5.9958
82	A	1209.4416	11.1561	346.2493	8.2800
83	A	1212.9487	11.1674	308.7730	13.1168
84	A	1254.8981	10.1049	864.9263	32.8815
85	A	1258.4551	11.4211	202.6890	24.2778
86	A	1259.7999	11.7640	120.1926	148.6843
87	A	1263.1431	11.5751	267.9297	1.1840
88	A	1285.6117	3.3975	58.5603	101.6747
89	A	1350.6765	5.4699	3.3371	17.1968
90	A	1371.3596	1.4404	0.1657	0.3129
91	A	1501.4075	3.0067	7.6153	18.6699
92	A	1530.7403	3.1876	70.5592	32.5142
93	A	1632.6274	8.8333	12.2620	50.9719
94	A	1643.9084	5.8363	40.6155	49.4466
95	A	1661.6966	2.0427	77.5390	16.5217
96	A	3161.7286	6.4088	5.9455	26.9808
97	A	3164.2432	6.4195	4.1237	51.1812
98	A	3178.3713	6.4866	1.6253	108.7862
99	A	3184.7297	6.5358	11.3861	45.3684
100	A	3198.9615	6.6178	7.1147	240.8279
101	A	3536.9125	7.7273	20.7317	155.8499
102	A	3627.3187	8.5087	20.2324	29.9061

ALN_ic3F7I_trm2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.4366	0.0000	0.0189	0.2233
2	A	2.8306	0.0001	0.0173	0.0453
3	A	6.4721	0.0003	0.4492	0.2245
4	A	7.6786	0.0005	0.4182	0.2735
5	A	17.0751	0.0030	0.0243	1.0485
6	A	19.1390	0.0029	0.0081	1.1844
7	A	24.2828	0.0064	0.0719	0.2529
8	A	40.0993	0.0174	0.0455	0.0035
9	A	40.2464	0.0180	0.0109	0.0084
10	A	46.8325	0.0075	0.5708	3.3676
11	A	49.4361	0.0143	0.4068	1.4327
12	A	51.8582	0.0097	0.6445	0.8720
13	A	70.2359	0.0130	1.0433	13.4443
14	A	75.3973	0.0655	0.0424	0.5391
15	A	77.9351	0.0740	0.0149	0.2426
16	A	119.8461	0.0489	22.5282	17.7378
17	A	131.0899	0.2360	0.3136	1.2619
18	A	133.0289	0.2116	0.0574	0.2013
19	A	142.6088	0.2803	0.9151	6.2447
20	A	143.1937	0.2480	17.0378	5.4954
21	A	177.5133	0.3601	2.4649	2.5594
22	A	178.5626	0.3675	1.5246	5.3935
23	A	237.8154	0.7533	11.2338	78.2183
24	A	244.2514	0.7624	3.6325	85.4831
25	A	252.5115	0.1524	1.1765	18.4199
26	A	254.7567	0.6959	0.7940	0.1659
27	A	255.0319	0.6548	0.4743	0.5083
28	A	281.5258	0.7847	1.7345	2.2907
29	A	281.9678	0.8809	1.9733	4.1025
30	A	298.2315	0.9575	0.4097	0.6899
31	A	298.9068	0.9466	0.3182	0.7594
32	A	324.2526	1.1346	0.1033	2.1452
33	A	325.0289	1.1309	0.1199	2.3393
34	A	343.0523	1.2877	0.1099	1.3677
35	A	343.1768	1.2259	0.0308	1.0969
36	A	356.9682	0.1052	7.4496	0.3114
37	A	409.8494	0.2789	1.8389	3.4337
38	A	427.2388	0.2017	3.3998	1.8916
39	A	462.5003	2.2650	1.8679	2.8245
40	A	462.5976	2.2564	3.2441	4.5893
41	A	511.2234	0.4167	37.9191	16.1349
42	A	529.9532	2.9703	3.2778	0.4625
43	A	529.9987	2.9703	3.4513	0.4388
44	A	532.9514	2.8213	4.4864	19.8628
45	A	533.7326	2.9856	7.5524	19.5522
46	A	541.6611	1.1002	1.0419	7.1474
47	A	556.7503	3.2837	0.2043	0.0484
48	A	556.9082	3.2947	0.3108	0.0777
49	A	606.6315	3.8737	6.0921	1.7154
50	A	606.9650	3.8962	2.4906	2.2950
51	A	635.9479	1.5182	0.5271	5.8589
52	A	700.4510	0.6884	36.6357	3.9314
53	A	701.9127	4.7103	39.5405	0.0200
54	A	702.8025	3.9551	44.9525	0.1246
55	A	736.9447	0.6014	131.0858	99.8628
56	A	741.5333	5.3672	19.4759	48.5170
57	A	742.2789	1.1768	27.8325	1.8877
58	A	783.5981	0.6772	396.5117	103.8851
59	A	834.6735	0.5301	1.5527	7.7182
60	A	837.2642	1.1600	35.6210	48.1616
61	A	884.2664	5.1712	191.5120	49.7767
62	A	884.8977	4.7592	38.3337	185.4282
63	A	895.0289	0.7072	21.4923	17.1007
64	A	948.8274	7.5307	82.1946	0.2750
65	A	948.8907	7.4748	126.5476	0.2155
66	A	970.1025	0.7467	1.2896	5.3724

67	A	987.8348	0.7347	0.3351	2.3846
68	A	1018.2642	3.6287	0.3238	46.0712
69	A	1049.9145	1.3837	2.1859	14.3822
70	A	1075.9480	1.0872	3.5574	3.9423
71	A	1097.3214	9.5391	88.9613	27.6953
72	A	1103.5981	9.6536	107.3923	16.1325
73	A	1129.4752	9.8372	36.6773	2.1288
74	A	1135.7442	10.0200	33.5131	1.9400
75	A	1141.8565	0.9630	3.5249	1.3462
76	A	1158.3061	10.2999	8.4443	0.3677
77	A	1161.6773	10.3966	7.3776	0.5546
78	A	1184.5334	0.9157	1.9648	10.8542
79	A	1195.5736	10.9209	377.3211	23.0876
80	A	1200.3553	10.8321	287.2851	11.3533
81	A	1202.5912	0.9650	7.5245	6.0447
82	A	1209.3559	11.1206	262.7901	12.3514
83	A	1212.8908	11.1684	322.9029	12.1516
84	A	1255.2850	10.3403	881.7071	25.6922
85	A	1258.4488	11.4241	122.8850	14.9226
86	A	1260.2649	11.7729	316.4273	144.8611
87	A	1263.5301	11.5816	263.9828	0.5903
88	A	1285.3211	3.3753	25.4568	95.6915
89	A	1350.6450	5.4653	3.3262	17.4590
90	A	1371.3627	1.4404	0.1625	0.3074
91	A	1501.3721	3.0061	7.5983	18.6695
92	A	1530.7150	3.1872	71.4835	31.4991
93	A	1632.5990	8.8295	12.3136	50.6255
94	A	1643.8635	5.8195	41.6029	50.7847
95	A	1661.5258	2.0441	77.9193	16.5133
96	A	3161.7342	6.4088	6.0566	27.2813
97	A	3164.2858	6.4197	4.2441	51.4633
98	A	3178.3654	6.4866	1.6331	108.9869
99	A	3184.7282	6.5358	11.4150	46.2136
100	A	3198.9447	6.6178	7.2173	244.1530
101	A	3536.6801	7.7265	20.0087	155.8574
102	A	3626.8854	8.5064	20.1471	29.3787

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.5086	0.0001	0.1378	0.1750
2	A	10.4050	0.0011	0.0644	1.1884
3	A	12.8576	0.0015	0.0124	0.0742
4	A	14.5173	0.0014	0.0098	0.0389
5	A	16.4472	0.0029	0.0162	0.0474
6	A	18.4343	0.0036	0.0331	0.3006
7	A	26.7285	0.0048	0.3783	0.1410
8	A	33.8388	0.0166	0.0371	0.3282
9	A	35.5676	0.0160	0.0192	0.1360
10	A	43.2826	0.0096	0.2059	1.1344
11	A	46.2953	0.0081	0.2252	1.4491
12	A	61.2210	0.0107	0.1503	4.8215
13	A	69.0042	0.0191	1.7190	5.0325
14	A	71.0394	0.0578	0.0747	0.2052
15	A	75.0342	0.0461	0.0068	0.2546
16	A	104.8956	0.0371	6.9119	18.8035
17	A	111.8960	0.1271	1.8542	0.8480
18	A	116.4327	0.1736	0.8539	0.0773
19	A	158.0894	0.3808	4.1366	10.7440
20	A	160.0204	0.3787	1.9207	8.9586
21	A	214.4148	0.4898	0.0704	0.0388
22	A	214.8597	0.4896	4.7161	0.2979
23	A	231.6591	0.5938	0.0275	0.0145
24	A	231.9474	0.5948	0.0664	0.0066
25	A	244.2285	0.1324	1.1496	11.9362
26	A	262.1545	0.8778	2.9864	33.9641
27	A	262.7622	0.6620	0.0661	2.0605
28	A	266.1189	0.8082	0.0969	1.0872
29	A	269.3173	0.9296	0.1900	20.9577

30	A	287.0817	0.8953	4.3911	1.2586
31	A	288.5058	0.9120	4.8236	0.3577
32	A	336.6815	1.2474	0.8295	0.8791
33	A	337.7280	1.2549	0.4497	1.9958
34	A	353.4237	0.1005	7.0212	0.0438
35	A	371.4591	1.5207	0.0085	0.7581
36	A	372.3337	1.5259	0.0544	1.5577
37	A	379.0178	1.2562	0.1122	0.8061
38	A	379.5179	1.5267	0.5900	0.6075
39	A	408.5128	0.2730	0.0553	0.0964
40	A	421.5000	0.2082	1.6169	0.2867
41	A	506.8071	2.4675	0.6399	0.2225
42	A	507.1134	2.2634	3.3545	0.3682
43	A	508.1747	0.4150	35.1823	6.1487
44	A	526.5281	2.8860	12.5668	2.2382
45	A	527.0511	2.9169	6.2805	2.6637
46	A	539.9979	1.0916	1.6805	3.5855
47	A	579.7951	3.4292	4.7755	9.4029
48	A	582.0439	3.4550	9.6068	6.3301
49	A	596.3477	3.7662	0.1276	2.1232
50	A	596.6257	3.7739	0.2536	1.6801
51	A	635.9821	1.5172	0.1555	3.3015
52	A	665.2185	3.8865	48.0413	0.9659
53	A	667.3725	4.4078	68.0946	1.7689
54	A	696.4091	0.6884	68.2111	15.0891
55	A	714.3917	0.4896	194.5301	84.5657
56	A	726.5070	3.8946	144.2771	36.1185
57	A	727.9970	1.4030	20.9037	3.1579
58	A	776.1282	0.6437	254.0544	27.0558
59	A	805.5220	5.0339	51.1892	1.0318
60	A	808.5620	4.7060	135.0465	22.7334
61	A	831.0631	0.5137	1.1452	0.4252
62	A	834.6308	1.4775	3.7135	24.8693
63	A	892.2109	0.6934	6.5559	7.5236
64	A	970.7213	0.7518	0.0035	0.0859
65	A	983.1878	0.7124	0.6386	1.6632
66	A	1017.2637	3.6952	1.4596	36.9526
67	A	1045.8053	3.2136	31.3149	12.5572
68	A	1048.5531	1.8794	36.8466	17.3660
69	A	1057.8334	8.6186	1.1700	100.1438
70	A	1073.8367	1.0750	2.0950	0.0670
71	A	1109.9654	9.8325	82.5586	1.1868
72	A	1112.8006	9.6683	48.6008	0.9655
73	A	1119.2537	10.0209	248.3171	0.4905
74	A	1129.0144	9.9716	47.8451	0.0781
75	A	1140.1745	0.9595	4.2881	1.5265
76	A	1166.1678	10.3870	88.7441	0.6478
77	A	1170.5819	10.4773	95.3151	0.6399
78	A	1181.7636	10.8553	574.2292	6.9575
79	A	1183.0157	0.9112	0.7715	4.2169
80	A	1186.4179	10.9480	44.3584	16.5905
81	A	1202.5347	0.9626	8.8747	6.4160
82	A	1206.7555	11.2765	12.7128	0.7990
83	A	1214.0333	11.4267	793.2606	1.1198
84	A	1245.3229	11.0090	33.3445	1.4693
85	A	1249.9802	11.4242	28.1717	8.5336
86	A	1285.5514	3.4047	126.3371	30.4371
87	A	1298.9676	11.2030	97.7470	4.2592
88	A	1300.8451	11.6543	299.7620	9.9742
89	A	1351.6564	5.6742	1.3511	4.8409
90	A	1370.3949	1.4321	0.0134	0.1240
91	A	1503.0296	3.0551	4.5642	3.3329
92	A	1530.3262	3.1916	68.8148	8.1099
93	A	1630.6152	8.9269	3.9928	3.2351
94	A	1643.6419	5.0329	38.1746	45.9058
95	A	1660.4161	2.1633	114.1215	29.1746
96	A	3161.4692	6.4026	11.2733	18.2738
97	A	3162.5787	6.4146	1.7634	74.5201
98	A	3175.8128	6.4758	2.7534	104.1615
99	A	3183.4536	6.5310	13.0937	40.8575
100	A	3195.6850	6.6048	5.4115	229.1886

101	A	3543.6783	7.7553	24.2642	192.2258
102	A	3636.5064	8.5549	20.5781	44.9466

ALN_nc3F7I_trm2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.6659	0.0000	0.0243	0.0314
2	A	2.1666	0.0000	0.0380	0.1916
3	A	6.3052	0.0003	0.2733	0.1268
4	A	7.1662	0.0004	0.2317	0.1700
5	A	12.6682	0.0017	0.0048	0.6431
6	A	15.9919	0.0019	0.0193	0.7006
7	A	21.3316	0.0049	0.1676	0.2434
8	A	25.0650	0.0046	0.3722	0.1728
9	A	31.9487	0.0104	0.0381	0.7024
10	A	45.4033	0.0080	0.2249	3.4833
11	A	46.8158	0.0113	0.2722	1.9100
12	A	52.1733	0.0118	0.5233	0.4597
13	A	66.6005	0.0132	0.8397	11.1346
14	A	71.5373	0.0602	0.0425	0.1761
15	A	75.0217	0.0413	0.0771	1.0358
16	A	109.2744	0.1153	0.4970	1.9015
17	A	111.3109	0.0902	3.3879	5.6505
18	A	118.6952	0.0643	22.4132	9.3927
19	A	157.4401	0.3661	6.5503	19.0636
20	A	159.0308	0.3743	2.1611	16.7967
21	A	213.2634	0.4880	2.2453	0.3601
22	A	213.5973	0.4790	2.6826	0.2270
23	A	231.1627	0.5910	0.1017	0.0024
24	A	231.4972	0.5930	0.1011	0.0038
25	A	247.2151	0.1458	0.7840	61.5704
26	A	262.6653	0.6384	0.0019	1.4299
27	A	264.3137	0.7964	2.9864	2.9999
28	A	265.0876	0.6601	1.2184	25.9817
29	A	266.6184	0.8983	0.9407	52.1311
30	A	286.6885	0.8894	4.7824	1.2825
31	A	287.2644	0.8984	3.2839	1.1652
32	A	336.7807	1.2474	0.8269	1.2416
33	A	337.0494	1.2500	0.5206	2.0908
34	A	350.7718	0.0938	9.0141	0.5018
35	A	371.2929	1.5198	0.0158	0.9267
36	A	371.4057	1.5192	0.0560	1.1319
37	A	378.9199	1.1967	0.1488	0.4013
38	A	379.2929	1.5160	0.4957	0.7198
39	A	406.9803	0.2635	1.4839	1.7355
40	A	419.5184	0.2358	1.8324	2.6289
41	A	506.3266	2.4097	2.9532	0.8713
42	A	506.7276	2.6049	1.5884	0.3160
43	A	510.5880	0.4167	38.8192	11.0288
44	A	526.6229	2.9184	7.9688	3.0452
45	A	526.9104	2.9121	6.6287	2.7962
46	A	541.2027	1.0922	1.4190	7.6328
47	A	580.1972	3.4249	8.4076	14.9476
48	A	582.3517	3.4572	11.2316	14.0084
49	A	596.2284	3.7650	0.0849	2.2492
50	A	596.4272	3.7717	0.1642	2.1555
51	A	636.1351	1.5184	0.4967	5.2508
52	A	665.9918	4.4046	74.9518	0.7516
53	A	666.9277	4.3782	34.9092	1.3673
54	A	699.5476	0.6678	60.0110	4.5999
55	A	722.9409	1.1270	281.1210	54.0937
56	A	725.9140	4.8908	15.2401	81.2845
57	A	730.2272	0.5532	110.9610	40.0941
58	A	774.0960	0.6568	346.7530	55.4801
59	A	805.8293	5.2251	169.6710	27.6677
60	A	806.8326	5.2276	46.7278	65.2027
61	A	833.3285	0.5338	2.1536	5.0518
62	A	836.0109	1.2615	9.6414	37.7789
63	A	893.1049	0.6777	39.0515	21.2097

64	A	969.2232	0.7445	0.8253	4.7591
65	A	986.7014	0.7320	0.2720	2.0167
66	A	1017.9617	3.6343	0.3404	41.1810
67	A	1049.8959	1.4074	6.3253	14.4015
68	A	1052.1859	8.0495	43.6566	64.7762
69	A	1053.9004	8.1644	32.4919	113.2369
70	A	1074.8190	1.0834	3.9127	3.3565
71	A	1112.8120	9.9180	317.2827	0.7167
72	A	1113.7423	9.6632	52.7246	0.4017
73	A	1116.2078	9.9986	196.3479	0.4916
74	A	1124.1685	9.8768	50.9923	0.4461
75	A	1141.1986	0.9628	3.3854	1.4309
76	A	1167.1463	10.4138	86.6117	0.6824
77	A	1169.0729	10.4573	85.2806	0.9149
78	A	1183.4958	10.5983	283.6294	18.1428
79	A	1184.0008	0.9296	1.0934	12.1883
80	A	1186.1596	9.3077	281.1674	14.3668
81	A	1202.4973	0.9624	6.6889	5.4162
82	A	1208.3323	11.3110	412.2134	1.0737
83	A	1211.1168	11.3616	426.1975	1.1577
84	A	1246.0974	11.0147	131.9618	11.9443
85	A	1247.1291	11.3573	43.8754	33.7596
86	A	1285.1467	3.4375	122.2417	62.0923
87	A	1299.0145	11.8556	238.2061	9.0159
88	A	1300.7524	10.9800	156.7488	6.5518
89	A	1350.5177	5.5156	3.2564	14.5046
90	A	1371.0464	1.4385	0.1643	0.3080
91	A	1501.4656	3.0167	7.3176	16.6113
92	A	1530.9056	3.1962	67.3228	24.1089
93	A	1632.3578	8.8571	10.1871	41.1077
94	A	1644.3002	5.6154	39.3635	39.9908
95	A	1661.9057	2.0748	80.0126	17.0128
96	A	3161.0374	6.4047	6.7262	26.1523
97	A	3163.2419	6.4151	3.8906	54.0422
98	A	3177.4140	6.4828	1.8303	111.1499
99	A	3183.7364	6.5318	12.8574	42.7123
100	A	3198.1646	6.6144	7.6991	240.5733
101	A	3540.1886	7.7408	20.1877	155.5769
102	A	3631.2422	8.5277	19.5267	32.0444

ANL2_01

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.9331	0.0001	0.3980	8.2020
2	A	30.1373	0.0021	0.3266	6.5253
3	A	35.8144	0.0040	0.0062	3.5232
4	A	55.8542	0.0085	0.0499	0.6728
5	A	65.7013	0.0107	0.5339	0.6944
6	A	109.4347	0.0374	1.5482	2.7721
7	A	221.9289	0.1023	1.9515	0.5632
8	A	234.3823	0.1196	2.2666	0.9285
9	A	306.6779	0.0585	17.2256	0.1979
10	A	380.2876	0.1860	5.2842	0.6299
11	A	398.2540	0.2206	3.9604	0.4838
12	A	407.6974	0.1798	28.0728	1.8637
13	A	414.8042	0.2778	2.1421	0.1460
14	A	422.2249	0.2261	16.8991	0.4964
15	A	509.1510	0.3901	39.1196	0.2445
16	A	517.4390	0.4024	12.6519	0.1474
17	A	539.8296	1.0855	2.9545	5.0442
18	A	540.1107	1.0737	0.9374	3.6782
19	A	636.5687	1.5194	0.0984	3.0035
20	A	637.4477	1.5124	0.9545	5.0905
21	A	661.8116	0.3105	223.0496	4.4156
22	A	695.1664	0.4629	171.3745	4.5739
23	A	701.8481	0.4503	35.0865	1.2441
24	A	703.0479	0.5225	27.4747	0.2024
25	A	760.6233	0.6340	55.3379	1.2386
26	A	769.9022	0.6410	131.2362	2.9333

27	A	825.1750	0.5052	0.7616	0.6817
28	A	831.5752	0.5267	0.7274	1.0505
29	A	833.0225	1.5777	3.7028	19.7822
30	A	835.4862	1.6448	2.0957	27.2328
31	A	883.8457	0.7145	3.9492	0.3393
32	A	894.9299	0.7060	14.4877	0.6758
33	A	962.7920	0.7281	0.1474	0.0883
34	A	973.0736	0.7570	0.0452	0.0345
35	A	981.1468	0.7241	0.0186	0.3321
36	A	991.6442	0.7387	0.1966	0.5854
37	A	1013.1334	3.5544	4.4932	39.7501
38	A	1016.6217	3.6253	0.5290	21.5421
39	A	1048.4279	1.3847	3.8934	15.7371
40	A	1049.8163	1.3794	3.3924	21.6999
41	A	1071.8749	1.0768	4.5717	0.0726
42	A	1074.5737	1.0838	4.0241	0.1101
43	A	1139.7775	0.9602	2.1793	2.3448
44	A	1143.2571	0.9581	0.9108	3.7603
45	A	1177.7620	0.8933	2.0736	4.6977
46	A	1181.9960	0.9044	1.2081	3.5172
47	A	1200.9571	0.9577	20.2497	1.9385
48	A	1201.9780	0.9585	2.0925	2.7624
49	A	1286.4337	3.2091	32.6182	10.5823
50	A	1305.6606	3.2519	70.9669	15.0018
51	A	1350.3775	5.7085	4.6165	1.2094
52	A	1351.0854	5.7860	10.7233	1.9946
53	A	1368.3121	1.4213	0.0692	0.1795
54	A	1368.8983	1.4331	0.0660	0.1488
55	A	1499.6483	3.0906	2.1670	0.4799
56	A	1501.6350	3.0609	3.4852	1.3845
57	A	1530.4953	3.2255	20.8531	1.7324
58	A	1531.1686	3.2772	86.5353	1.9290
59	A	1624.3903	8.7662	1.5678	7.4527
60	A	1632.5989	9.0195	3.5903	4.1901
61	A	1644.2673	5.3579	28.3310	20.8079
62	A	1648.1254	5.8476	51.0469	21.1848
63	A	1660.6596	2.2694	94.2313	19.2887
64	A	1681.8481	1.9921	107.2352	14.8594
65	A	3147.5454	6.3431	13.3495	61.0046
66	A	3158.3471	6.3908	9.0395	43.7574
67	A	3161.5917	6.4058	3.9996	67.3655
68	A	3161.9376	6.4025	0.5700	82.3530
69	A	3169.7100	6.4653	33.0921	87.0856
70	A	3174.9860	6.4725	3.5529	127.7425
71	A	3181.9230	6.5247	21.2406	29.7546
72	A	3188.3974	6.5653	20.3424	184.1817
73	A	3196.3001	6.6073	8.8560	222.7968
74	A	3210.5489	6.6262	0.0832	238.3525
75	A	3508.8403	7.6509	231.9251	288.1388
76	A	3546.7204	7.7672	12.4262	161.6798
77	A	3638.8158	8.5629	16.4627	53.1072
78	A	3641.5216	8.5404	62.0543	91.7851

ANL2_02

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.9289	0.0001	0.3980	8.2016
2	A	30.1362	0.0021	0.3266	6.5255
3	A	35.8139	0.0040	0.0062	3.5231
4	A	55.8551	0.0085	0.0499	0.6730
5	A	65.6996	0.0107	0.5339	0.6944
6	A	109.4366	0.0374	1.5483	2.7721
7	A	221.9288	0.1023	1.9516	0.5632
8	A	234.3824	0.1196	2.2667	0.9284
9	A	306.6753	0.0585	17.2230	0.1979
10	A	380.2861	0.1860	5.2861	0.6300
11	A	398.2539	0.2206	3.9613	0.4837
12	A	407.6937	0.1797	28.0826	1.8642
13	A	414.8039	0.2778	2.1408	0.1459

14	A	422.2230	0.2261	16.8905	0.4961
15	A	509.1508	0.3901	39.1211	0.2444
16	A	517.4387	0.4024	12.6515	0.1474
17	A	539.8294	1.0855	2.9546	5.0429
18	A	540.1108	1.0737	0.9375	3.6794
19	A	636.5687	1.5194	0.0984	3.0035
20	A	637.4476	1.5124	0.9545	5.0904
21	A	661.8055	0.3105	223.0304	4.4154
22	A	695.1621	0.4628	171.4133	4.5757
23	A	701.8470	0.4504	35.0597	1.2425
24	A	703.0474	0.5225	27.4740	0.2023
25	A	760.6226	0.6340	55.3345	1.2385
26	A	769.9013	0.6410	131.2335	2.9333
27	A	825.1743	0.5052	0.7615	0.6817
28	A	831.5749	0.5267	0.7271	1.0499
29	A	833.0224	1.5777	3.7026	19.7830
30	A	835.4863	1.6449	2.0958	27.2323
31	A	883.8449	0.7145	3.9490	0.3392
32	A	894.9296	0.7060	14.4875	0.6757
33	A	962.7916	0.7281	0.1474	0.0883
34	A	973.0733	0.7570	0.0452	0.0345
35	A	981.1463	0.7241	0.0186	0.3321
36	A	991.6441	0.7387	0.1966	0.5854
37	A	1013.1333	3.5544	4.4935	39.7498
38	A	1016.6216	3.6253	0.5290	21.5423
39	A	1048.4278	1.3847	3.8934	15.7372
40	A	1049.8162	1.3794	3.3924	21.6999
41	A	1071.8742	1.0768	4.5709	0.0726
42	A	1074.5731	1.0838	4.0244	0.1101
43	A	1139.7769	0.9602	2.1792	2.3449
44	A	1143.2563	0.9581	0.9111	3.7602
45	A	1177.7618	0.8933	2.0736	4.6977
46	A	1181.9959	0.9044	1.2081	3.5172
47	A	1200.9569	0.9577	20.2499	1.9385
48	A	1201.9779	0.9585	2.0926	2.7624
49	A	1286.4338	3.2091	32.6179	10.5822
50	A	1305.6610	3.2519	70.9685	15.0020
51	A	1350.3774	5.7086	4.6166	1.2095
52	A	1351.0853	5.7861	10.7230	1.9945
53	A	1368.3118	1.4213	0.0692	0.1795
54	A	1368.8982	1.4331	0.0660	0.1488
55	A	1499.6480	3.0906	2.1669	0.4799
56	A	1501.6349	3.0609	3.4852	1.3846
57	A	1530.4952	3.2255	20.8530	1.7326
58	A	1531.1686	3.2772	86.5362	1.9289
59	A	1624.3900	8.7662	1.5680	7.4526
60	A	1632.5990	9.0195	3.5903	4.1901
61	A	1644.2670	5.3577	28.3312	20.8078
62	A	1648.1253	5.8475	51.0455	21.1842
63	A	1660.6588	2.2695	94.2332	19.2894
64	A	1681.8482	1.9921	107.2378	14.8593
65	A	3147.5460	6.3431	13.3495	61.0048
66	A	3158.3479	6.3908	9.0397	43.7539
67	A	3161.5913	6.4058	4.0008	67.3394
68	A	3161.9383	6.4025	0.5688	82.3835
69	A	3169.7107	6.4653	33.0923	87.0844
70	A	3174.9865	6.4725	3.5525	127.7416
71	A	3181.9236	6.5247	21.2406	29.7556
72	A	3188.3979	6.5653	20.3425	184.1826
73	A	3196.3007	6.6073	8.8560	222.7972
74	A	3210.5501	6.6262	0.0832	238.3499
75	A	3508.8425	7.6509	231.9414	288.1440
76	A	3546.7232	7.7672	12.4264	161.6787
77	A	3638.8195	8.5629	16.4630	53.1068
78	A	3641.5263	8.5404	62.0557	91.7853

ANL2_03

 NM# Symm Wavenumber Force Const IR Intens Raman Activ

1	A	15.3479	0.0007	0.1905	2.8260
2	A	27.6339	0.0020	0.5097	2.1012
3	A	36.9562	0.0036	1.2749	1.5743
4	A	66.2105	0.0103	0.4425	5.9392
5	A	68.7641	0.0109	0.2798	2.7296
6	A	128.6486	0.0505	0.2218	9.5836
7	A	232.3533	0.1135	8.4326	0.9530
8	A	233.2502	0.1160	0.1748	2.0859
9	A	319.5189	0.0650	28.1785	0.3480
10	A	345.2833	0.0775	28.0729	0.7337
11	A	389.0402	0.2427	3.3707	0.2416
12	A	395.8288	0.2589	1.0024	1.2734
13	A	419.6804	0.3082	0.6488	0.1890
14	A	421.3627	0.3040	1.1851	0.2437
15	A	508.6031	0.3813	2.0898	1.0295
16	A	513.2829	0.3888	78.2849	1.3576
17	A	539.2461	1.1219	5.2100	3.8623
18	A	539.9729	1.0882	3.1243	3.5980
19	A	636.4050	1.4905	1.9472	6.6098
20	A	636.4923	1.4869	0.7575	0.8798
21	A	671.0791	0.3658	187.2156	6.2645
22	A	701.0701	0.6529	42.5748	0.8376
23	A	706.8558	0.5396	40.3656	0.1973
24	A	717.8727	0.3810	202.5022	7.4437
25	A	766.8031	0.6395	173.4427	1.9467
26	A	772.5863	0.6496	103.9956	3.7952
27	A	830.9667	0.6000	0.7544	3.1951
28	A	833.0560	0.9844	5.9723	15.4578
29	A	835.5147	0.5654	1.6249	1.1692
30	A	840.6500	1.3504	14.6741	31.2184
31	A	887.8761	0.7106	25.0895	1.3824
32	A	897.9612	0.7059	9.5191	0.1260
33	A	970.0719	0.7482	0.1763	0.0389
34	A	972.4669	0.7492	0.2361	0.0153
35	A	984.8453	0.7198	0.1481	0.3866
36	A	989.9424	0.7361	0.6759	0.1901
37	A	1014.3961	3.5626	1.4248	43.8601
38	A	1015.7446	3.5988	0.7976	19.7654
39	A	1048.0849	1.3690	4.1869	15.7380
40	A	1049.0763	1.3811	3.5468	21.1687
41	A	1073.7676	1.0852	4.2013	0.4064
42	A	1080.2408	1.1276	6.5749	0.3458
43	A	1141.5621	0.9631	2.4379	1.4105
44	A	1154.3499	0.9762	1.7792	1.4082
45	A	1178.5727	0.8955	1.1432	3.9427
46	A	1180.1381	0.9010	1.0872	3.6587
47	A	1198.6557	0.9534	9.1927	2.5718
48	A	1202.2896	0.9600	9.4644	2.1015
49	A	1288.5371	3.2043	47.4415	10.6693
50	A	1308.1899	3.2231	48.9752	17.9948
51	A	1350.1443	5.6908	4.9652	0.8734
52	A	1354.1102	4.6669	6.5959	0.3328
53	A	1369.5161	1.4282	0.0505	0.1594
54	A	1370.4445	1.5013	0.9922	0.2480
55	A	1501.1234	3.0626	2.1889	0.7753
56	A	1501.3845	3.0627	2.9324	2.0680
57	A	1530.2945	3.2171	51.7616	1.9035
58	A	1531.1760	3.3116	49.5904	1.4074
59	A	1626.1839	8.6317	4.7241	3.6912
60	A	1630.1872	8.2633	3.7654	7.8301
61	A	1643.3923	4.7361	33.0118	29.2853
62	A	1647.5486	5.5792	49.7986	15.6727
63	A	1659.6615	2.4735	110.5013	22.0457
64	A	1679.9167	1.9912	72.3347	10.3372
65	A	3152.9376	6.3681	9.5641	58.3513
66	A	3154.9232	6.3648	12.7801	6.6216
67	A	3158.0619	6.3876	0.1689	105.5866
68	A	3166.5793	6.4185	0.2295	60.3586
69	A	3171.2655	6.4638	8.1744	123.0151
70	A	3174.1844	6.4771	9.0984	107.0718
71	A	3174.8018	6.4972	35.0757	31.5640

72	A	3182.7269	6.5263	19.4970	15.8402
73	A	3191.5183	6.5845	13.5531	237.8512
74	A	3193.6447	6.5975	9.5894	265.2668
75	A	3529.7895	7.7129	54.4116	153.3645
76	A	3550.5605	7.7827	11.0861	156.0469
77	A	3626.9919	8.4822	20.1345	33.6269
78	A	3645.0094	8.5950	16.8305	48.2795

ANL2_04

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3477	0.0007	0.1905	2.8261
2	A	27.6342	0.0020	0.5097	2.1010
3	A	36.9568	0.0036	1.2748	1.5743
4	A	66.2099	0.0103	0.4425	5.9393
5	A	68.7642	0.0109	0.2798	2.7295
6	A	128.6487	0.0505	0.2218	9.5836
7	A	232.3532	0.1135	8.4328	0.9529
8	A	233.2502	0.1160	0.1747	2.0859
9	A	319.5179	0.0650	28.1796	0.3480
10	A	345.2873	0.0775	28.0716	0.7337
11	A	389.0405	0.2427	3.3708	0.2416
12	A	395.8287	0.2589	1.0022	1.2734
13	A	419.6800	0.3082	0.6489	0.1890
14	A	421.3624	0.3040	1.1850	0.2437
15	A	508.6029	0.3813	2.0895	1.0295
16	A	513.2826	0.3888	78.2868	1.3576
17	A	539.2461	1.1219	5.2099	3.8622
18	A	539.9730	1.0882	3.1244	3.5980
19	A	636.4050	1.4904	1.9485	6.6101
20	A	636.4923	1.4869	0.7571	0.8794
21	A	671.0720	0.3658	187.2211	6.2647
22	A	701.0702	0.6529	42.5651	0.8373
23	A	706.8556	0.5396	40.3657	0.1972
24	A	717.8753	0.3810	202.4984	7.4437
25	A	766.8028	0.6395	173.4229	1.9467
26	A	772.5876	0.6496	104.0206	3.7953
27	A	830.9669	0.6000	0.7546	3.1951
28	A	833.0559	0.9844	5.9719	15.4574
29	A	835.5147	0.5654	1.6250	1.1694
30	A	840.6502	1.3503	14.6754	31.2187
31	A	887.8764	0.7106	25.0903	1.3825
32	A	897.9610	0.7059	9.5185	0.1260
33	A	970.0718	0.7482	0.1763	0.0389
34	A	972.4668	0.7492	0.2360	0.0153
35	A	984.8454	0.7198	0.1481	0.3866
36	A	989.9425	0.7361	0.6759	0.1901
37	A	1014.3963	3.5626	1.4247	43.8619
38	A	1015.7446	3.5988	0.7977	19.7637
39	A	1048.0850	1.3690	4.1869	15.7378
40	A	1049.0763	1.3811	3.5468	21.1687
41	A	1073.7673	1.0852	4.2013	0.4063
42	A	1080.2414	1.1276	6.5750	0.3458
43	A	1141.5619	0.9631	2.4379	1.4106
44	A	1154.3511	0.9762	1.7792	1.4082
45	A	1178.5726	0.8955	1.1432	3.9427
46	A	1180.1381	0.9010	1.0872	3.6587
47	A	1198.6557	0.9534	9.1925	2.5718
48	A	1202.2896	0.9600	9.4645	2.1015
49	A	1288.5375	3.2043	47.4423	10.6690
50	A	1308.1888	3.2231	48.9745	17.9952
51	A	1350.1445	5.6908	4.9653	0.8734
52	A	1354.1104	4.6668	6.5959	0.3328
53	A	1369.5160	1.4282	0.0504	0.1594
54	A	1370.4448	1.5013	0.9923	0.2480
55	A	1501.1233	3.0626	2.1888	0.7754
56	A	1501.3846	3.0627	2.9324	2.0680
57	A	1530.2946	3.2171	51.7636	1.9036
58	A	1531.1759	3.3116	49.5879	1.4073

59	A	1626.1844	8.6317	4.7240	3.6912
60	A	1630.1874	8.2633	3.7655	7.8302
61	A	1643.3922	4.7361	33.0117	29.2853
62	A	1647.5485	5.5792	49.7981	15.6724
63	A	1659.6614	2.4735	110.5020	22.0458
64	A	1679.9167	1.9912	72.3334	10.3371
65	A	3152.9379	6.3681	9.5638	58.3495
66	A	3154.9229	6.3648	12.7794	6.6249
67	A	3158.0620	6.3876	0.1691	105.5858
68	A	3166.5786	6.4185	0.2294	60.3587
69	A	3171.2654	6.4638	8.1761	123.0055
70	A	3174.1839	6.4771	9.1013	107.0909
71	A	3174.8019	6.4972	35.0714	31.5487
72	A	3182.7260	6.5263	19.4976	15.8391
73	A	3191.5176	6.5845	13.5528	237.8535
74	A	3193.6440	6.5975	9.5894	265.2685
75	A	3529.7849	7.7129	54.4116	153.3585
76	A	3550.5628	7.7827	11.0862	156.0524
77	A	3626.9888	8.4822	20.1338	33.6271
78	A	3645.0128	8.5951	16.8307	48.2796

 ANL2_05

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3507	0.0007	0.1906	2.8264
2	A	27.6381	0.0020	0.5098	2.1017
3	A	36.9527	0.0036	1.2748	1.5746
4	A	66.2166	0.0103	0.4426	5.9379
5	A	68.7634	0.0109	0.2797	2.7311
6	A	128.6574	0.0505	0.2218	9.5830
7	A	232.3526	0.1135	8.4329	0.9527
8	A	233.2549	0.1160	0.1742	2.0855
9	A	319.5205	0.0650	28.1836	0.3480
10	A	345.3030	0.0775	28.0601	0.7338
11	A	389.0410	0.2427	3.3722	0.2415
12	A	395.8316	0.2588	1.0011	1.2733
13	A	419.6799	0.3082	0.6486	0.1891
14	A	421.3624	0.3040	1.1853	0.2437
15	A	508.6028	0.3813	2.0921	1.0297
16	A	513.2837	0.3888	78.2711	1.3574
17	A	539.2462	1.1219	5.2099	3.8623
18	A	539.9730	1.0882	3.1246	3.5980
19	A	636.4052	1.4906	1.9426	6.6083
20	A	636.4924	1.4868	0.7588	0.8807
21	A	671.1027	0.3659	187.1862	6.2640
22	A	701.0707	0.6529	42.5391	0.8367
23	A	706.8562	0.5396	40.3639	0.1974
24	A	717.8832	0.3811	202.5158	7.4440
25	A	766.8053	0.6395	173.4669	1.9473
26	A	772.5895	0.6496	104.0315	3.7954
27	A	830.9662	0.6000	0.7544	3.1951
28	A	833.0561	0.9844	5.9740	15.4581
29	A	835.5149	0.5654	1.6239	1.1693
30	A	840.6511	1.3503	14.6800	31.2181
31	A	887.8759	0.7106	25.0915	1.3824
32	A	897.9633	0.7059	9.5209	0.1260
33	A	970.0718	0.7482	0.1763	0.0389
34	A	972.4667	0.7492	0.2361	0.0153
35	A	984.8451	0.7198	0.1482	0.3867
36	A	989.9438	0.7361	0.6760	0.1901
37	A	1014.3963	3.5625	1.4249	43.8559
38	A	1015.7452	3.5988	0.7973	19.7674
39	A	1048.0847	1.3690	4.1865	15.7382
40	A	1049.0765	1.3811	3.5470	21.1681
41	A	1073.7682	1.0852	4.2014	0.4062
42	A	1080.2434	1.1277	6.5751	0.3459
43	A	1141.5628	0.9631	2.4377	1.4105
44	A	1154.3546	0.9763	1.7798	1.4084
45	A	1178.5724	0.8955	1.1432	3.9429

46	A	1180.1382	0.9010	1.0871	3.6586
47	A	1198.6551	0.9534	9.1928	2.5718
48	A	1202.2900	0.9600	9.4636	2.1013
49	A	1288.5332	3.2043	47.4376	10.6686
50	A	1308.1891	3.2231	48.9742	17.9946
51	A	1350.1443	5.6907	4.9648	0.8735
52	A	1354.1104	4.6666	6.5957	0.3329
53	A	1369.5165	1.4282	0.0505	0.1594
54	A	1370.4449	1.5014	0.9926	0.2480
55	A	1501.1238	3.0626	2.1892	0.7758
56	A	1501.3847	3.0627	2.9322	2.0676
57	A	1530.2943	3.2171	51.7610	1.9035
58	A	1531.1757	3.3116	49.5886	1.4072
59	A	1626.1840	8.6317	4.7240	3.6914
60	A	1630.1888	8.2638	3.7648	7.8296
61	A	1643.3922	4.7362	33.0103	29.2871
62	A	1647.5488	5.5790	49.8006	15.6726
63	A	1659.6614	2.4735	110.5045	22.0441
64	A	1679.9206	1.9912	72.3234	10.3355
65	A	3152.9369	6.3681	9.5643	58.3542
66	A	3154.9228	6.3648	12.7801	6.6214
67	A	3158.0615	6.3876	0.1689	105.5847
68	A	3166.5801	6.4185	0.2298	60.3565
69	A	3171.2651	6.4638	8.1740	123.0171
70	A	3174.1846	6.4771	9.0950	107.0495
71	A	3174.8016	6.4972	35.0796	31.5837
72	A	3182.7274	6.5263	19.4968	15.8430
73	A	3191.5179	6.5845	13.5528	237.8533
74	A	3193.6451	6.5975	9.5890	265.2529
75	A	3529.7719	7.7129	54.4406	153.3682
76	A	3550.5572	7.7826	11.0845	156.0507
77	A	3626.9854	8.4821	20.1390	33.6321
78	A	3645.0041	8.5950	16.8278	48.2793

ANL2_06

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3465	0.0007	0.1905	2.8260
2	A	27.6327	0.0020	0.5097	2.1013
3	A	36.9568	0.0036	1.2749	1.5744
4	A	66.2120	0.0103	0.4425	5.9393
5	A	68.7652	0.0109	0.2798	2.7296
6	A	128.6496	0.0505	0.2218	9.5834
7	A	232.3530	0.1135	8.4327	0.9531
8	A	233.2500	0.1160	0.1750	2.0857
9	A	319.5210	0.0650	28.1785	0.3479
10	A	345.2830	0.0775	28.0726	0.7337
11	A	389.0406	0.2427	3.3709	0.2416
12	A	395.8289	0.2589	1.0026	1.2734
13	A	419.6805	0.3082	0.6488	0.1890
14	A	421.3625	0.3040	1.1851	0.2437
15	A	508.6031	0.3813	2.0899	1.0294
16	A	513.2829	0.3888	78.2870	1.3576
17	A	539.2462	1.1219	5.2102	3.8622
18	A	539.9731	1.0882	3.1242	3.5980
19	A	636.4050	1.4904	1.9482	6.6101
20	A	636.4923	1.4869	0.7570	0.8796
21	A	671.0783	0.3658	187.2205	6.2646
22	A	701.0695	0.6529	42.6024	0.8384
23	A	706.8557	0.5396	40.3669	0.1972
24	A	717.8658	0.3810	202.5040	7.4435
25	A	766.8028	0.6395	173.4641	1.9467
26	A	772.5837	0.6496	103.9490	3.7949
27	A	830.9669	0.6000	0.7544	3.1951
28	A	833.0564	0.9843	5.9719	15.4574
29	A	835.5146	0.5654	1.6252	1.1695
30	A	840.6493	1.3504	14.6705	31.2181
31	A	887.8759	0.7106	25.0871	1.3823
32	A	897.9607	0.7059	9.5195	0.1260

33	A	970.0720	0.7482	0.1763	0.0389
34	A	972.4668	0.7492	0.2361	0.0153
35	A	984.8453	0.7198	0.1481	0.3866
36	A	989.9422	0.7361	0.6759	0.1901
37	A	1014.3959	3.5626	1.4249	43.8596
38	A	1015.7445	3.5988	0.7977	19.7663
39	A	1048.0849	1.3690	4.1869	15.7384
40	A	1049.0763	1.3811	3.5468	21.1687
41	A	1073.7677	1.0852	4.2013	0.4063
42	A	1080.2402	1.1276	6.5748	0.3458
43	A	1141.5624	0.9631	2.4378	1.4105
44	A	1154.3488	0.9762	1.7792	1.4083
45	A	1178.5727	0.8955	1.1432	3.9426
46	A	1180.1381	0.9010	1.0873	3.6588
47	A	1198.6560	0.9534	9.1928	2.5718
48	A	1202.2896	0.9600	9.4645	2.1014
49	A	1288.5389	3.2043	47.4428	10.6695
50	A	1308.1917	3.2230	48.9758	17.9950
51	A	1350.1444	5.6908	4.9655	0.8733
52	A	1354.1103	4.6670	6.5959	0.3328
53	A	1369.5162	1.4282	0.0505	0.1594
54	A	1370.4444	1.5013	0.9921	0.2480
55	A	1501.1235	3.0626	2.1889	0.7751
56	A	1501.3846	3.0627	2.9323	2.0682
57	A	1530.2946	3.2171	51.7617	1.9036
58	A	1531.1763	3.3116	49.5914	1.4075
59	A	1626.1834	8.6317	4.7240	3.6911
60	A	1630.1869	8.2634	3.7653	7.8302
61	A	1643.3927	4.7362	33.0147	29.2861
62	A	1647.5489	5.5792	49.7972	15.6721
63	A	1659.6624	2.4734	110.4995	22.0454
64	A	1679.9163	1.9912	72.3385	10.3378
65	A	3152.9379	6.3681	9.5641	58.3505
66	A	3154.9229	6.3648	12.7805	6.6214
67	A	3158.0615	6.3876	0.1689	105.5859
68	A	3166.5793	6.4185	0.2295	60.3596
69	A	3171.2653	6.4638	8.1738	123.0176
70	A	3174.1844	6.4771	9.0974	107.0690
71	A	3174.8016	6.4972	35.0771	31.5681
72	A	3182.7269	6.5263	19.4969	15.8399
73	A	3191.5182	6.5845	13.5532	237.8505
74	A	3193.6447	6.5975	9.5895	265.2693
75	A	3529.7920	7.7129	54.4099	153.3673
76	A	3550.5595	7.7826	11.0863	156.0442
77	A	3626.9949	8.4822	20.1347	33.6269
78	A	3645.0082	8.5950	16.8307	48.2802

ANL2_07

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3479	0.0007	0.1905	2.8259
2	A	27.6340	0.0020	0.5096	2.1013
3	A	36.9563	0.0036	1.2748	1.5745
4	A	66.2112	0.0103	0.4425	5.9390
5	A	68.7643	0.0109	0.2798	2.7297
6	A	128.6479	0.0504	0.2217	9.5834
7	A	232.3539	0.1135	8.4328	0.9528
8	A	233.2504	0.1160	0.1745	2.0860
9	A	319.5213	0.0650	28.1811	0.3480
10	A	345.2886	0.0775	28.0712	0.7337
11	A	389.0410	0.2427	3.3711	0.2416
12	A	395.8293	0.2589	1.0024	1.2734
13	A	419.6805	0.3082	0.6488	0.1890
14	A	421.3626	0.3040	1.1852	0.2436
15	A	508.6036	0.3813	2.0894	1.0294
16	A	513.2836	0.3888	78.2798	1.3576
17	A	539.2459	1.1219	5.2103	3.8619
18	A	539.9731	1.0882	3.1232	3.5985
19	A	636.4052	1.4906	1.9433	6.6086

20	A	636.4925	1.4868	0.7589	0.8810
21	A	671.0993	0.3658	187.2156	6.2643
22	A	701.0711	0.6529	42.5431	0.8370
23	A	706.8565	0.5396	40.3628	0.1973
24	A	717.8797	0.3811	202.5018	7.4438
25	A	766.8052	0.6395	173.4590	1.9468
26	A	772.5890	0.6496	104.0171	3.7955
27	A	830.9671	0.6000	0.7542	3.1953
28	A	833.0573	0.9844	5.9733	15.4579
29	A	835.5156	0.5654	1.6247	1.1688
30	A	840.6505	1.3503	14.6786	31.2196
31	A	887.8769	0.7106	25.0917	1.3825
32	A	897.9624	0.7059	9.5199	0.1260
33	A	970.0723	0.7482	0.1763	0.0389
34	A	972.4676	0.7492	0.2360	0.0153
35	A	984.8457	0.7198	0.1481	0.3866
36	A	989.9430	0.7361	0.6759	0.1901
37	A	1014.3963	3.5626	1.4247	43.8615
38	A	1015.7448	3.5988	0.7976	19.7639
39	A	1048.0852	1.3690	4.1870	15.7375
40	A	1049.0764	1.3811	3.5468	21.1692
41	A	1073.7694	1.0852	4.2015	0.4063
42	A	1080.2416	1.1276	6.5750	0.3458
43	A	1141.5641	0.9631	2.4376	1.4105
44	A	1154.3512	0.9762	1.7791	1.4082
45	A	1178.5730	0.8955	1.1432	3.9427
46	A	1180.1382	0.9010	1.0873	3.6587
47	A	1198.6560	0.9534	9.1926	2.5718
48	A	1202.2900	0.9600	9.4642	2.1014
49	A	1288.5377	3.2043	47.4411	10.6688
50	A	1308.1875	3.2230	48.9744	17.9953
51	A	1350.1450	5.6907	4.9654	0.8734
52	A	1354.1107	4.6668	6.5955	0.3328
53	A	1369.5167	1.4282	0.0505	0.1594
54	A	1370.4451	1.5013	0.9922	0.2480
55	A	1501.1238	3.0626	2.1891	0.7751
56	A	1501.3848	3.0627	2.9324	2.0682
57	A	1530.2949	3.2171	51.7632	1.9037
58	A	1531.1761	3.3116	49.5877	1.4073
59	A	1626.1848	8.6317	4.7239	3.6911
60	A	1630.1878	8.2634	3.7650	7.8302
61	A	1643.3931	4.7366	33.0196	29.2902
62	A	1647.5489	5.5794	49.7950	15.6695
63	A	1659.6633	2.4733	110.4969	22.0444
64	A	1679.9177	1.9912	72.3323	10.3366
65	A	3152.9355	6.3681	9.5644	58.3544
66	A	3154.9228	6.3648	12.7792	6.6242
67	A	3158.0619	6.3876	0.1691	105.5893
68	A	3166.5784	6.4185	0.2295	60.3561
69	A	3171.2654	6.4638	8.1767	123.0049
70	A	3174.1834	6.4771	9.1027	107.0982
71	A	3174.8016	6.4972	35.0696	31.5407
72	A	3182.7260	6.5263	19.4967	15.8407
73	A	3191.5173	6.5845	13.5527	237.8556
74	A	3193.6439	6.5975	9.5896	265.2646
75	A	3529.7811	7.7129	54.4106	153.3614
76	A	3550.5539	7.7826	11.0850	156.0501
77	A	3626.9848	8.4821	20.1327	33.6273
78	A	3645.0007	8.5950	16.8293	48.2797

ANL2_08

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3488	0.0007	0.1905	2.8262
2	A	27.6367	0.0020	0.5096	2.1008
3	A	36.9560	0.0036	1.2749	1.5746
4	A	66.2108	0.0103	0.4425	5.9388
5	A	68.7636	0.0109	0.2797	2.7300
6	A	128.6521	0.0505	0.2218	9.5837

7	A	232.3538	0.1135	8.4326	0.9529
8	A	233.2510	0.1160	0.1747	2.0857
9	A	319.5205	0.0650	28.1809	0.3480
10	A	345.2935	0.0775	28.0687	0.7337
11	A	389.0413	0.2427	3.3715	0.2416
12	A	395.8296	0.2589	1.0020	1.2734
13	A	419.6804	0.3082	0.6489	0.1890
14	A	421.3626	0.3040	1.1851	0.2437
15	A	508.6031	0.3813	2.0897	1.0295
16	A	513.2829	0.3888	78.2841	1.3576
17	A	539.2460	1.1219	5.2099	3.8621
18	A	539.9730	1.0882	3.1241	3.5981
19	A	636.4050	1.4905	1.9472	6.6098
20	A	636.4923	1.4869	0.7577	0.8798
21	A	671.0780	0.3658	187.2184	6.2645
22	A	701.0704	0.6529	42.5601	0.8372
23	A	706.8558	0.5396	40.3639	0.1972
24	A	717.8764	0.3810	202.5036	7.4437
25	A	766.8028	0.6395	173.4379	1.9468
26	A	772.5871	0.6496	104.0139	3.7953
27	A	830.9667	0.6000	0.7548	3.1941
28	A	833.0562	0.9844	5.9715	15.4580
29	A	835.5141	0.5654	1.6248	1.1696
30	A	840.6500	1.3504	14.6764	31.2190
31	A	887.8764	0.7106	25.0902	1.3825
32	A	897.9610	0.7059	9.5189	0.1260
33	A	970.0709	0.7482	0.1763	0.0389
34	A	972.4665	0.7492	0.2361	0.0153
35	A	984.8446	0.7198	0.1482	0.3866
36	A	989.9422	0.7361	0.6759	0.1901
37	A	1014.3962	3.5626	1.4248	43.8644
38	A	1015.7444	3.5988	0.7977	19.7613
39	A	1048.0848	1.3690	4.1868	15.7385
40	A	1049.0764	1.3811	3.5468	21.1679
41	A	1073.7673	1.0852	4.2014	0.4064
42	A	1080.2415	1.1276	6.5750	0.3458
43	A	1141.5618	0.9631	2.4378	1.4105
44	A	1154.3516	0.9762	1.7793	1.4081
45	A	1178.5725	0.8955	1.1432	3.9428
46	A	1180.1379	0.9010	1.0872	3.6587
47	A	1198.6552	0.9534	9.1925	2.5718
48	A	1202.2894	0.9600	9.4643	2.1015
49	A	1288.5380	3.2043	47.4421	10.6687
50	A	1308.1885	3.2230	48.9755	17.9955
51	A	1350.1438	5.6908	4.9654	0.8735
52	A	1354.1101	4.6669	6.5957	0.3328
53	A	1369.5159	1.4282	0.0505	0.1594
54	A	1370.4445	1.5013	0.9922	0.2480
55	A	1501.1229	3.0626	2.1888	0.7759
56	A	1501.3845	3.0627	2.9325	2.0675
57	A	1530.2945	3.2171	51.7680	1.9038
58	A	1531.1756	3.3116	49.5840	1.4071
59	A	1626.1842	8.6317	4.7241	3.6912
60	A	1630.1875	8.2634	3.7654	7.8302
61	A	1643.3917	4.7363	33.0133	29.2862
62	A	1647.5481	5.5795	49.8012	15.6735
63	A	1659.6621	2.4734	110.5004	22.0446
64	A	1679.9180	1.9912	72.3316	10.3366
65	A	3152.9388	6.3681	9.5638	58.3502
66	A	3154.9238	6.3648	12.7798	6.6254
67	A	3158.0624	6.3876	0.1691	105.5737
68	A	3166.5795	6.4185	0.2296	60.3476
69	A	3171.2653	6.4638	8.1733	123.0135
70	A	3174.1843	6.4771	9.1017	107.1167
71	A	3174.8028	6.4973	35.0697	31.5397
72	A	3182.7248	6.5263	19.4994	15.8384
73	A	3191.5181	6.5845	13.5533	237.8631
74	A	3193.6451	6.5975	9.5908	265.2578
75	A	3529.7809	7.7129	54.4169	153.3611
76	A	3550.5608	7.7827	11.0861	156.0531
77	A	3626.9857	8.4821	20.1347	33.6278

78 A 3645.0098 8.5950 16.8302 48.2791

ANL2_09

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3213	0.0007	0.1909	2.8241
2	A	27.6697	0.0020	0.5107	2.1156
3	A	36.9487	0.0036	1.2778	1.5772
4	A	66.3021	0.0104	0.4442	5.9311
5	A	68.7785	0.0109	0.2780	2.7445
6	A	128.7779	0.0506	0.2235	9.5725
7	A	232.3560	0.1133	8.4542	0.9430
8	A	233.2854	0.1162	0.1612	2.0797
9	A	319.6607	0.0651	28.1406	0.3478
10	A	345.6331	0.0777	27.9958	0.7367
11	A	389.0768	0.2425	3.4061	0.2425
12	A	395.9115	0.2587	1.0115	1.2753
13	A	419.6891	0.3082	0.6495	0.1905
14	A	421.3626	0.3039	1.1940	0.2428
15	A	508.6083	0.3813	2.0347	1.0221
16	A	513.2844	0.3887	78.4290	1.3641
17	A	539.2425	1.1219	5.2176	3.8548
18	A	539.9797	1.0882	3.1273	3.6024
19	A	636.4003	1.4856	2.1241	6.6395
20	A	636.4885	1.4889	0.6893	0.8490
21	A	670.3011	0.3648	187.6802	6.2781
22	A	701.1268	0.6524	41.2010	0.8015
23	A	706.8465	0.5404	40.5932	0.1967
24	A	718.2496	0.3818	202.0794	7.4398
25	A	766.7485	0.6390	170.9257	1.9418
26	A	772.7277	0.6502	107.2846	3.8054
27	A	830.9833	0.6021	0.7648	3.2728
28	A	833.0387	0.9816	5.9626	15.4100
29	A	835.5090	0.5648	1.6340	1.1529
30	A	840.6862	1.3471	14.8478	31.2073
31	A	887.9145	0.7107	25.2097	1.3946
32	A	897.9511	0.7058	9.4357	0.1281
33	A	970.0814	0.7482	0.1772	0.0393
34	A	972.4661	0.7492	0.2359	0.0153
35	A	984.8605	0.7198	0.1487	0.3887
36	A	989.9506	0.7362	0.6756	0.1902
37	A	1014.4067	3.5622	1.4160	44.0234
38	A	1015.7385	3.5985	0.8078	19.5983
39	A	1048.0823	1.3690	4.1858	15.7306
40	A	1049.0770	1.3811	3.5489	21.1749
41	A	1073.7267	1.0850	4.1983	0.4070
42	A	1080.2979	1.1278	6.5870	0.3489
43	A	1141.5212	0.9631	2.4399	1.4141
44	A	1154.4548	0.9765	1.7889	1.4061
45	A	1178.5743	0.8955	1.1413	3.9417
46	A	1180.1410	0.9010	1.0887	3.6612
47	A	1198.6407	0.9534	9.1872	2.5732
48	A	1202.2906	0.9600	9.4714	2.1002
49	A	1288.5616	3.2045	47.5436	10.6430
50	A	1308.0958	3.2232	48.9104	18.0244
51	A	1350.1365	5.6932	4.9748	0.8762
52	A	1354.1125	4.6596	6.5908	0.3345
53	A	1369.5149	1.4281	0.0495	0.1605
54	A	1370.4544	1.5020	1.0028	0.2486
55	A	1501.1262	3.0627	2.1834	0.7821
56	A	1501.3825	3.0623	2.9362	2.0607
57	A	1530.2938	3.2174	51.9994	1.9121
58	A	1531.1602	3.3110	49.3716	1.3968
59	A	1626.2041	8.6296	4.7353	3.6898
60	A	1630.1831	8.2603	3.7621	7.8311
61	A	1643.3650	4.7140	32.8251	29.1299
62	A	1647.5310	5.5679	49.8719	15.7697
63	A	1659.5862	2.4828	110.7402	22.1272
64	A	1679.9557	1.9906	72.1333	10.3030

65	A	3152.9251	6.3681	9.5719	58.3828
66	A	3154.9284	6.3649	12.7755	6.6270
67	A	3158.0660	6.3876	0.1687	105.5293
68	A	3166.5805	6.4185	0.2289	60.4227
69	A	3171.2644	6.4638	8.1690	123.0203
70	A	3174.1883	6.4771	9.1443	107.0616
71	A	3174.8090	6.4973	35.0592	31.5318
72	A	3182.7389	6.5263	19.4750	15.8535
73	A	3191.5132	6.5845	13.5474	237.8874
74	A	3193.6432	6.5975	9.5854	265.3641
75	A	3529.3923	7.7115	54.8733	153.2681
76	A	3550.7689	7.7835	11.1194	156.3930
77	A	3626.7392	8.4806	20.2131	33.7405
78	A	3645.3546	8.5969	16.9045	48.2469

ANL2_10

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3213	0.0007	0.1909	2.8240
2	A	27.6697	0.0020	0.5107	2.1157
3	A	36.9487	0.0036	1.2778	1.5772
4	A	66.3023	0.0104	0.4442	5.9311
5	A	68.7784	0.0109	0.2780	2.7445
6	A	128.7777	0.0506	0.2235	9.5724
7	A	232.3559	0.1133	8.4542	0.9430
8	A	233.2855	0.1162	0.1612	2.0797
9	A	319.6609	0.0651	28.1404	0.3478
10	A	345.6330	0.0777	27.9959	0.7367
11	A	389.0768	0.2425	3.4061	0.2425
12	A	395.9117	0.2587	1.0115	1.2753
13	A	419.6891	0.3082	0.6495	0.1905
14	A	421.3626	0.3039	1.1940	0.2428
15	A	508.6084	0.3813	2.0348	1.0221
16	A	513.2844	0.3887	78.4284	1.3641
17	A	539.2425	1.1219	5.2176	3.8548
18	A	539.9796	1.0882	3.1273	3.6024
19	A	636.4003	1.4856	2.1238	6.6395
20	A	636.4886	1.4889	0.6894	0.8490
21	A	670.3027	0.3648	187.6798	6.2781
22	A	701.1269	0.6524	41.1973	0.8015
23	A	706.8465	0.5404	40.5935	0.1967
24	A	718.2507	0.3818	202.0779	7.4398
25	A	766.7487	0.6390	170.9241	1.9418
26	A	772.7282	0.6502	107.2909	3.8055
27	A	830.9833	0.6021	0.7648	3.2731
28	A	833.0387	0.9815	5.9628	15.4098
29	A	835.5090	0.5648	1.6339	1.1529
30	A	840.6863	1.3471	14.8484	31.2074
31	A	887.9146	0.7107	25.2101	1.3947
32	A	897.9512	0.7058	9.4357	0.1281
33	A	970.0815	0.7482	0.1772	0.0393
34	A	972.4662	0.7492	0.2359	0.0153
35	A	984.8605	0.7198	0.1487	0.3887
36	A	989.9507	0.7362	0.6756	0.1902
37	A	1014.4067	3.5622	1.4160	44.0236
38	A	1015.7385	3.5985	0.8077	19.5981
39	A	1048.0823	1.3690	4.1858	15.7306
40	A	1049.0769	1.3811	3.5489	21.1749
41	A	1073.7269	1.0850	4.1984	0.4070
42	A	1080.2980	1.1278	6.5871	0.3489
43	A	1141.5213	0.9631	2.4399	1.4141
44	A	1154.4551	0.9765	1.7889	1.4061
45	A	1178.5743	0.8955	1.1413	3.9417
46	A	1180.1410	0.9010	1.0887	3.6612
47	A	1198.6407	0.9534	9.1872	2.5732
48	A	1202.2906	0.9600	9.4714	2.1002
49	A	1288.5612	3.2045	47.5435	10.6430
50	A	1308.0956	3.2232	48.9102	18.0244
51	A	1350.1365	5.6932	4.9748	0.8762

52	A	1354.1125	4.6596	6.5908	0.3345
53	A	1369.5149	1.4281	0.0495	0.1605
54	A	1370.4545	1.5020	1.0029	0.2486
55	A	1501.1262	3.0627	2.1834	0.7821
56	A	1501.3826	3.0623	2.9363	2.0607
57	A	1530.2937	3.2174	51.9994	1.9121
58	A	1531.1602	3.3110	49.3713	1.3967
59	A	1626.2042	8.6296	4.7352	3.6899
60	A	1630.1832	8.2603	3.7620	7.8311
61	A	1643.3650	4.7140	32.8251	29.1300
62	A	1647.5310	5.5679	49.8719	15.7697
63	A	1659.5861	2.4828	110.7400	22.1272
64	A	1679.9558	1.9906	72.1327	10.3029
65	A	3152.9251	6.3681	9.5720	58.3828
66	A	3154.9284	6.3649	12.7755	6.6270
67	A	3158.0660	6.3876	0.1687	105.5292
68	A	3166.5806	6.4185	0.2289	60.4234
69	A	3171.2644	6.4638	8.1689	123.0205
70	A	3174.1884	6.4771	9.1442	107.0590
71	A	3174.8090	6.4973	35.0595	31.5335
72	A	3182.7391	6.5263	19.4748	15.8536
73	A	3191.5132	6.5845	13.5474	237.8870
74	A	3193.6432	6.5975	9.5854	265.3648
75	A	3529.3919	7.7115	54.8740	153.2687
76	A	3550.7684	7.7835	11.1194	156.3927
77	A	3626.7388	8.4806	20.2134	33.7407
78	A	3645.3540	8.5969	16.9044	48.2468

ANL2_11

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.9210	0.0001	0.3980	8.2021
2	A	30.1358	0.0021	0.3266	6.5250
3	A	35.8132	0.0040	0.0062	3.5232
4	A	55.8549	0.0085	0.0499	0.6729
5	A	65.6995	0.0107	0.5339	0.6943
6	A	109.4388	0.0374	1.5483	2.7722
7	A	221.9287	0.1023	1.9515	0.5632
8	A	234.3831	0.1196	2.2666	0.9284
9	A	306.6802	0.0585	17.2242	0.1979
10	A	380.2881	0.1860	5.2836	0.6300
11	A	398.2555	0.2206	3.9593	0.4838
12	A	407.6983	0.1797	28.0726	1.8636
13	A	414.8046	0.2778	2.1418	0.1460
14	A	422.2255	0.2261	16.9019	0.4966
15	A	509.1508	0.3901	39.1207	0.2444
16	A	517.4387	0.4024	12.6513	0.1474
17	A	539.8296	1.0855	2.9545	5.0436
18	A	540.1107	1.0737	0.9374	3.6788
19	A	636.5688	1.5194	0.0985	3.0036
20	A	637.4478	1.5124	0.9546	5.0905
21	A	661.8198	0.3105	223.0399	4.4157
22	A	695.1649	0.4628	171.3902	4.5746
23	A	701.8474	0.4503	35.0768	1.2433
24	A	703.0473	0.5225	27.4745	0.2025
25	A	760.6230	0.6340	55.3384	1.2386
26	A	769.9015	0.6410	131.2348	2.9333
27	A	825.1742	0.5052	0.7616	0.6817
28	A	831.5745	0.5267	0.7274	1.0506
29	A	833.0228	1.5777	3.7024	19.7816
30	A	835.4865	1.6448	2.0956	27.2331
31	A	883.8452	0.7145	3.9493	0.3393
32	A	894.9292	0.7060	14.4877	0.6758
33	A	962.7917	0.7281	0.1474	0.0883
34	A	973.0733	0.7570	0.0452	0.0345
35	A	981.1463	0.7241	0.0186	0.3321
36	A	991.6442	0.7387	0.1965	0.5855
37	A	1013.1336	3.5544	4.4932	39.7500
38	A	1016.6218	3.6253	0.5290	21.5423

39	A	1048.4286	1.3847	3.8934	15.7373
40	A	1049.8169	1.3794	3.3923	21.6996
41	A	1071.8755	1.0768	4.5711	0.0726
42	A	1074.5744	1.0839	4.0246	0.1102
43	A	1139.7774	0.9602	2.1797	2.3443
44	A	1143.2581	0.9581	0.9104	3.7608
45	A	1177.7623	0.8933	2.0736	4.6978
46	A	1181.9961	0.9044	1.2080	3.5173
47	A	1200.9568	0.9577	20.2493	1.9384
48	A	1201.9777	0.9585	2.0927	2.7624
49	A	1286.4340	3.2091	32.6176	10.5822
50	A	1305.6603	3.2519	70.9676	15.0020
51	A	1350.3776	5.7085	4.6150	1.2092
52	A	1351.0862	5.7861	10.7245	1.9949
53	A	1368.3122	1.4213	0.0692	0.1795
54	A	1368.8982	1.4331	0.0660	0.1487
55	A	1499.6485	3.0906	2.1671	0.4799
56	A	1501.6342	3.0609	3.4852	1.3845
57	A	1530.4957	3.2255	20.8525	1.7330
58	A	1531.1690	3.2772	86.5363	1.9284
59	A	1624.3913	8.7662	1.5679	7.4527
60	A	1632.6002	9.0196	3.5904	4.1901
61	A	1644.2665	5.3577	28.3281	20.8073
62	A	1648.1252	5.8479	51.0518	21.1861
63	A	1660.6592	2.2694	94.2321	19.2885
64	A	1681.8492	1.9921	107.2328	14.8588
65	A	3147.5471	6.3431	13.3487	61.0024
66	A	3158.3482	6.3908	9.0394	43.7564
67	A	3161.5931	6.4058	3.9993	67.3729
68	A	3161.9387	6.4025	0.5698	82.3500
69	A	3169.7108	6.4653	33.0934	87.0823
70	A	3174.9870	6.4725	3.5529	127.7455
71	A	3181.9236	6.5247	21.2409	29.7533
72	A	3188.3976	6.5653	20.3424	184.1835
73	A	3196.3010	6.6073	8.8560	222.7976
74	A	3210.5504	6.6262	0.0832	238.3505
75	A	3508.8333	7.6509	231.9460	288.1428
76	A	3546.7204	7.7672	12.4269	161.6814
77	A	3638.8163	8.5629	16.4631	53.1067
78	A	3641.5189	8.5404	62.0541	91.7860

ANL2_12

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	7.9284	0.0001	0.3978	8.2011
2	A	30.1361	0.0021	0.3268	6.5255
3	A	35.8122	0.0040	0.0062	3.5229
4	A	55.8575	0.0085	0.0500	0.6737
5	A	65.6962	0.0107	0.5337	0.6943
6	A	109.4395	0.0374	1.5486	2.7721
7	A	221.9291	0.1023	1.9515	0.5633
8	A	234.3829	0.1196	2.2666	0.9284
9	A	306.6766	0.0585	17.2171	0.1979
10	A	380.2854	0.1860	5.2843	0.6299
11	A	398.2557	0.2206	3.9542	0.4840
12	A	407.6969	0.1797	28.0754	1.8631
13	A	414.8045	0.2778	2.1405	0.1459
14	A	422.2252	0.2261	16.8987	0.4965
15	A	509.1508	0.3901	39.1219	0.2443
16	A	517.4391	0.4024	12.6513	0.1473
17	A	539.8294	1.0856	2.9542	5.0407
18	A	540.1108	1.0737	0.9377	3.6816
19	A	636.5687	1.5194	0.0985	3.0037
20	A	637.4476	1.5124	0.9546	5.0901
21	A	661.8145	0.3105	222.9980	4.4159
22	A	695.1620	0.4627	171.4404	4.5764
23	A	701.8470	0.4504	35.0528	1.2419
24	A	703.0472	0.5225	27.4757	0.2026
25	A	760.6221	0.6340	55.3355	1.2385

26	A	769.9012	0.6410	131.2357	2.9332
27	A	825.1746	0.5052	0.7614	0.6818
28	A	831.5750	0.5267	0.7267	1.0492
29	A	833.0223	1.5778	3.7027	19.7852
30	A	835.4868	1.6448	2.0952	27.2312
31	A	883.8450	0.7145	3.9491	0.3392
32	A	894.9297	0.7060	14.4872	0.6756
33	A	962.7920	0.7281	0.1474	0.0883
34	A	973.0736	0.7570	0.0452	0.0345
35	A	981.1464	0.7241	0.0187	0.3320
36	A	991.6448	0.7387	0.1966	0.5854
37	A	1013.1334	3.5544	4.4935	39.7493
38	A	1016.6215	3.6253	0.5290	21.5420
39	A	1048.4278	1.3847	3.8934	15.7374
40	A	1049.8162	1.3794	3.3923	21.6997
41	A	1071.8752	1.0768	4.5692	0.0726
42	A	1074.5735	1.0838	4.0257	0.1102
43	A	1139.7772	0.9602	2.1794	2.3441
44	A	1143.2574	0.9581	0.9110	3.7609
45	A	1177.7619	0.8933	2.0738	4.6978
46	A	1181.9961	0.9044	1.2081	3.5172
47	A	1200.9570	0.9577	20.2507	1.9386
48	A	1201.9780	0.9585	2.0920	2.7624
49	A	1286.4344	3.2091	32.6169	10.5820
50	A	1305.6621	3.2519	70.9690	15.0024
51	A	1350.3773	5.7085	4.6147	1.2093
52	A	1351.0857	5.7860	10.7245	1.9944
53	A	1368.3121	1.4213	0.0692	0.1795
54	A	1368.8981	1.4331	0.0660	0.1488
55	A	1499.6484	3.0906	2.1668	0.4798
56	A	1501.6348	3.0609	3.4852	1.3846
57	A	1530.4952	3.2255	20.8517	1.7328
58	A	1531.1688	3.2772	86.5367	1.9289
59	A	1624.3900	8.7662	1.5682	7.4525
60	A	1632.5989	9.0196	3.5903	4.1901
61	A	1644.2670	5.3576	28.3284	20.8073
62	A	1648.1257	5.8475	51.0476	21.1845
63	A	1660.6588	2.2695	94.2317	19.2894
64	A	1681.8492	1.9921	107.2396	14.8584
65	A	3147.5450	6.3431	13.3497	61.0059
66	A	3158.3484	6.3908	9.0403	43.7424
67	A	3161.5893	6.4058	4.0020	67.3047
68	A	3161.9376	6.4025	0.5673	82.4290
69	A	3169.7099	6.4653	33.0926	87.0841
70	A	3174.9860	6.4725	3.5519	127.7425
71	A	3181.9228	6.5247	21.2410	29.7557
72	A	3188.3973	6.5653	20.3426	184.1791
73	A	3196.3001	6.6073	8.8559	222.7964
74	A	3210.5483	6.6262	0.0833	238.3504
75	A	3508.8360	7.6509	231.9617	288.1500
76	A	3546.7227	7.7672	12.4271	161.6803
77	A	3638.8190	8.5629	16.4632	53.1059
78	A	3641.5219	8.5404	62.0568	91.7857

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3937	0.0006	2.0331	1.6087
2	A	20.4568	0.0011	1.1224	3.4780
3	A	29.3915	0.0025	0.8001	5.1301
4	A	51.5870	0.0070	0.1811	4.4140
5	A	69.6112	0.0104	0.0513	2.2512
6	A	92.9714	0.0223	0.0888	6.5204
7	A	223.4053	0.0869	15.9938	2.2629
8	A	228.6460	0.1105	3.8863	2.1084
9	A	292.3774	0.0536	19.3162	0.6657
10	A	303.3873	0.0569	11.5924	0.2466
11	A	345.0341	0.0960	263.4817	2.4597
12	A	385.6917	0.2477	1.1632	0.3500

13	A	389.4243	0.2623	3.1393	1.1366
14	A	418.1621	0.3048	0.0967	0.1009
15	A	421.5399	0.3124	1.3392	0.3064
16	A	504.6585	0.3499	78.1866	0.8017
17	A	514.2912	0.4235	4.3707	0.7445
18	A	538.6122	1.0885	4.8872	3.6208
19	A	540.6351	1.0175	0.3931	4.9136
20	A	609.2502	0.3083	194.8880	6.2254
21	A	636.5298	1.5066	1.2588	1.6529
22	A	636.8406	1.4592	2.6247	5.3104
23	A	699.1717	0.5658	16.3870	0.3803
24	A	704.3040	0.5635	42.0468	0.4327
25	A	758.7732	0.6100	130.1861	2.0078
26	A	759.3687	0.6014	9.8431	2.0902
27	A	825.7643	0.5086	0.8676	0.8280
28	A	831.1770	0.5672	1.5208	2.6392
29	A	834.4377	1.3337	4.2300	16.0086
30	A	837.2491	1.8977	4.5493	25.7545
31	A	880.0533	0.6945	9.9942	0.3023
32	A	891.7929	0.6952	13.3669	0.1710
33	A	965.5552	0.7310	0.3227	0.1177
34	A	967.7289	0.7423	0.3159	0.0904
35	A	982.7152	0.7162	0.0255	0.2190
36	A	983.2649	0.7219	1.3473	0.1844
37	A	1012.3480	3.5921	3.4446	36.9717
38	A	1014.4432	3.6052	1.4958	26.0693
39	A	1048.5545	1.3753	3.7362	8.0468
40	A	1048.7421	1.3735	3.2149	28.6726
41	A	1053.6940	1.0117	1.0357	0.1542
42	A	1071.6540	1.0790	3.9547	0.5364
43	A	1130.2136	0.9731	5.3480	1.6946
44	A	1140.2727	0.9611	2.6909	2.0768
45	A	1178.0829	0.8952	1.4142	4.4692
46	A	1178.9856	0.8947	1.2604	3.1376
47	A	1200.7387	0.9572	10.8555	1.8455
48	A	1201.3209	0.9586	12.6972	2.6875
49	A	1296.7345	3.2070	50.6847	14.7365
50	A	1317.5480	3.1726	57.3428	12.4130
51	A	1351.6348	5.9293	8.0674	0.9401
52	A	1352.1806	6.3308	5.8601	0.1802
53	A	1366.7399	1.4225	0.1148	0.3177
54	A	1368.1239	1.4249	0.0093	0.1149
55	A	1499.5907	3.1240	1.9521	1.9983
56	A	1500.7821	3.0890	1.1953	0.6254
57	A	1530.6151	3.2571	44.9843	1.7797
58	A	1533.0558	3.3203	61.9905	2.6756
59	A	1622.8889	8.8420	4.3895	3.3981
60	A	1628.3983	8.0334	4.6415	6.7102
61	A	1642.3419	3.5701	18.3171	17.2655
62	A	1644.4273	3.6195	6.7458	3.4078
63	A	1659.6016	2.6747	114.7671	26.0421
64	A	1661.0508	2.7913	193.4126	33.8060
65	A	3150.5555	6.3542	10.6036	54.8417
66	A	3155.5566	6.3669	11.8966	6.9182
67	A	3158.7784	6.3917	0.4103	114.5995
68	A	3162.3079	6.4003	0.1677	69.5745
69	A	3170.6859	6.4646	22.4603	103.2231
70	A	3172.7797	6.4715	8.9499	117.8387
71	A	3175.6283	6.5008	27.7403	17.7448
72	A	3180.4573	6.5141	19.8955	19.3968
73	A	3190.2543	6.5829	11.6257	232.5054
74	A	3192.3156	6.5871	12.1025	269.3392
75	A	3560.4530	7.8229	9.3998	183.4542
76	A	3598.7826	7.9839	29.4213	165.6382
77	A	3659.1268	8.6674	15.3617	49.0092
78	A	3707.3325	8.9214	20.3848	42.6374

ANL2_14

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
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1	A	12.3916	0.0004	0.5002	0.0000
2	A	36.4828	0.0038	0.0000	6.7216
3	A	46.9066	0.0070	0.0000	4.1302
4	A	53.8455	0.0070	1.4373	0.0000
5	A	59.2135	0.0076	0.9063	0.0000
6	A	106.1410	0.0289	0.0000	10.5142
7	A	228.0582	0.1118	0.0000	1.7171
8	A	230.0496	0.1084	11.1254	0.0000
9	A	280.1550	0.0480	42.3048	0.0000
10	A	281.1536	0.0484	0.0001	0.3127
11	A	384.1142	0.2577	0.4244	0.0000
12	A	384.1433	0.2575	0.0000	1.1768
13	A	412.7637	0.2931	0.6809	0.0000
14	A	417.6921	0.3004	0.0000	0.1747
15	A	499.6744	0.3263	0.0000	1.5541
16	A	504.5674	0.3406	131.7666	0.0000
17	A	538.0630	1.0719	0.0000	5.6470
18	A	538.8462	1.0972	7.2179	0.0000
19	A	593.8535	0.2938	0.0003	14.6849
20	A	603.3890	0.2995	369.3771	0.0000
21	A	636.0335	1.5152	0.4919	0.0000
22	A	637.1509	1.5102	0.0000	5.0343
23	A	698.1139	0.5269	66.6982	0.0000
24	A	698.9045	0.5464	0.0000	0.2480
25	A	757.5247	0.6417	151.9413	0.0000
26	A	761.3120	0.6283	0.0000	4.5258
27	A	821.2756	0.5053	0.0000	1.3283
28	A	823.6237	0.5046	2.3217	0.0000
29	A	833.7390	1.7484	0.0000	38.9324
30	A	833.9841	1.8083	6.3983	0.0000
31	A	882.9873	0.6992	0.0000	1.2940
32	A	883.9340	0.6934	20.0452	0.0000
33	A	965.4181	0.7438	0.6891	0.0000
34	A	966.5333	0.7442	0.0000	0.4488
35	A	985.5058	0.7333	0.0000	1.3381
36	A	985.7318	0.7331	0.7027	0.0000
37	A	1015.1665	3.5239	2.7067	0.0000
38	A	1015.3184	3.5280	0.0000	50.6312
39	A	1049.7729	1.3771	0.0000	33.2287
40	A	1050.2715	1.3737	5.3423	0.0000
41	A	1067.6465	1.0588	0.0000	0.1618
42	A	1067.8654	1.0585	5.5844	0.0000
43	A	1136.9479	0.9576	6.1444	0.0020
44	A	1136.9676	0.9566	0.0032	3.8988
45	A	1178.5384	0.8942	0.0000	6.8677
46	A	1178.7567	0.8954	2.8708	0.0000
47	A	1199.7217	0.9533	14.4514	0.0000
48	A	1200.6657	0.9562	0.0000	5.1104
49	A	1296.6870	3.2218	104.3964	0.0000
50	A	1297.6773	3.1996	0.0001	25.3198
51	A	1351.3767	6.0224	11.6762	0.0000
52	A	1353.4645	6.0216	0.0000	3.3297
53	A	1366.4675	1.4228	0.0696	0.0000
54	A	1366.5206	1.4278	0.0000	0.2627
55	A	1500.3066	3.1055	3.5479	0.0000
56	A	1501.0792	3.1101	0.0000	2.9824
57	A	1530.6909	3.2757	0.0000	2.3664
58	A	1531.5877	3.2774	102.7579	0.0000
59	A	1629.7949	9.0129	8.5700	0.0000
60	A	1629.8974	8.9665	0.0000	5.8934
61	A	1644.5911	4.1262	0.0000	22.4327
62	A	1645.8422	4.1056	27.8104	0.0000
63	A	1661.5586	2.4466	277.7600	0.0000
64	A	1662.3582	2.4386	0.0000	48.9290
65	A	3149.5512	6.3509	21.4574	0.0183
66	A	3149.5603	6.3510	0.0032	121.4232
67	A	3163.4793	6.4101	15.6588	0.0002
68	A	3163.6388	6.4118	0.0000	54.0100
69	A	3168.6813	6.4558	0.0000	277.4664
70	A	3168.8912	6.4566	23.8361	0.0001

71	A	3181.0938	6.5112	0.0000	61.9109
72	A	3181.3465	6.5117	42.3431	0.0000
73	A	3195.6318	6.6033	0.0000	354.5824
74	A	3195.8869	6.6038	18.1135	0.0001
75	A	3565.1075	7.8439	28.2990	1.0946
76	A	3565.1616	7.8443	0.0805	385.2400
77	A	3662.0341	8.6803	3.5446	95.1226
78	A	3662.0449	8.6804	23.3209	14.4588

ANL2_15

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	12.3908	0.0004	0.5002	0.0000
2	A	36.4810	0.0038	0.0000	6.7214
3	A	46.9055	0.0070	0.0000	4.1303
4	A	53.8440	0.0070	1.4375	0.0000
5	A	59.2124	0.0076	0.9061	0.0000
6	A	106.1405	0.0289	0.0000	10.5140
7	A	228.0584	0.1118	0.0000	1.7172
8	A	230.0488	0.1084	11.1254	0.0000
9	A	280.1561	0.0480	42.3054	0.0000
10	A	281.1549	0.0484	0.0000	0.3127
11	A	384.1143	0.2577	0.4244	0.0000
12	A	384.1434	0.2575	0.0000	1.1768
13	A	412.7636	0.2931	0.6809	0.0000
14	A	417.6918	0.3004	0.0000	0.1747
15	A	499.6742	0.3263	0.0000	1.5541
16	A	504.5673	0.3406	131.7684	0.0000
17	A	538.0630	1.0719	0.0000	5.6470
18	A	538.8463	1.0972	7.2176	0.0000
19	A	593.8516	0.2938	0.0001	14.6848
20	A	603.3875	0.2995	369.3746	0.0000
21	A	636.0336	1.5152	0.4919	0.0000
22	A	637.1509	1.5102	0.0000	5.0343
23	A	698.1140	0.5269	66.6985	0.0000
24	A	698.9044	0.5464	0.0000	0.2480
25	A	757.5243	0.6417	151.9404	0.0000
26	A	761.3117	0.6283	0.0000	4.5258
27	A	821.2757	0.5053	0.0000	1.3282
28	A	823.6236	0.5046	2.3215	0.0000
29	A	833.7391	1.7484	0.0000	38.9324
30	A	833.9842	1.8083	6.3983	0.0000
31	A	882.9872	0.6992	0.0000	1.2938
32	A	883.9339	0.6934	20.0457	0.0000
33	A	965.4181	0.7438	0.6892	0.0000
34	A	966.5334	0.7442	0.0000	0.4488
35	A	985.5056	0.7333	0.0000	1.3382
36	A	985.7316	0.7331	0.7026	0.0000
37	A	1015.1666	3.5239	2.7067	0.0001
38	A	1015.3184	3.5280	0.0000	50.6308
39	A	1049.7733	1.3771	0.0000	33.2290
40	A	1050.2719	1.3737	5.3423	0.0000
41	A	1067.6466	1.0588	0.0000	0.1618
42	A	1067.8655	1.0585	5.5844	0.0000
43	A	1136.9479	0.9576	6.1451	0.0016
44	A	1136.9676	0.9566	0.0025	3.8992
45	A	1178.5385	0.8942	0.0000	6.8677
46	A	1178.7568	0.8954	2.8708	0.0000
47	A	1199.7220	0.9533	14.4515	0.0000
48	A	1200.6659	0.9562	0.0000	5.1104
49	A	1296.6876	3.2218	104.3959	0.0000
50	A	1297.6777	3.1996	0.0000	25.3199
51	A	1351.3771	6.0224	11.6760	0.0000
52	A	1353.4647	6.0216	0.0000	3.3295
53	A	1366.4675	1.4228	0.0696	0.0000
54	A	1366.5207	1.4278	0.0000	0.2627
55	A	1500.3067	3.1055	3.5479	0.0000
56	A	1501.0793	3.1101	0.0000	2.9823
57	A	1530.6912	3.2757	0.0000	2.3665

58	A	1531.5880	3.2774	102.7575	0.0000
59	A	1629.7951	9.0129	8.5702	0.0001
60	A	1629.8976	8.9665	0.0002	5.8932
61	A	1644.5911	4.1261	0.0000	22.4326
62	A	1645.8424	4.1055	27.8085	0.0000
63	A	1661.5587	2.4466	277.7620	0.0000
64	A	1662.3583	2.4386	0.0000	48.9294
65	A	3149.5512	6.3509	21.4479	0.0716
66	A	3149.5602	6.3510	0.0126	121.3702
67	A	3163.4793	6.4101	15.6598	0.0000
68	A	3163.6387	6.4118	0.0000	54.0072
69	A	3168.6812	6.4558	0.0000	277.4698
70	A	3168.8911	6.4566	23.8364	0.0000
71	A	3181.0943	6.5112	0.0001	61.9159
72	A	3181.3469	6.5117	42.3419	0.0001
73	A	3195.6324	6.6033	0.0001	354.5780
74	A	3195.8875	6.6038	18.1138	0.0016
75	A	3565.1073	7.8439	28.3691	0.1389
76	A	3565.1611	7.8443	0.0102	386.1956
77	A	3662.0352	8.6803	0.7752	106.4196
78	A	3662.0436	8.6804	26.0904	3.1619

ANL2_16

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3487	0.0007	0.1905	2.8260
2	A	27.6344	0.0020	0.5097	2.1012
3	A	36.9569	0.0036	1.2749	1.5744
4	A	66.2112	0.0103	0.4425	5.9391
5	A	68.7652	0.0109	0.2798	2.7296
6	A	128.6497	0.0505	0.2217	9.5835
7	A	232.3536	0.1135	8.4328	0.9529
8	A	233.2505	0.1160	0.1747	2.0859
9	A	319.5182	0.0650	28.1787	0.3480
10	A	345.2827	0.0775	28.0721	0.7337
11	A	389.0401	0.2427	3.3706	0.2416
12	A	395.8289	0.2589	1.0024	1.2734
13	A	419.6803	0.3082	0.6488	0.1890
14	A	421.3628	0.3040	1.1850	0.2437
15	A	508.6029	0.3813	2.0902	1.0296
16	A	513.2830	0.3888	78.2857	1.3576
17	A	539.2460	1.1219	5.2104	3.8622
18	A	539.9729	1.0882	3.1244	3.5980
19	A	636.4050	1.4905	1.9479	6.6099
20	A	636.4923	1.4869	0.7574	0.8796
21	A	671.0755	0.3658	187.2146	6.2645
22	A	701.0697	0.6529	42.5899	0.8380
23	A	706.8560	0.5396	40.3660	0.1973
24	A	717.8704	0.3810	202.5006	7.4436
25	A	766.8033	0.6395	173.4443	1.9468
26	A	772.5858	0.6496	103.9817	3.7951
27	A	830.9671	0.6000	0.7541	3.1962
28	A	833.0559	0.9843	5.9726	15.4571
29	A	835.5149	0.5654	1.6248	1.1689
30	A	840.6497	1.3504	14.6734	31.2181
31	A	887.8763	0.7106	25.0883	1.3824
32	A	897.9615	0.7059	9.5192	0.1260
33	A	970.0721	0.7482	0.1763	0.0389
34	A	972.4673	0.7492	0.2361	0.0153
35	A	984.8457	0.7198	0.1481	0.3866
36	A	989.9429	0.7361	0.6759	0.1901
37	A	1014.3961	3.5626	1.4248	43.8615
38	A	1015.7446	3.5988	0.7977	19.7642
39	A	1048.0850	1.3690	4.1869	15.7378
40	A	1049.0763	1.3811	3.5468	21.1688
41	A	1073.7673	1.0852	4.2012	0.4064
42	A	1080.2408	1.1276	6.5750	0.3458
43	A	1141.5619	0.9631	2.4379	1.4105
44	A	1154.3499	0.9762	1.7792	1.4082

45	A	1178.5728	0.8955	1.1432	3.9427
46	A	1180.1383	0.9010	1.0873	3.6587
47	A	1198.6557	0.9534	9.1927	2.5718
48	A	1202.2898	0.9600	9.4645	2.1014
49	A	1288.5367	3.2043	47.4419	10.6692
50	A	1308.1889	3.2231	48.9757	17.9949
51	A	1350.1443	5.6908	4.9653	0.8734
52	A	1354.1104	4.6669	6.5959	0.3328
53	A	1369.5163	1.4282	0.0505	0.1594
54	A	1370.4446	1.5013	0.9922	0.2480
55	A	1501.1235	3.0626	2.1889	0.7754
56	A	1501.3846	3.0627	2.9324	2.0679
57	A	1530.2945	3.2171	51.7631	1.9036
58	A	1531.1758	3.3116	49.5890	1.4074
59	A	1626.1842	8.6317	4.7241	3.6912
60	A	1630.1873	8.2634	3.7654	7.8302
61	A	1643.3921	4.7360	33.0102	29.2843
62	A	1647.5484	5.5791	49.7988	15.6732
63	A	1659.6611	2.4735	110.5024	22.0460
64	A	1679.9158	1.9912	72.3348	10.3373
65	A	3152.9386	6.3681	9.5633	58.3462
66	A	3154.9221	6.3648	12.7796	6.6228
67	A	3158.0610	6.3876	0.1689	105.5880
68	A	3166.5781	6.4185	0.2295	60.3623
69	A	3171.2644	6.4638	8.1755	123.0091
70	A	3174.1832	6.4771	9.1000	107.0796
71	A	3174.8009	6.4972	35.0743	31.5568
72	A	3182.7254	6.5263	19.4972	15.8397
73	A	3191.5166	6.5845	13.5528	237.8553
74	A	3193.6433	6.5975	9.5892	265.2674
75	A	3529.7911	7.7129	54.4122	153.3637
76	A	3550.5622	7.7827	11.0861	156.0470
77	A	3626.9952	8.4822	20.1345	33.6270
78	A	3645.0120	8.5951	16.8304	48.2792

ANL2_17

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3479	0.0007	0.1905	2.8261
2	A	27.6343	0.0020	0.5097	2.1010
3	A	36.9561	0.0036	1.2748	1.5744
4	A	66.2105	0.0103	0.4425	5.9391
5	A	68.7641	0.0109	0.2798	2.7297
6	A	128.6498	0.0505	0.2217	9.5837
7	A	232.3537	0.1135	8.4325	0.9530
8	A	233.2502	0.1160	0.1748	2.0859
9	A	319.5185	0.0650	28.1800	0.3480
10	A	345.2858	0.0775	28.0720	0.7337
11	A	389.0402	0.2427	3.3708	0.2416
12	A	395.8286	0.2589	1.0023	1.2734
13	A	419.6803	0.3082	0.6488	0.1890
14	A	421.3626	0.3040	1.1851	0.2437
15	A	508.6030	0.3813	2.0897	1.0295
16	A	513.2829	0.3888	78.2838	1.3576
17	A	539.2461	1.1219	5.2100	3.8622
18	A	539.9730	1.0882	3.1242	3.5981
19	A	636.4050	1.4905	1.9462	6.6094
20	A	636.4923	1.4869	0.7579	0.8801
21	A	671.0842	0.3658	187.2123	6.2644
22	A	701.0699	0.6529	42.5763	0.8377
23	A	706.8558	0.5396	40.3642	0.1973
24	A	717.8723	0.3810	202.5043	7.4437
25	A	766.8036	0.6395	173.4598	1.9468
26	A	772.5859	0.6496	103.9811	3.7952
27	A	830.9666	0.6000	0.7545	3.1942
28	A	833.0561	0.9844	5.9721	15.4580
29	A	835.5147	0.5654	1.6249	1.1695
30	A	840.6499	1.3504	14.6740	31.2189
31	A	887.8757	0.7106	25.0890	1.3824

32	A	897.9613	0.7059	9.5197	0.1260
33	A	970.0717	0.7482	0.1763	0.0389
34	A	972.4668	0.7492	0.2360	0.0153
35	A	984.8451	0.7198	0.1481	0.3866
36	A	989.9424	0.7361	0.6759	0.1901
37	A	1014.3960	3.5626	1.4249	43.8590
38	A	1015.7447	3.5988	0.7976	19.7664
39	A	1048.0849	1.3690	4.1869	15.7381
40	A	1049.0762	1.3811	3.5468	21.1687
41	A	1073.7681	1.0852	4.2013	0.4064
42	A	1080.2408	1.1276	6.5749	0.3458
43	A	1141.5626	0.9631	2.4379	1.4105
44	A	1154.3499	0.9762	1.7792	1.4082
45	A	1178.5727	0.8955	1.1432	3.9428
46	A	1180.1381	0.9010	1.0872	3.6587
47	A	1198.6557	0.9534	9.1927	2.5718
48	A	1202.2895	0.9600	9.4643	2.1015
49	A	1288.5375	3.2043	47.4407	10.6693
50	A	1308.1903	3.2231	48.9756	17.9947
51	A	1350.1443	5.6908	4.9652	0.8734
52	A	1354.1102	4.6669	6.5960	0.3328
53	A	1369.5161	1.4282	0.0505	0.1594
54	A	1370.4446	1.5013	0.9922	0.2480
55	A	1501.1235	3.0626	2.1889	0.7753
56	A	1501.3846	3.0627	2.9323	2.0680
57	A	1530.2945	3.2171	51.7615	1.9035
58	A	1531.1761	3.3116	49.5907	1.4074
59	A	1626.1838	8.6317	4.7241	3.6912
60	A	1630.1871	8.2632	3.7654	7.8301
61	A	1643.3925	4.7363	33.0137	29.2867
62	A	1647.5487	5.5793	49.7982	15.6719
63	A	1659.6622	2.4734	110.4999	22.0452
64	A	1679.9169	1.9912	72.3351	10.3373
65	A	3152.9381	6.3681	9.5638	58.3504
66	A	3154.9234	6.3648	12.7799	6.6208
67	A	3158.0622	6.3876	0.1688	105.5895
68	A	3166.5792	6.4185	0.2295	60.3573
69	A	3171.2658	6.4638	8.1750	123.0131
70	A	3174.1844	6.4771	9.0986	107.0777
71	A	3174.8019	6.4972	35.0749	31.5583
72	A	3182.7265	6.5263	19.4976	15.8395
73	A	3191.5182	6.5845	13.5530	237.8524
74	A	3193.6446	6.5975	9.5895	265.2661
75	A	3529.7896	7.7129	54.4110	153.3647
76	A	3550.5591	7.7826	11.0858	156.0468
77	A	3626.9914	8.4822	20.1345	33.6264
78	A	3645.0074	8.5950	16.8301	48.2793

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3487	0.0007	0.1906	2.8261
2	A	27.6347	0.0020	0.5097	2.1011
3	A	36.9566	0.0036	1.2748	1.5744
4	A	66.2110	0.0103	0.4425	5.9392
5	A	68.7648	0.0109	0.2798	2.7296
6	A	128.6495	0.0505	0.2218	9.5835
7	A	232.3536	0.1135	8.4327	0.9529
8	A	233.2506	0.1160	0.1747	2.0860
9	A	319.5178	0.0650	28.1793	0.3480
10	A	345.2840	0.0775	28.0719	0.7337
11	A	389.0402	0.2427	3.3706	0.2416
12	A	395.8286	0.2589	1.0021	1.2734
13	A	419.6802	0.3082	0.6488	0.1890
14	A	421.3627	0.3040	1.1850	0.2437
15	A	508.6030	0.3813	2.0898	1.0295
16	A	513.2828	0.3888	78.2854	1.3576
17	A	539.2461	1.1219	5.2100	3.8622
18	A	539.9729	1.0882	3.1244	3.5980

19	A	636.4050	1.4905	1.9477	6.6098
20	A	636.4923	1.4869	0.7576	0.8797
21	A	671.0745	0.3658	187.2178	6.2646
22	A	701.0703	0.6529	42.5659	0.8374
23	A	706.8558	0.5396	40.3655	0.1973
24	A	717.8755	0.3810	202.4985	7.4437
25	A	766.8030	0.6395	173.4266	1.9468
26	A	772.5876	0.6496	104.0190	3.7953
27	A	830.9670	0.6000	0.7543	3.1955
28	A	833.0560	0.9844	5.9722	15.4574
29	A	835.5148	0.5654	1.6248	1.1691
30	A	840.6502	1.3503	14.6757	31.2186
31	A	887.8765	0.7106	25.0907	1.3825
32	A	897.9611	0.7059	9.5185	0.1260
33	A	970.0720	0.7482	0.1763	0.0389
34	A	972.4669	0.7492	0.2360	0.0153
35	A	984.8454	0.7198	0.1482	0.3866
36	A	989.9427	0.7361	0.6759	0.1901
37	A	1014.3962	3.5626	1.4247	43.8618
38	A	1015.7446	3.5988	0.7977	19.7635
39	A	1048.0850	1.3690	4.1868	15.7378
40	A	1049.0763	1.3811	3.5468	21.1688
41	A	1073.7672	1.0852	4.2012	0.4063
42	A	1080.2412	1.1276	6.5750	0.3458
43	A	1141.5617	0.9631	2.4380	1.4105
44	A	1154.3506	0.9762	1.7792	1.4082
45	A	1178.5727	0.8955	1.1432	3.9428
46	A	1180.1382	0.9010	1.0872	3.6587
47	A	1198.6557	0.9534	9.1926	2.5718
48	A	1202.2896	0.9600	9.4644	2.1014
49	A	1288.5374	3.2043	47.4416	10.6690
50	A	1308.1888	3.2231	48.9745	17.9951
51	A	1350.1443	5.6908	4.9652	0.8734
52	A	1354.1104	4.6668	6.5958	0.3328
53	A	1369.5160	1.4282	0.0504	0.1594
54	A	1370.4447	1.5013	0.9923	0.2480
55	A	1501.1234	3.0626	2.1889	0.7755
56	A	1501.3847	3.0627	2.9324	2.0679
57	A	1530.2945	3.2171	51.7625	1.9036
58	A	1531.1759	3.3116	49.5888	1.4074
59	A	1626.1843	8.6317	4.7240	3.6911
60	A	1630.1871	8.2633	3.7652	7.8301
61	A	1643.3923	4.7361	33.0115	29.2855
62	A	1647.5485	5.5792	49.7981	15.6725
63	A	1659.6613	2.4735	110.5028	22.0458
64	A	1679.9169	1.9912	72.3327	10.3369
65	A	3152.9369	6.3681	9.5641	58.3516
66	A	3154.9230	6.3648	12.7799	6.6206
67	A	3158.0616	6.3876	0.1687	105.5866
68	A	3166.5789	6.4185	0.2294	60.3614
69	A	3171.2651	6.4638	8.1743	123.0153
70	A	3174.1842	6.4771	9.0986	107.0597
71	A	3174.8014	6.4972	35.0768	31.5689
72	A	3182.7272	6.5263	19.4965	15.8407
73	A	3191.5177	6.5845	13.5530	237.8523
74	A	3193.6443	6.5975	9.5888	265.2665
75	A	3529.7878	7.7129	54.4106	153.3597
76	A	3550.5625	7.7827	11.0862	156.0503
77	A	3626.9897	8.4822	20.1342	33.6266
78	A	3645.0119	8.5951	16.8304	48.2795

ANL2_19

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3525	0.0007	0.1906	2.8264
2	A	27.6365	0.0020	0.5097	2.1011
3	A	36.9534	0.0036	1.2746	1.5747
4	A	66.2135	0.0103	0.4426	5.9384
5	A	68.7640	0.0109	0.2797	2.7302

6	A	128.6493	0.0505	0.2217	9.5831
7	A	232.3532	0.1135	8.4324	0.9530
8	A	233.2517	0.1160	0.1746	2.0861
9	A	319.5182	0.0650	28.1831	0.3481
10	A	345.2899	0.0775	28.0650	0.7335
11	A	389.0394	0.2427	3.3702	0.2415
12	A	395.8289	0.2589	1.0015	1.2733
13	A	419.6796	0.3082	0.6486	0.1891
14	A	421.3624	0.3040	1.1850	0.2437
15	A	508.6022	0.3813	2.0920	1.0299
16	A	513.2826	0.3888	78.2774	1.3574
17	A	539.2462	1.1219	5.2102	3.8622
18	A	539.9729	1.0882	3.1240	3.5982
19	A	636.4052	1.4906	1.9437	6.6084
20	A	636.4924	1.4868	0.7592	0.8807
21	A	671.0913	0.3658	187.1890	6.2640
22	A	701.0690	0.6529	42.5802	0.8376
23	A	706.8560	0.5396	40.3599	0.1974
24	A	717.8732	0.3810	202.5135	7.4438
25	A	766.8042	0.6395	173.4691	1.9472
26	A	772.5863	0.6496	103.9865	3.7952
27	A	830.9661	0.5999	0.7542	3.1933
28	A	833.0559	0.9846	5.9729	15.4595
29	A	835.5151	0.5654	1.6237	1.1689
30	A	840.6503	1.3504	14.6753	31.2179
31	A	887.8752	0.7106	25.0895	1.3820
32	A	897.9627	0.7059	9.5206	0.1260
33	A	970.0716	0.7482	0.1763	0.0389
34	A	972.4665	0.7492	0.2361	0.0153
35	A	984.8448	0.7198	0.1482	0.3866
36	A	989.9431	0.7361	0.6760	0.1901
37	A	1014.3962	3.5626	1.4249	43.8564
38	A	1015.7451	3.5988	0.7974	19.7674
39	A	1048.0849	1.3690	4.1866	15.7375
40	A	1049.0764	1.3811	3.5468	21.1683
41	A	1073.7679	1.0852	4.2011	0.4063
42	A	1080.2416	1.1276	6.5748	0.3458
43	A	1141.5624	0.9631	2.4379	1.4105
44	A	1154.3512	0.9762	1.7793	1.4083
45	A	1178.5724	0.8955	1.1432	3.9430
46	A	1180.1380	0.9010	1.0871	3.6584
47	A	1198.6556	0.9534	9.1928	2.5718
48	A	1202.2898	0.9600	9.4640	2.1014
49	A	1288.5344	3.2043	47.4370	10.6691
50	A	1308.1897	3.2231	48.9747	17.9939
51	A	1350.1444	5.6908	4.9648	0.8734
52	A	1354.1106	4.6667	6.5957	0.3328
53	A	1369.5164	1.4282	0.0505	0.1594
54	A	1370.4448	1.5013	0.9924	0.2480
55	A	1501.1237	3.0626	2.1892	0.7758
56	A	1501.3848	3.0627	2.9323	2.0676
57	A	1530.2944	3.2171	51.7542	1.9033
58	A	1531.1761	3.3116	49.5948	1.4075
59	A	1626.1844	8.6317	4.7239	3.6913
60	A	1630.1881	8.2635	3.7653	7.8295
61	A	1643.3924	4.7362	33.0081	29.2863
62	A	1647.5488	5.5791	49.7992	15.6719
63	A	1659.6616	2.4735	110.5053	22.0444
64	A	1679.9173	1.9912	72.3304	10.3369
65	A	3152.9373	6.3681	9.5639	58.3529
66	A	3154.9230	6.3648	12.7789	6.6260
67	A	3158.0624	6.3876	0.1692	105.5882
68	A	3166.5794	6.4185	0.2298	60.3537
69	A	3171.2658	6.4638	8.1774	122.9997
70	A	3174.1839	6.4771	9.1008	107.0934
71	A	3174.8022	6.4972	35.0699	31.5462
72	A	3182.7260	6.5263	19.4984	15.8423
73	A	3191.5175	6.5845	13.5523	237.8559
74	A	3193.6444	6.5975	9.5891	265.2502
75	A	3529.7870	7.7129	54.4156	153.3602
76	A	3550.5592	7.7826	11.0848	156.0486

77	A	3626.9915	8.4822	20.1360	33.6269
78	A	3645.0068	8.5950	16.8276	48.2800

ANL2_20

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3484	0.0007	0.1905	2.8260
2	A	27.6345	0.0020	0.5097	2.1011
3	A	36.9563	0.0036	1.2749	1.5744
4	A	66.2104	0.0103	0.4425	5.9391
5	A	68.7643	0.0109	0.2798	2.7296
6	A	128.6487	0.0505	0.2217	9.5836
7	A	232.3536	0.1135	8.4327	0.9529
8	A	233.2502	0.1160	0.1747	2.0860
9	A	319.5174	0.0650	28.1792	0.3480
10	A	345.2828	0.0775	28.0722	0.7337
11	A	389.0400	0.2427	3.3705	0.2416
12	A	395.8284	0.2589	1.0022	1.2734
13	A	419.6803	0.3082	0.6488	0.1890
14	A	421.3630	0.3040	1.1850	0.2437
15	A	508.6029	0.3813	2.0899	1.0295
16	A	513.2828	0.3888	78.2856	1.3576
17	A	539.2460	1.1219	5.2101	3.8622
18	A	539.9729	1.0882	3.1244	3.5980
19	A	636.4050	1.4904	1.9480	6.6100
20	A	636.4923	1.4869	0.7571	0.8795
21	A	671.0764	0.3658	187.2162	6.2645
22	A	701.0698	0.6529	42.5816	0.8378
23	A	706.8560	0.5396	40.3635	0.1973
24	A	717.8715	0.3810	202.5026	7.4437
25	A	766.8033	0.6395	173.4478	1.9468
26	A	772.5860	0.6496	103.9851	3.7952
27	A	830.9666	0.6000	0.7545	3.1942
28	A	833.0561	0.9845	5.9722	15.4590
29	A	835.5149	0.5654	1.6247	1.1689
30	A	840.6498	1.3504	14.6736	31.2183
31	A	887.8758	0.7106	25.0892	1.3823
32	A	897.9609	0.7059	9.5191	0.1260
33	A	970.0718	0.7482	0.1763	0.0389
34	A	972.4670	0.7492	0.2360	0.0153
35	A	984.8453	0.7198	0.1481	0.3865
36	A	989.9432	0.7361	0.6759	0.1901
37	A	1014.3961	3.5626	1.4248	43.8618
38	A	1015.7445	3.5988	0.7977	19.7640
39	A	1048.0849	1.3690	4.1868	15.7386
40	A	1049.0765	1.3811	3.5468	21.1679
41	A	1073.7672	1.0852	4.2013	0.4063
42	A	1080.2407	1.1276	6.5749	0.3458
43	A	1141.5617	0.9631	2.4379	1.4105
44	A	1154.3498	0.9762	1.7792	1.4082
45	A	1178.5726	0.8955	1.1432	3.9427
46	A	1180.1382	0.9010	1.0873	3.6587
47	A	1198.6556	0.9534	9.1927	2.5718
48	A	1202.2896	0.9600	9.4645	2.1015
49	A	1288.5376	3.2043	47.4415	10.6691
50	A	1308.1893	3.2231	48.9752	17.9949
51	A	1350.1440	5.6908	4.9652	0.8734
52	A	1354.1102	4.6668	6.5960	0.3328
53	A	1369.5162	1.4282	0.0505	0.1594
54	A	1370.4446	1.5013	0.9922	0.2480
55	A	1501.1231	3.0626	2.1888	0.7757
56	A	1501.3846	3.0627	2.9324	2.0676
57	A	1530.2947	3.2171	51.7638	1.9036
58	A	1531.1759	3.3116	49.5883	1.4073
59	A	1626.1841	8.6317	4.7239	3.6912
60	A	1630.1873	8.2633	3.7652	7.8301
61	A	1643.3920	4.7362	33.0111	29.2850
62	A	1647.5486	5.5794	49.8004	15.6736
63	A	1659.6615	2.4734	110.5014	22.0452

64	A	1679.9165	1.9912	72.3348	10.3372
65	A	3152.9377	6.3681	9.5641	58.3484
66	A	3154.9233	6.3648	12.7794	6.6239
67	A	3158.0624	6.3876	0.1690	105.5888
68	A	3166.5772	6.4185	0.2288	60.3640
69	A	3171.2658	6.4638	8.1763	123.0061
70	A	3174.1839	6.4771	9.1062	107.0881
71	A	3174.8021	6.4973	35.0698	31.5400
72	A	3182.7266	6.5263	19.4947	15.8365
73	A	3191.5179	6.5845	13.5528	237.8462
74	A	3193.6433	6.5975	9.5891	265.2841
75	A	3529.7904	7.7129	54.4102	153.3623
76	A	3550.5622	7.7827	11.0861	156.0482
77	A	3626.9924	8.4822	20.1343	33.6266
78	A	3645.0114	8.5951	16.8303	48.2792

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3464	0.0007	0.1905	2.8260
2	A	27.6334	0.0020	0.5097	2.1011
3	A	36.9563	0.0036	1.2749	1.5743
4	A	66.2094	0.0103	0.4425	5.9392
5	A	68.7629	0.0109	0.2798	2.7297
6	A	128.6482	0.0505	0.2218	9.5836
7	A	232.3532	0.1135	8.4328	0.9530
8	A	233.2498	0.1160	0.1748	2.0858
9	A	319.5201	0.0650	28.1787	0.3480
10	A	345.2869	0.0775	28.0726	0.7337
11	A	389.0405	0.2427	3.3709	0.2416
12	A	395.8289	0.2589	1.0023	1.2734
13	A	419.6803	0.3082	0.6488	0.1890
14	A	421.3623	0.3040	1.1852	0.2437
15	A	508.6030	0.3813	2.0897	1.0294
16	A	513.2827	0.3888	78.2856	1.3576
17	A	539.2460	1.1219	5.2099	3.8623
18	A	539.9730	1.0882	3.1246	3.5980
19	A	636.4050	1.4904	1.9481	6.6101
20	A	636.4923	1.4869	0.7571	0.8795
21	A	671.0766	0.3658	187.2199	6.2646
22	A	701.0700	0.6529	42.5732	0.8376
23	A	706.8553	0.5396	40.3670	0.1973
24	A	717.8725	0.3810	202.5008	7.4437
25	A	766.8027	0.6395	173.4365	1.9467
26	A	772.5862	0.6496	103.9999	3.7952
27	A	830.9664	0.5999	0.7551	3.1932
28	A	833.0561	0.9844	5.9713	15.4585
29	A	835.5139	0.5654	1.6253	1.1700
30	A	840.6498	1.3504	14.6741	31.2188
31	A	887.8757	0.7106	25.0896	1.3824
32	A	897.9601	0.7059	9.5188	0.1260
33	A	970.0716	0.7482	0.1763	0.0389
34	A	972.4664	0.7492	0.2360	0.0153
35	A	984.8451	0.7198	0.1481	0.3865
36	A	989.9420	0.7361	0.6758	0.1901
37	A	1014.3960	3.5626	1.4248	43.8600
38	A	1015.7446	3.5988	0.7977	19.7660
39	A	1048.0848	1.3690	4.1869	15.7380
40	A	1049.0762	1.3811	3.5468	21.1686
41	A	1073.7676	1.0852	4.2013	0.4063
42	A	1080.2409	1.1276	6.5751	0.3458
43	A	1141.5620	0.9631	2.4379	1.4105
44	A	1154.3503	0.9762	1.7792	1.4082
45	A	1178.5725	0.8955	1.1432	3.9427
46	A	1180.1378	0.9010	1.0872	3.6587
47	A	1198.6555	0.9534	9.1926	2.5718
48	A	1202.2893	0.9600	9.4644	2.1015
49	A	1288.5378	3.2043	47.4426	10.6691
50	A	1308.1890	3.2231	48.9750	17.9952

51	A	1350.1442	5.6908	4.9653	0.8733
52	A	1354.1099	4.6668	6.5959	0.3328
53	A	1369.5158	1.4282	0.0505	0.1594
54	A	1370.4445	1.5013	0.9923	0.2480
55	A	1501.1229	3.0626	2.1889	0.7753
56	A	1501.3842	3.0627	2.9323	2.0680
57	A	1530.2946	3.2171	51.7650	1.9037
58	A	1531.1758	3.3116	49.5873	1.4073
59	A	1626.1840	8.6317	4.7240	3.6912
60	A	1630.1875	8.2633	3.7654	7.8301
61	A	1643.3922	4.7365	33.0170	29.2883
62	A	1647.5483	5.5793	49.7960	15.6706
63	A	1659.6621	2.4734	110.4991	22.0449
64	A	1679.9163	1.9912	72.3346	10.3372
65	A	3152.9391	6.3681	9.5638	58.3493
66	A	3154.9239	6.3648	12.7797	6.6219
67	A	3158.0628	6.3876	0.1689	105.5899
68	A	3166.5799	6.4185	0.2294	60.3601
69	A	3171.2663	6.4638	8.1756	123.0102
70	A	3174.1852	6.4771	9.0982	107.0738
71	A	3174.8025	6.4972	35.0756	31.5619
72	A	3182.7276	6.5263	19.4972	15.8392
73	A	3191.5186	6.5845	13.5528	237.8552
74	A	3193.6454	6.5975	9.5894	265.2667
75	A	3529.7859	7.7129	54.4142	153.3643
76	A	3550.5601	7.7827	11.0863	156.0493
77	A	3626.9916	8.4822	20.1340	33.6278
78	A	3645.0091	8.5950	16.8308	48.2791

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	15.3473	0.0007	0.1906	2.8260
2	A	27.6341	0.0020	0.5097	2.1012
3	A	36.9561	0.0036	1.2748	1.5743
4	A	66.2104	0.0103	0.4425	5.9392
5	A	68.7640	0.0109	0.2798	2.7295
6	A	128.6489	0.0505	0.2218	9.5836
7	A	232.3534	0.1135	8.4325	0.9530
8	A	233.2505	0.1160	0.1749	2.0858
9	A	319.5187	0.0650	28.1787	0.3480
10	A	345.2836	0.0775	28.0730	0.7337
11	A	389.0401	0.2427	3.3706	0.2416
12	A	395.8287	0.2589	1.0024	1.2734
13	A	419.6802	0.3082	0.6488	0.1890
14	A	421.3627	0.3040	1.1851	0.2437
15	A	508.6029	0.3813	2.0897	1.0295
16	A	513.2828	0.3888	78.2850	1.3577
17	A	539.2461	1.1219	5.2100	3.8623
18	A	539.9729	1.0882	3.1246	3.5979
19	A	636.4050	1.4905	1.9471	6.6097
20	A	636.4923	1.4869	0.7575	0.8798
21	A	671.0803	0.3658	187.2152	6.2645
22	A	701.0700	0.6529	42.5793	0.8377
23	A	706.8561	0.5396	40.3646	0.1973
24	A	717.8720	0.3810	202.5032	7.4437
25	A	766.8032	0.6395	173.4453	1.9467
26	A	772.5860	0.6496	103.9900	3.7952
27	A	830.9666	0.6000	0.7544	3.1947
28	A	833.0561	0.9844	5.9725	15.4582
29	A	835.5146	0.5654	1.6248	1.1692
30	A	840.6500	1.3504	14.6738	31.2183
31	A	887.8758	0.7106	25.0888	1.3824
32	A	897.9613	0.7059	9.5195	0.1260
33	A	970.0719	0.7482	0.1763	0.0389
34	A	972.4665	0.7492	0.2360	0.0153
35	A	984.8454	0.7198	0.1481	0.3866
36	A	989.9424	0.7361	0.6759	0.1901
37	A	1014.3961	3.5626	1.4248	43.8597

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38	A	1015.7447	3.5988	0.7976	19.7660
39	A	1048.0849	1.3690	4.1869	15.7382
40	A	1049.0763	1.3811	3.5468	21.1684
41	A	1073.7677	1.0852	4.2013	0.4063
42	A	1080.2408	1.1276	6.5749	0.3458
43	A	1141.5623	0.9631	2.4379	1.4105
44	A	1154.3500	0.9762	1.7792	1.4082
45	A	1178.5726	0.8955	1.1432	3.9427
46	A	1180.1380	0.9010	1.0872	3.6587
47	A	1198.6558	0.9534	9.1927	2.5718
48	A	1202.2896	0.9600	9.4643	2.1014
49	A	1288.5368	3.2043	47.4415	10.6694
50	A	1308.1901	3.2231	48.9755	17.9947
51	A	1350.1446	5.6908	4.9652	0.8734
52	A	1354.1103	4.6668	6.5959	0.3328
53	A	1369.5160	1.4282	0.0505	0.1594
54	A	1370.4446	1.5013	0.9922	0.2480
55	A	1501.1234	3.0626	2.1889	0.7752
56	A	1501.3845	3.0627	2.9323	2.0681
57	A	1530.2944	3.2171	51.7608	1.9035
58	A	1531.1760	3.3116	49.5912	1.4075
59	A	1626.1840	8.6317	4.7241	3.6912
60	A	1630.1872	8.2633	3.7654	7.8301
61	A	1643.3925	4.7362	33.0132	29.2861
62	A	1647.5487	5.5792	49.7982	15.6720
63	A	1659.6618	2.4735	110.5007	22.0457
64	A	1679.9170	1.9912	72.3349	10.3372
65	A	3152.9383	6.3681	9.5646	58.3531
66	A	3154.9232	6.3648	12.7798	6.6216
67	A	3158.0620	6.3876	0.1688	105.5890
68	A	3166.5790	6.4185	0.2290	60.3541
69	A	3171.2655	6.4638	8.1749	123.0118
70	A	3174.1857	6.4771	9.0883	107.0378
71	A	3174.8017	6.4972	35.0840	31.5935
72	A	3182.7271	6.5263	19.4985	15.8351
73	A	3191.5179	6.5845	13.5529	237.8531
74	A	3193.6445	6.5975	9.5893	265.2776
75	A	3529.7899	7.7129	54.4112	153.3647
76	A	3550.5600	7.7827	11.0860	156.0462
77	A	3626.9922	8.4822	20.1345	33.6267
78	A	3645.0089	8.5950	16.8305	48.2797

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-2.0350	0.0000	0.0007	0.4966
2	A	9.7099	0.0002	0.5345	7.2144
3	A	13.1241	0.0005	0.3823	5.6546
4	A	39.2993	0.0066	0.7606	0.1207
5	A	45.2899	0.0059	1.0747	0.2040
6	A	80.4401	0.0211	2.8298	18.1499
7	A	227.8804	0.1101	0.6071	4.2722
8	A	249.0096	0.0824	0.4418	18.0332
9	A	250.9797	0.0412	0.0967	0.2194
10	A	262.0652	0.0929	0.9058	0.6595
11	A	282.4895	0.0593	0.1358	10.1317
12	A	317.7943	0.0638	7.4034	0.6193
13	A	387.5295	0.2575	0.1893	0.4500
14	A	398.2733	0.2065	0.8411	4.3454
15	A	415.2630	0.2961	0.1455	0.0185
16	A	488.8874	0.3937	21.8613	89.2683
17	A	503.6871	0.3492	58.4671	0.5855
18	A	539.5003	1.0990	5.1130	3.3634
19	A	598.9327	0.2900	299.9461	16.7083
20	A	636.7996	1.5196	0.2080	3.9396
21	A	697.6760	0.5575	30.4990	0.4243
22	A	757.2579	0.6096	87.8708	1.9110
23	A	822.5675	0.5022	0.2369	0.4003
24	A	833.6269	1.8179	3.8286	20.3569

25	A	881.1502	0.6888	13.7125	0.3928
26	A	885.5749	1.2436	3.9636	21.6237
27	A	942.6571	0.5981	0.9628	0.1567
28	A	959.5256	0.7740	0.4651	0.8098
29	A	961.7786	0.7356	0.0837	0.0652
30	A	978.1768	0.7105	0.1526	0.5146
31	A	1014.6553	3.6403	1.2476	35.8091
32	A	1038.0107	0.7591	5.4801	3.0083
33	A	1048.9372	1.3753	4.0139	18.2076
34	A	1065.7267	1.0493	2.3450	0.0870
35	A	1134.9618	0.9734	4.7700	2.5605
36	A	1137.5534	1.7325	1.1116	1.7240
37	A	1171.9223	1.4437	64.9554	32.5557
38	A	1180.0884	0.9043	1.3626	4.0485
39	A	1200.6743	0.9575	9.5096	3.3017
40	A	1232.4108	1.2171	56.8172	30.5761
41	A	1295.9880	3.2221	67.3320	15.5941
42	A	1349.6780	5.9334	4.4971	1.6685
43	A	1355.8321	1.4417	0.8466	2.6323
44	A	1367.9945	1.4241	0.0018	0.1645
45	A	1407.2279	1.4719	11.7453	2.1721
46	A	1422.3253	1.4567	6.2637	3.5200
47	A	1481.7991	1.3506	3.2880	6.7478
48	A	1487.3170	1.3622	0.3070	9.4872
49	A	1494.6287	1.3717	13.7558	12.9228
50	A	1501.2088	3.0793	1.9380	1.6706
51	A	1506.3947	1.3980	5.1086	1.7476
52	A	1531.4525	3.2456	61.5750	2.1366
53	A	1630.5369	9.0027	4.6569	4.2042
54	A	1645.3634	4.2278	32.3833	23.1109
55	A	1661.8143	2.3929	131.7247	27.7147
56	A	3007.0022	5.5662	12.8821	43.0602
57	A	3012.4781	5.5830	71.4626	582.7441
58	A	3076.0636	6.0767	11.5873	155.1754
59	A	3077.7390	6.0864	3.3186	12.7523
60	A	3097.6461	6.1612	13.7875	113.2687
61	A	3112.2216	6.2891	12.2497	30.4971
62	A	3120.4509	6.3045	24.2931	49.6918
63	A	3153.8976	6.3645	15.6136	9.1575
64	A	3155.4338	6.3810	1.5656	96.1241
65	A	3169.2794	6.4509	5.2302	138.8077
66	A	3174.9720	6.4968	30.1545	29.0320
67	A	3190.9271	6.5833	13.0998	260.9123
68	A	3565.7516	7.8465	19.6145	184.7435
69	A	3664.3350	8.6951	17.5316	48.2901

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.2564	0.0000	0.0153	0.5027
2	A	9.4347	0.0002	0.5224	7.5966
3	A	13.3226	0.0005	0.3924	5.0328
4	A	38.5768	0.0061	0.6818	0.2484
5	A	45.7095	0.0063	1.1356	0.1356
6	A	80.4072	0.0211	2.8462	17.9121
7	A	227.8385	0.1103	0.6326	4.5168
8	A	248.6559	0.0800	0.4922	16.9602
9	A	250.6483	0.0410	0.0686	0.3596
10	A	263.0292	0.0977	0.6288	0.8834
11	A	282.1757	0.0594	0.1234	10.3886
12	A	316.6993	0.0628	7.8901	0.5035
13	A	387.0425	0.2549	0.2039	0.4393
14	A	398.7781	0.2083	1.0366	4.3809
15	A	415.2505	0.2958	0.1617	0.0460
16	A	489.0907	0.3948	20.0207	89.6524
17	A	503.5819	0.3482	59.7448	0.5616
18	A	539.4687	1.0994	5.1188	3.4229
19	A	598.9294	0.2900	298.5736	16.8324
20	A	636.8179	1.5197	0.2073	3.9216

21	A	697.5672	0.5571	30.5906	0.4769
22	A	757.2629	0.6096	87.7694	1.9357
23	A	822.5097	0.5021	0.2513	0.4098
24	A	833.6136	1.8174	3.8452	20.3980
25	A	881.1873	0.6889	13.6775	0.3957
26	A	885.5665	1.2446	4.1156	20.9822
27	A	942.5586	0.5980	0.9847	0.1999
28	A	959.4935	0.7738	0.4730	0.8050
29	A	961.6729	0.7354	0.0872	0.0663
30	A	978.1074	0.7104	0.1560	0.5048
31	A	1014.6861	3.6410	1.2504	35.6245
32	A	1038.2149	0.7599	5.6344	3.5629
33	A	1048.9549	1.3753	4.0151	18.2125
34	A	1065.7722	1.0494	2.3641	0.0741
35	A	1135.0233	0.9673	5.0455	1.9552
36	A	1137.5364	1.7515	0.7655	2.1303
37	A	1171.8984	1.4442	65.2677	32.3814
38	A	1180.0920	0.9043	1.3604	4.0019
39	A	1200.6919	0.9575	9.4637	3.3096
40	A	1232.4866	1.2164	56.9498	30.9789
41	A	1295.9304	3.2217	67.0937	15.5585
42	A	1349.6912	5.9327	4.5068	1.6115
43	A	1355.6710	1.4422	0.9127	2.7715
44	A	1368.0101	1.4241	0.0023	0.1703
45	A	1407.2157	1.4714	11.7580	2.1495
46	A	1422.3858	1.4570	5.9941	3.8662
47	A	1481.7671	1.3507	3.4019	6.4879
48	A	1487.1768	1.3620	0.3670	9.6157
49	A	1494.5526	1.3716	13.7097	12.5717
50	A	1501.2194	3.0786	2.0127	1.7263
51	A	1506.2368	1.3978	5.4065	1.7795
52	A	1531.4624	3.2455	61.5538	2.1524
53	A	1630.5595	9.0031	4.6072	4.2242
54	A	1645.3683	4.2213	32.4031	22.9060
55	A	1661.8027	2.3950	131.2508	27.8894
56	A	3006.9627	5.5663	12.7115	42.6020
57	A	3012.4481	5.5831	72.1873	585.1951
58	A	3075.8150	6.0763	11.5231	149.5859
59	A	3077.7485	6.0862	3.4702	18.2229
60	A	3097.7297	6.1608	14.0556	111.1718
61	A	3112.4563	6.2894	12.0192	30.5269
62	A	3120.4995	6.3052	24.0276	47.7878
63	A	3153.8694	6.3646	15.4202	10.7109
64	A	3155.4682	6.3809	1.7668	94.8029
65	A	3169.2731	6.4509	5.2559	138.8464
66	A	3174.9610	6.4968	30.1622	29.1223
67	A	3190.9139	6.5832	13.1292	261.3771
68	A	3565.7623	7.8465	19.5042	184.8640
69	A	3664.3295	8.6950	17.5294	48.4959

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.5148	0.0001	0.3459	0.2829
2	A	10.7842	0.0007	0.0276	1.5405
3	A	15.0008	0.0012	0.1111	1.5692
4	A	21.3717	0.0013	0.0022	5.4390
5	A	47.4921	0.0130	0.0831	2.9511
6	A	57.3906	0.0124	0.3714	1.1244
7	A	80.9316	0.0754	0.1241	0.0169
8	A	106.7738	0.0473	5.6179	8.1820
9	A	120.0371	0.1081	10.5152	7.5674
10	A	160.0349	0.2843	1.0285	2.2744
11	A	220.2511	0.5286	1.0851	2.0529
12	A	235.8806	0.4164	5.9086	50.0350
13	A	247.7488	0.1616	1.3816	0.1401
14	A	256.7718	0.6706	1.8847	3.7983
15	A	275.5193	0.7360	3.9246	3.8947
16	A	302.4539	0.9573	1.7825	0.8531

17	A	324.4975	1.1301	0.4546	2.3197
18	A	345.6812	0.2666	2.3565	0.9544
19	A	351.5715	0.1366	5.8298	0.4277
20	A	394.0062	1.2314	0.6886	2.2108
21	A	409.9111	0.2749	0.1765	0.4055
22	A	422.3956	0.2227	1.7731	0.4161
23	A	461.7503	2.0210	2.5237	4.5534
24	A	508.1462	0.3983	24.1689	4.9743
25	A	527.7465	2.9347	9.1282	0.7178
26	A	540.7115	1.0853	1.2207	5.3582
27	A	578.3796	3.5154	0.5976	8.8832
28	A	613.3350	3.8272	5.3243	1.2379
29	A	636.6881	1.5224	0.1316	4.1086
30	A	644.5515	4.2767	7.8776	10.8970
31	A	699.0823	0.5870	37.8982	2.5293
32	A	732.4641	0.4675	74.1397	71.2366
33	A	741.5766	3.0592	51.0423	6.1115
34	A	781.0279	0.6650	281.1328	52.8639
35	A	827.3827	0.5073	0.2359	0.2950
36	A	834.5500	1.2805	12.3154	33.7576
37	A	874.7515	5.1096	168.9463	45.1614
38	A	894.4891	0.7120	15.1445	1.4010
39	A	967.1106	0.7462	0.0664	0.0232
40	A	987.5002	0.7326	0.1381	0.7902
41	A	1017.4339	4.1941	47.8745	19.4940
42	A	1018.2063	6.5128	172.5316	47.4454
43	A	1049.5819	1.3813	3.6325	17.5401
44	A	1074.5043	1.0717	3.5292	0.0367
45	A	1100.0921	9.5151	89.3855	9.1021
46	A	1103.7847	9.4568	7.0990	1.0962
47	A	1139.7299	0.9580	4.7188	1.5046
48	A	1153.2288	10.2447	136.1136	8.4154
49	A	1182.6797	0.9121	0.3988	4.3909
50	A	1188.2007	10.8828	460.7453	5.8402
51	A	1201.5787	0.9875	14.7485	4.7258
52	A	1202.3964	8.3407	311.2999	4.7602
53	A	1231.2671	10.9659	170.5480	21.2480
54	A	1277.5654	3.2316	47.2708	40.9294
55	A	1318.1556	12.7438	59.9507	12.9703
56	A	1349.3473	5.5572	1.8917	3.2373
57	A	1369.9279	1.4335	0.0395	0.1043
58	A	1502.7436	3.0463	3.3624	2.0288
59	A	1530.9420	3.1939	56.0429	1.6485
60	A	1636.5523	9.1081	4.1157	4.8385
61	A	1645.4154	4.3420	29.6094	42.5860
62	A	1658.5296	2.3112	100.3506	28.4631
63	A	3157.4513	6.3855	13.5406	18.5847
64	A	3158.3823	6.3967	2.3327	79.5855
65	A	3173.3235	6.4647	3.0873	124.3463
66	A	3180.2768	6.5174	20.8047	41.1383
67	A	3194.5373	6.5997	10.4178	263.1253
68	A	3538.0659	7.7314	20.4621	182.5084
69	A	3629.5513	8.5185	19.2160	47.1451

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.5117	0.0001	0.3459	0.2831
2	A	10.7845	0.0007	0.0277	1.5402
3	A	15.0017	0.0012	0.1111	1.5690
4	A	21.3762	0.0013	0.0022	5.4386
5	A	47.4939	0.0130	0.0831	2.9516
6	A	57.3930	0.0124	0.3714	1.1249
7	A	80.9317	0.0754	0.1241	0.0169
8	A	106.7772	0.0473	5.6154	8.1790
9	A	120.0380	0.1081	10.5180	7.5695
10	A	160.0351	0.2843	1.0285	2.2744
11	A	220.2512	0.5286	1.0851	2.0528
12	A	235.8816	0.4165	5.9085	50.0343

13	A	247.7508	0.1616	1.3827	0.1404
14	A	256.7721	0.6706	1.8846	3.7979
15	A	275.5194	0.7360	3.9246	3.8949
16	A	302.4537	0.9573	1.7824	0.8531
17	A	324.4976	1.1301	0.4546	2.3197
18	A	345.6830	0.2669	2.3534	0.9548
19	A	351.5747	0.1366	5.8322	0.4272
20	A	394.0064	1.2315	0.6886	2.2110
21	A	409.9129	0.2749	0.1764	0.4053
22	A	422.3995	0.2227	1.7739	0.4162
23	A	461.7505	2.0209	2.5239	4.5534
24	A	508.1470	0.3983	24.1673	4.9741
25	A	527.7463	2.9347	9.1281	0.7178
26	A	540.7115	1.0853	1.2206	5.3582
27	A	578.3797	3.5154	0.5976	8.8832
28	A	613.3351	3.8272	5.3243	1.2379
29	A	636.6880	1.5224	0.1316	4.1086
30	A	644.5514	4.2767	7.8776	10.8968
31	A	699.0833	0.5870	37.8976	2.5294
32	A	732.4653	0.4675	74.1382	71.2364
33	A	741.5766	3.0589	51.0441	6.1106
34	A	781.0273	0.6650	281.1334	52.8617
35	A	827.3839	0.5073	0.2359	0.2950
36	A	834.5499	1.2806	12.3150	33.7569
37	A	874.7518	5.1096	168.9475	45.1611
38	A	894.4891	0.7120	15.1440	1.4007
39	A	967.1118	0.7462	0.0664	0.0232
40	A	987.5010	0.7326	0.1381	0.7902
41	A	1017.4339	4.1941	47.8708	19.4946
42	A	1018.2063	6.5129	172.5339	47.4446
43	A	1049.5821	1.3813	3.6325	17.5400
44	A	1074.5037	1.0717	3.5291	0.0367
45	A	1100.0908	9.5151	89.3996	9.1007
46	A	1103.7859	9.4568	7.0886	1.0968
47	A	1139.7298	0.9580	4.7188	1.5047
48	A	1153.2296	10.2447	136.1105	8.4155
49	A	1182.6797	0.9121	0.3988	4.3909
50	A	1188.2002	10.8828	460.7628	5.8394
51	A	1201.5792	0.9875	14.7371	4.7261
52	A	1202.3973	8.3433	311.2863	4.7608
53	A	1231.2664	10.9659	170.5576	21.2474
54	A	1277.5657	3.2316	47.2713	40.9280
55	A	1318.1563	12.7439	59.9503	12.9703
56	A	1349.3473	5.5573	1.8918	3.2372
57	A	1369.9281	1.4335	0.0395	0.1043
58	A	1502.7435	3.0463	3.3623	2.0288
59	A	1530.9421	3.1939	56.0428	1.6484
60	A	1636.5522	9.1081	4.1158	4.8385
61	A	1645.4154	4.3420	29.6092	42.5840
62	A	1658.5296	2.3112	100.3520	28.4632
63	A	3157.4511	6.3855	13.5398	18.5917
64	A	3158.3823	6.3967	2.3338	79.5786
65	A	3173.3235	6.4647	3.0871	124.3467
66	A	3180.2768	6.5174	20.8047	41.1386
67	A	3194.5375	6.5997	10.4180	263.1241
68	A	3538.0685	7.7314	20.4627	182.5094
69	A	3629.5540	8.5185	19.2161	47.1450

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.9100	0.0000	0.2089	0.2713
2	A	13.1703	0.0008	0.0067	3.1369
3	A	18.1557	0.0010	0.1977	3.2007
4	A	26.3500	0.0036	0.1106	2.6224
5	A	46.6729	0.0130	0.0746	2.9500
6	A	54.7673	0.0126	0.4059	1.0394
7	A	74.9384	0.0509	0.0012	0.0120
8	A	106.5756	0.0436	7.7229	10.9100

9	A	116.2344	0.1067	7.2080	3.5415
10	A	156.9533	0.3651	5.5407	18.2594
11	A	213.6580	0.4784	2.5228	0.2172
12	A	231.0259	0.5904	0.1027	0.0034
13	A	244.5438	0.1448	5.5803	23.4180
14	A	262.1637	0.6348	0.0390	1.3990
15	A	264.2697	0.6276	2.0982	29.7213
16	A	286.5344	0.8872	3.4519	1.1855
17	A	336.6112	1.2449	0.6137	1.3063
18	A	349.7720	0.0978	8.2052	0.2282
19	A	371.2247	1.5191	0.0128	0.8868
20	A	378.7739	1.2283	0.2107	0.4743
21	A	409.8958	0.2705	0.1528	0.2416
22	A	423.1997	0.2188	1.6613	0.1635
23	A	506.7065	2.5169	1.8449	0.3600
24	A	508.1780	0.3996	24.9806	6.2223
25	A	526.5418	2.9158	6.6564	3.0092
26	A	540.8327	1.0870	1.5039	5.9335
27	A	579.5281	3.4155	7.0167	13.5400
28	A	596.1350	3.7630	0.0749	2.2396
29	A	636.6838	1.5224	0.1234	4.2428
30	A	665.7056	4.4047	44.5633	0.7944
31	A	699.0253	0.5891	40.7128	3.9233
32	A	724.3291	2.8555	120.1671	77.1971
33	A	733.9359	0.4670	80.2662	45.2441
34	A	780.6591	0.6726	292.4266	69.7632
35	A	806.5128	4.9314	78.0038	35.7788
36	A	827.6287	0.5076	0.1839	0.3005
37	A	834.7023	1.2733	8.3503	33.5915
38	A	894.2171	0.7021	20.6910	4.2015
39	A	967.5914	0.7470	0.0678	0.0276
40	A	987.2939	0.7316	0.1103	0.9484
41	A	1017.4482	3.6817	0.3277	37.1847
42	A	1049.4552	1.3931	6.7567	23.1645
43	A	1053.6872	8.0857	33.3230	77.5411
44	A	1074.6801	1.0727	3.5130	0.0249
45	A	1110.5575	9.6016	56.8530	0.4123
46	A	1111.8797	9.9033	241.7368	1.4577
47	A	1139.8751	0.9580	5.0222	1.4995
48	A	1166.6392	10.4040	89.7187	0.6971
49	A	1182.6258	0.9298	6.5351	4.8701
50	A	1182.6788	8.8360	282.6032	16.9312
51	A	1201.5528	0.9591	7.1958	6.0624
52	A	1207.4790	11.2950	415.4870	1.0600
53	A	1245.9210	10.9610	92.7295	25.5552
54	A	1277.6502	3.2949	68.0331	45.6966
55	A	1300.4488	11.7802	199.9867	6.6493
56	A	1349.2984	5.5473	1.9160	3.6734
57	A	1369.9351	1.4336	0.0353	0.0974
58	A	1502.6899	3.0456	3.2749	2.1541
59	A	1530.8916	3.1942	58.1397	1.9798
60	A	1636.3209	9.0997	4.1973	4.8186
61	A	1645.3846	4.4152	31.9996	49.5999
62	A	1658.7224	2.2917	100.6425	29.7047
63	A	3157.3889	6.3849	14.0902	16.6258
64	A	3158.3125	6.3965	2.1122	81.9007
65	A	3173.1950	6.4643	3.1346	125.6285
66	A	3180.1265	6.5169	21.0972	42.0543
67	A	3194.4108	6.5991	10.6812	266.9506
68	A	3538.1809	7.7320	20.0270	182.4460
69	A	3629.6619	8.5191	19.2248	46.2240

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.7089	0.0000	0.0636	0.2505
2	A	14.9611	0.0012	0.0032	3.3074
3	A	17.3010	0.0009	0.1938	3.3086
4	A	26.4547	0.0037	0.1130	2.4845

5	A	43.6369	0.0109	0.1672	3.4224
6	A	54.6967	0.0126	0.4020	1.0531
7	A	74.9541	0.0513	0.0011	0.0202
8	A	108.3954	0.0383	13.2850	16.2546
9	A	115.2856	0.1636	1.6336	0.5351
10	A	157.5770	0.3776	6.6035	18.6581
11	A	213.6074	0.4783	2.5344	0.2201
12	A	231.2676	0.5917	0.0872	0.0066
13	A	246.2149	0.1359	2.8370	12.9804
14	A	261.5805	0.8567	4.4034	49.2035
15	A	261.8284	0.6370	0.1678	2.6327
16	A	286.5503	0.8897	5.1041	0.9860
17	A	336.6495	1.2465	1.2588	2.1890
18	A	350.0785	0.0986	8.0089	0.1534
19	A	371.3064	1.5195	0.0965	1.1896
20	A	378.7850	1.2333	0.1979	0.6908
21	A	410.3297	0.2725	0.1293	0.1812
22	A	424.1102	0.2168	1.6857	0.1519
23	A	506.6732	2.4913	1.8604	0.3108
24	A	508.0346	0.3998	27.5467	9.3461
25	A	526.5533	2.8741	8.1727	3.4036
26	A	540.8893	1.0892	1.7319	6.2465
27	A	579.3384	3.4283	6.6128	16.8834
28	A	596.1117	3.7627	0.1058	2.2063
29	A	636.6744	1.5224	0.1247	4.3693
30	A	665.2021	4.2124	64.0612	1.0077
31	A	698.8916	0.5924	41.5652	5.0147
32	A	723.0745	1.8911	182.9633	95.4284
33	A	735.8544	0.5164	39.0164	42.8863
34	A	780.8667	0.7071	315.6604	82.3160
35	A	808.5836	3.7077	37.1384	13.9665
36	A	827.7414	0.5078	0.1278	0.3200
37	A	835.0380	1.2448	9.2749	35.3860
38	A	894.2511	0.7029	21.1701	4.8579
39	A	967.8748	0.7476	0.0629	0.0309
40	A	987.2588	0.7311	0.1018	1.0342
41	A	1017.3925	3.6812	0.3717	39.3750
42	A	1049.4139	1.3932	3.0717	25.3509
43	A	1053.9306	8.0704	25.9951	88.6945
44	A	1074.9228	1.0739	3.5467	0.0332
45	A	1111.2068	9.6708	102.9176	0.6778
46	A	1111.6003	9.8119	169.0805	0.5817
47	A	1140.0226	0.9581	6.3133	1.3938
48	A	1165.2333	10.3655	97.6904	0.6616
49	A	1182.5943	0.9126	1.0180	4.8327
50	A	1182.7278	10.7398	318.2302	17.7743
51	A	1201.4697	0.9589	6.5798	6.2277
52	A	1208.3250	11.3079	413.5761	1.0539
53	A	1246.5071	11.0507	46.9525	12.1052
54	A	1277.8560	3.2814	104.3609	47.7166
55	A	1300.5895	11.8747	204.6924	6.0455
56	A	1349.3372	5.5374	1.9628	4.0265
57	A	1369.9421	1.4340	0.0372	0.0970
58	A	1502.6769	3.0451	3.2266	2.2568
59	A	1530.9011	3.1952	62.3764	1.8168
60	A	1636.2842	9.0973	4.2740	4.8138
61	A	1645.4453	4.4781	35.4871	55.0102
62	A	1658.9601	2.2759	103.6697	29.8457
63	A	3157.5263	6.3855	14.5483	16.4365
64	A	3158.4787	6.3970	2.2033	82.0439
65	A	3173.2732	6.4647	3.1683	126.5141
66	A	3180.2047	6.5172	21.2639	44.3069
67	A	3194.4671	6.5993	11.0545	275.3956
68	A	3537.9840	7.7314	18.7247	177.4003
69	A	3629.2209	8.5167	19.1634	43.7432

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
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1	A	13.2228	0.0003	0.4487	2.0085
2	A	18.0242	0.0007	0.6623	2.9648
3	A	30.2872	0.0028	0.4131	2.0430
4	A	42.7825	0.0044	0.6318	1.7338
5	A	53.5924	0.0069	0.5126	2.1525
6	A	68.4071	0.0165	0.5134	5.5551
7	A	129.5014	0.0223	0.0819	0.4073
8	A	198.1943	0.0375	0.2088	1.9060
9	A	229.5660	0.1108	3.0812	1.7407
10	A	270.0972	0.0632	0.6865	1.7554
11	A	303.5440	0.0565	10.8252	0.0885
12	A	386.1820	0.2573	0.1745	0.4926
13	A	388.1049	0.2068	1.0868	4.3390
14	A	414.7538	0.2969	0.2099	0.0117
15	A	500.9224	0.3453	63.3294	12.7382
16	A	504.8170	0.4409	19.4625	24.3833
17	A	538.3805	1.0663	7.0941	3.1758
18	A	583.3585	0.2873	189.9776	8.2831
19	A	636.7505	1.5181	0.2255	3.0578
20	A	697.7849	0.5658	29.8906	0.3453
21	A	757.7558	0.6092	85.6162	2.6938
22	A	771.1785	0.4446	7.8013	5.5060
23	A	824.2815	0.5053	0.9696	0.3995
24	A	828.4891	0.5669	4.3962	2.6729
25	A	834.4791	1.8243	3.1340	19.8373
26	A	882.7104	0.6837	9.6930	0.3651
27	A	887.6006	0.9313	3.6425	3.2483
28	A	964.7233	0.7405	0.0409	0.0319
29	A	984.0655	0.7215	0.1459	0.3898
30	A	1014.9926	3.6308	1.6546	27.3622
31	A	1027.2378	0.8070	1.0255	2.8040
32	A	1046.0998	0.8533	1.3886	1.4140
33	A	1049.3251	1.3633	2.8427	16.7350
34	A	1065.7401	1.0522	2.2990	0.1143
35	A	1088.5694	1.4741	1.4124	2.9507
36	A	1135.7954	0.9619	4.1311	1.9524
37	A	1179.8008	0.9025	1.4524	3.4272
38	A	1200.8876	0.9580	8.2229	2.9866
39	A	1216.9806	1.2351	6.9004	5.7158
40	A	1228.1913	1.2037	32.7710	8.8731
41	A	1298.0452	2.8225	37.6147	12.6824
42	A	1307.5927	1.2136	34.7257	5.2324
43	A	1350.4088	5.9606	4.6209	0.9208
44	A	1368.0278	1.4240	0.0063	0.1879
45	A	1375.9254	1.5784	3.3202	0.4024
46	A	1419.9377	1.4780	5.0886	0.6166
47	A	1473.1583	1.4034	4.2315	11.1666
48	A	1478.5670	1.3852	5.0369	9.5599
49	A	1498.9241	1.3834	14.1218	4.0289
50	A	1500.9396	2.9795	2.8924	1.7069
51	A	1507.9333	1.4379	2.4760	2.5757
52	A	1532.0259	3.2593	50.3710	1.1591
53	A	1629.7628	8.9741	3.6437	3.7471
54	A	1645.2282	4.2591	20.4028	14.4091
55	A	1662.6772	2.3902	133.2143	23.2489
56	A	2991.4035	5.6383	34.0348	252.4383
57	A	3025.1408	5.6103	19.1248	155.9400
58	A	3051.9847	5.9757	8.9207	68.4748
59	A	3086.4133	6.1535	21.2733	71.2321
60	A	3092.6327	5.9786	24.9549	117.6769
61	A	3113.6167	6.2816	14.2480	36.2066
62	A	3154.0235	6.3644	13.0073	9.3043
63	A	3155.7494	6.3933	3.0039	96.2549
64	A	3155.9436	6.5033	2.9891	64.8507
65	A	3169.4047	6.4524	4.9004	137.7824
66	A	3174.6838	6.4960	29.1230	20.9587
67	A	3191.0037	6.5832	10.9668	223.7322
68	A	3568.6543	7.8589	21.6620	192.4562
69	A	3667.2497	8.7091	17.0409	53.7081

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.2816	0.0000	0.0019	0.1939
2	A	9.9519	0.0002	0.4447	6.8384
3	A	15.3350	0.0007	0.3164	4.5744
4	A	36.7746	0.0052	0.5002	0.7618
5	A	52.6381	0.0061	1.5256	0.2552
6	A	82.3354	0.0223	3.1825	18.9072
7	A	125.8756	0.0212	0.2966	0.7343
8	A	195.5415	0.0364	0.4761	2.8302
9	A	228.9185	0.1121	0.4467	5.2222
10	A	270.2525	0.0649	0.1843	6.7672
11	A	318.2993	0.0628	8.2075	0.3070
12	A	387.0566	0.2183	0.1298	12.7956
13	A	388.4637	0.2356	0.3201	5.9930
14	A	415.1541	0.2957	0.1506	0.0113
15	A	502.1498	0.4747	1.0150	90.6187
16	A	503.7954	0.3514	63.4666	3.8158
17	A	539.6252	1.1032	4.8005	3.3904
18	A	609.7444	0.2972	323.5645	23.0573
19	A	636.8017	1.5198	0.2056	4.0934
20	A	697.4880	0.5575	30.1315	0.4264
21	A	757.6263	0.6102	91.2293	2.2122
22	A	772.1031	0.4463	8.9643	5.8365
23	A	822.6353	0.5027	0.3161	0.4065
24	A	826.7305	0.5577	3.9312	4.5218
25	A	833.5039	1.8038	4.1612	20.6888
26	A	881.6313	0.6883	12.6925	0.2272
27	A	889.0688	0.9454	3.9573	5.6707
28	A	961.5518	0.7352	0.0817	0.0802
29	A	977.9056	0.7100	0.1488	0.5461
30	A	1014.8049	3.6426	1.1593	37.9878
31	A	1027.4536	0.8157	1.6868	3.3911
32	A	1048.2305	0.8455	0.4070	2.8700
33	A	1048.9909	1.3755	4.2661	18.9036
34	A	1066.6109	1.0524	2.4938	0.0640
35	A	1089.0122	1.4887	2.2655	4.5660
36	A	1135.5248	0.9608	5.4055	1.8681
37	A	1180.2263	0.9047	1.3530	4.1939
38	A	1200.7142	0.9576	9.5946	3.4047
39	A	1219.2696	1.2469	4.1574	11.5989
40	A	1228.6601	1.1969	51.9900	23.2004
41	A	1294.6848	3.0971	82.4299	16.7562
42	A	1308.6579	1.1707	29.4260	5.6817
43	A	1349.6570	5.8996	4.3811	1.8689
44	A	1368.1487	1.4247	0.0036	0.1622
45	A	1376.2877	1.5724	6.3404	1.3596
46	A	1416.3438	1.4834	11.9075	1.0777
47	A	1473.0998	1.4039	3.3335	15.0536
48	A	1480.0638	1.3856	3.8139	14.9089
49	A	1499.7670	1.3847	8.9625	6.6694
50	A	1501.3063	3.0757	2.0138	1.7639
51	A	1507.5855	1.4151	6.0645	3.6409
52	A	1531.4276	3.2431	64.7278	1.8640
53	A	1630.8742	9.0052	4.6880	4.3446
54	A	1645.4396	4.2498	34.9976	25.5035
55	A	1661.8085	2.3833	132.8519	28.6918
56	A	2994.0793	5.6474	32.3881	298.7552
57	A	3024.6133	5.5916	23.8843	189.6613
58	A	3050.6769	5.9758	8.2057	88.3553
59	A	3086.0755	6.1048	15.6540	112.3070
60	A	3090.4019	6.0220	35.4639	88.4635
61	A	3099.5653	6.2350	30.5072	35.7209
62	A	3151.6147	6.4949	5.3265	57.2200
63	A	3154.0306	6.3655	16.3743	9.4023
64	A	3155.5053	6.3815	1.6473	97.8004
65	A	3169.4552	6.4514	5.1181	139.7168
66	A	3175.2381	6.4978	29.9697	31.8895
67	A	3191.1321	6.5842	13.4478	270.5583

68	A	3563.9009	7.8388	17.2799	179.5540
69	A	3661.8645	8.6822	17.2229	46.6296

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.1740	0.0001	0.2129	1.3044
2	A	12.4458	0.0004	0.3083	4.5191
3	A	13.0689	0.0003	0.2878	6.6235
4	A	36.4781	0.0062	0.3744	0.4547
5	A	49.5284	0.0040	0.8890	0.0872
6	A	82.7769	0.0225	2.9433	17.8064
7	A	113.9348	0.0202	1.0609	0.1727
8	A	198.7020	0.0829	0.8335	3.3326
9	A	229.2042	0.1135	0.4567	7.0755
10	A	238.5418	0.0363	0.0375	0.0395
11	A	279.1683	0.1691	0.1070	28.5706
12	A	318.6002	0.0629	8.3897	0.2758
13	A	387.9722	0.2573	0.1262	0.4430
14	A	415.0924	0.2954	0.1596	0.0172
15	A	503.7660	0.3511	63.3715	4.3180
16	A	539.5495	1.1015	4.3675	3.8137
17	A	594.9912	0.6788	42.5587	99.8724
18	A	610.9607	0.3146	262.8732	7.9538
19	A	636.8273	1.5198	0.2091	3.9137
20	A	697.5225	0.5564	30.3059	0.4122
21	A	733.5913	0.3468	3.5649	0.1269
22	A	757.6783	0.6113	90.3773	2.0494
23	A	822.6393	0.5021	0.2136	0.3806
24	A	833.4889	1.8043	3.5918	20.5685
25	A	836.1583	0.4882	0.0462	0.5442
26	A	881.6242	0.6885	13.0528	0.3029
27	A	900.6267	0.9264	5.7913	0.5361
28	A	961.5199	0.7351	0.0856	0.0593
29	A	978.0491	0.7103	0.1524	0.5172
30	A	1014.8602	3.6437	1.1612	35.1825
31	A	1028.0578	0.6880	1.2647	1.1141
32	A	1029.9393	1.7958	0.4906	29.4295
33	A	1048.9923	1.3756	3.9668	18.0234
34	A	1066.4348	1.0514	2.5008	0.0646
35	A	1105.8758	1.4341	2.0984	5.3234
36	A	1135.4107	0.9609	5.2805	1.9176
37	A	1180.1943	0.9046	1.3428	3.9852
38	A	1200.7320	0.9576	9.3443	3.3587
39	A	1215.3174	1.0857	72.6446	32.8640
40	A	1237.1834	1.3097	0.3676	0.5271
41	A	1294.9315	3.2220	66.0700	15.2982
42	A	1323.5165	1.1402	0.2987	6.6115
43	A	1349.6807	5.9078	4.3594	1.6103
44	A	1359.4215	1.5099	1.3250	19.0214
45	A	1368.1369	1.4246	0.0037	0.1645
46	A	1410.7550	1.4339	2.3245	0.7948
47	A	1479.8480	1.4259	1.3849	9.6551
48	A	1494.1327	1.3807	2.1087	12.4915
49	A	1498.8880	1.3753	8.8980	9.7549
50	A	1501.2957	3.0773	2.0618	1.6786
51	A	1509.2198	1.4564	7.7628	0.7594
52	A	1531.4238	3.2429	60.4923	2.0203
53	A	1630.8816	9.0075	4.5638	4.2850
54	A	1645.4196	4.2454	32.0535	22.7117
55	A	1661.7710	2.3847	128.4532	27.4657
56	A	3019.9511	5.5613	36.0892	197.9388
57	A	3037.6062	5.7605	6.3515	78.1714
58	A	3063.1871	6.0972	0.1637	102.3250
59	A	3084.1767	5.9637	11.0646	129.2519
60	A	3087.8985	6.2009	39.3937	10.5899
61	A	3089.0299	6.1404	37.9036	109.9432
62	A	3146.9476	6.4802	8.2809	50.7233
63	A	3154.0768	6.3654	15.3816	9.5366

64	A	3155.5999	6.3818	1.5489	95.5589
65	A	3169.4333	6.4515	5.1464	139.5957
66	A	3175.1730	6.4976	29.8778	28.9167
67	A	3191.0464	6.5838	12.9302	259.9994
68	A	3563.9207	7.8389	19.5382	185.3854
69	A	3661.9361	8.6827	17.5971	49.1247

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.5939	0.0000	0.0428	0.4872
2	A	8.3854	0.0001	0.3418	7.2349
3	A	13.7503	0.0006	0.2767	4.6519
4	A	35.7028	0.0056	0.3485	0.7116
5	A	49.8082	0.0041	0.9177	0.0635
6	A	82.8687	0.0225	3.5106	20.0272
7	A	114.1851	0.0202	1.0353	0.1995
8	A	199.1373	0.0833	1.1373	5.0015
9	A	229.2159	0.1132	0.2588	5.4788
10	A	238.1126	0.0362	0.0403	0.0258
11	A	278.9319	0.1698	0.1928	34.5692
12	A	319.4546	0.0633	8.2535	0.3225
13	A	388.1626	0.2573	0.1269	0.5232
14	A	415.1365	0.2953	0.1566	0.0099
15	A	503.9464	0.3524	62.3310	3.9767
16	A	539.6481	1.1029	4.5816	3.4249
17	A	596.0589	0.7745	5.4779	107.9775
18	A	611.6378	0.2984	327.9822	26.1363
19	A	636.8086	1.5198	0.2081	4.1163
20	A	697.6367	0.5550	30.3780	0.4449
21	A	733.7192	0.3469	3.6229	0.1124
22	A	757.8668	0.6126	90.6449	2.1828
23	A	822.5395	0.5021	0.1655	0.3826
24	A	833.4690	1.8015	4.1225	20.8547
25	A	836.4045	0.4882	0.0210	0.6687
26	A	881.6387	0.6891	12.8449	0.2689
27	A	900.8415	0.9260	6.2900	0.2082
28	A	961.5764	0.7354	0.0817	0.0725
29	A	978.1330	0.7108	0.1480	0.5851
30	A	1014.8206	3.6430	1.1581	37.9447
31	A	1028.2323	0.6886	1.4114	1.1303
32	A	1030.1492	1.7930	0.6098	33.1639
33	A	1048.9644	1.3754	4.2686	19.1138
34	A	1066.6628	1.0523	2.5378	0.0594
35	A	1106.3657	1.4358	2.8686	4.7486
36	A	1135.4573	0.9605	5.4148	1.8755
37	A	1180.2422	0.9048	1.3553	4.2351
38	A	1200.6544	0.9575	9.7342	3.5188
39	A	1215.9289	1.0869	76.5652	37.7751
40	A	1237.5207	1.3102	0.2417	0.5157
41	A	1294.8371	3.2196	74.1739	16.4908
42	A	1322.7490	1.1391	0.3221	7.1234
43	A	1349.6287	5.8980	4.3754	1.9699
44	A	1358.5988	1.5111	1.7259	22.3758
45	A	1368.1310	1.4248	0.0035	0.1611
46	A	1410.8672	1.4339	2.5882	0.9022
47	A	1479.8447	1.4261	2.1519	10.6752
48	A	1494.1142	1.3810	2.0899	13.0790
49	A	1498.7345	1.3750	9.0044	10.5491
50	A	1501.3035	3.0764	1.9914	1.8554
51	A	1509.1152	1.4557	6.5532	1.0398
52	A	1531.4009	3.2428	65.7441	1.9552
53	A	1630.9159	9.0072	4.6950	4.3487
54	A	1645.4395	4.2622	35.9606	26.1585
55	A	1661.7958	2.3792	132.9796	28.8994
56	A	3020.2271	5.5620	35.7897	213.8377
57	A	3036.2313	5.7548	9.4724	84.9729
58	A	3062.4267	6.0947	0.0046	103.6091
59	A	3084.3683	5.9713	10.8923	133.5492

60	A	3087.8476	6.2001	41.1699	12.8737
61	A	3088.9479	6.1336	39.6595	130.2324
62	A	3147.1291	6.4808	7.9399	39.6181
63	A	3154.0786	6.3657	16.3954	9.4221
64	A	3155.5455	6.3817	1.6750	97.4932
65	A	3169.4985	6.4516	5.0796	140.2952
66	A	3175.2871	6.4980	29.9642	32.0234
67	A	3191.1715	6.5844	13.4301	270.5682
68	A	3563.6243	7.8377	17.5545	181.6161
69	A	3661.5388	8.6806	17.3645	46.9218

pyCH3-iC3H7I

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-1.2377	0.0000	0.0027	1.6988
2	A	8.8002	0.0002	1.1536	0.4283
3	A	17.2346	0.0008	1.8324	0.2644
4	A	25.8740	0.0004	0.2074	1.1255
5	A	55.1623	0.0118	1.6436	3.0591
6	A	57.9868	0.0143	1.7002	4.5007
7	A	61.4360	0.0123	0.0649	0.2567
8	A	213.0162	0.1011	0.0069	1.2125
9	A	249.6421	0.0817	0.0351	21.6531
10	A	251.0047	0.0400	0.0210	0.2652
11	A	265.8876	0.1098	0.1533	1.1557
12	A	281.3381	0.0590	0.0795	14.9128
13	A	344.0061	0.1779	0.0110	0.1402
14	A	387.5491	0.2303	0.0025	0.0940
15	A	398.9015	0.2076	0.9470	4.5968
16	A	491.5168	0.4094	4.9293	74.7773
17	A	495.3231	0.4198	16.2258	45.0483
18	A	529.1400	0.9067	10.5115	13.3788
19	A	685.9858	1.9203	0.0034	4.8473
20	A	739.6573	1.1130	3.0549	0.7081
21	A	807.2149	0.5658	28.0062	5.8172
22	A	818.1694	1.1586	16.0521	19.9141
23	A	881.1752	0.5708	0.0117	0.0402
24	A	886.4212	1.2447	3.8685	27.6055
25	A	941.6775	0.5980	0.9307	0.2476
26	A	961.0772	0.7745	0.4278	0.9975
27	A	972.0624	0.7206	0.1011	0.5800
28	A	995.4278	0.8499	0.0000	0.0872
29	A	1005.7219	0.8586	0.0025	0.0396
30	A	1019.4118	4.5157	16.2980	27.8598
31	A	1037.6898	0.7581	6.0408	5.0684
32	A	1060.0224	1.0397	7.1043	0.9178
33	A	1096.4854	1.3714	9.9492	12.4350
34	A	1117.9099	1.0512	0.0500	0.0510
35	A	1136.2567	1.7779	0.4017	2.1925
36	A	1172.4374	1.4598	69.6823	43.0041
37	A	1232.1962	1.2151	76.8047	33.0670
38	A	1240.6907	1.8571	3.5609	48.4827
39	A	1246.8320	1.4869	7.0962	4.9710
40	A	1285.4313	8.8260	0.0029	0.8874
41	A	1355.4953	1.4374	0.9585	2.9314
42	A	1359.6518	1.4489	0.2842	1.9743
43	A	1406.1726	1.4685	11.4483	2.4349
44	A	1414.7517	1.4730	2.2616	20.0226
45	A	1421.4653	1.4561	5.5283	5.9286
46	A	1444.0772	2.3292	10.3319	1.7097
47	A	1482.6009	1.3520	3.2768	6.5994
48	A	1487.1705	1.3622	0.2310	9.3530
49	A	1488.9171	1.4677	21.6908	6.1986
50	A	1491.3003	1.3797	7.8855	10.6499
51	A	1495.1194	1.3728	12.6652	13.8856
52	A	1506.0380	1.3969	5.5877	1.9456
53	A	1528.5873	3.0544	0.8047	5.7429
54	A	1605.3556	9.0522	10.0490	6.4466
55	A	1641.2714	8.6535	81.4498	22.6151

56	A	3004.7421	5.5578	14.9469	48.4298
57	A	3010.1678	5.5747	90.4033	674.7131
58	A	3026.5350	5.6105	19.0301	274.3602
59	A	3072.1603	6.0598	11.6484	169.6698
60	A	3074.4552	6.0742	3.5894	12.6963
61	A	3082.7165	6.1326	15.2323	87.3523
62	A	3093.5098	6.1419	18.6894	124.1126
63	A	3108.9878	6.2805	12.5667	66.6102
64	A	3109.1179	6.2747	14.2968	29.7614
65	A	3116.7306	6.2911	27.1423	48.4296
66	A	3147.7553	6.3450	12.2059	77.6039
67	A	3149.5461	6.3698	2.7354	17.6254
68	A	3171.9444	6.4799	30.4826	39.7610
69	A	3174.3446	6.5044	5.9306	272.6369

pyCH3_nC3F7I_d

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.3312	0.0000	0.0127	5.2636
2	A	13.1535	0.0013	0.1136	0.1842
3	A	16.7113	0.0014	0.1899	0.4291
4	A	23.2010	0.0026	0.1096	0.5492
5	A	24.6429	0.0004	0.2273	1.1312
6	A	67.9746	0.0201	0.6341	0.3755
7	A	72.1484	0.0272	0.2897	0.5573
8	A	79.8544	0.0327	6.6101	1.3210
9	A	91.0658	0.0489	1.1716	0.5640
10	A	123.8596	0.1760	3.8384	1.1988
11	A	160.1835	0.2817	1.1328	2.8480
12	A	220.0014	0.4412	0.5662	3.2313
13	A	223.4229	0.1262	0.5482	1.2928
14	A	236.5626	0.7088	6.9670	47.7956
15	A	258.0098	0.7157	3.8702	5.0758
16	A	276.2752	0.8282	6.5904	4.3259
17	A	302.4393	1.0071	1.6433	0.9587
18	A	324.5399	1.0923	0.7374	2.8801
19	A	346.4226	0.2063	0.0048	0.2694
20	A	347.9077	0.7226	0.0749	1.2969
21	A	391.1483	0.2372	0.0034	0.0558
22	A	396.1780	1.6603	0.3944	1.8665
23	A	460.3292	2.2213	1.7103	4.0023
24	A	496.3143	0.4227	19.0240	0.9452
25	A	527.5056	2.9372	9.8865	0.7483
26	A	535.3736	0.9255	17.7581	7.3312
27	A	577.7684	3.5123	0.8164	8.9640
28	A	611.9062	3.8366	5.7574	1.2773
29	A	644.5499	4.2845	8.2305	10.4120
30	A	684.7652	1.9136	0.0220	5.2924
31	A	738.7579	1.0939	4.4863	1.6159
32	A	740.6626	5.3184	40.4793	16.0884
33	A	811.3918	0.5942	27.4069	9.0576
34	A	821.7080	1.1124	17.5391	28.9841
35	A	875.5709	6.0362	188.6400	46.4611
36	A	882.6164	0.5722	0.0218	0.0403
37	A	975.5040	0.7281	0.0854	0.5284
38	A	997.0411	0.8476	0.0014	0.0395
39	A	1007.7939	0.8604	0.0383	0.0885
40	A	1017.8625	8.0152	224.2870	25.2261
41	A	1026.9752	4.7000	22.2220	25.0180
42	A	1060.8087	1.0528	6.8417	0.6168
43	A	1093.2157	5.4816	101.5048	2.3341
44	A	1095.8038	1.7902	15.7383	12.1906
45	A	1101.1736	5.2990	12.1551	18.8259
46	A	1124.2138	1.0586	0.1285	0.0585
47	A	1151.0519	10.1939	137.8155	9.7418
48	A	1185.4968	10.7298	507.0448	4.2910
49	A	1199.9725	11.0845	313.0836	3.6271
50	A	1230.7173	7.7329	159.7981	20.5807
51	A	1240.7891	1.8038	5.9778	32.4175

52	A	1248.4428	1.6018	4.3069	14.7342
53	A	1289.1250	8.7981	0.1886	0.1870
54	A	1318.5452	12.7780	71.9734	12.5539
55	A	1360.9659	1.4502	0.4280	1.6944
56	A	1415.8941	1.4704	3.2024	24.0065
57	A	1447.7669	2.3333	11.6514	1.5338
58	A	1488.0783	1.4829	23.5780	5.7440
59	A	1491.5738	1.3823	8.3930	10.5833
60	A	1532.0577	3.0595	0.3862	3.3713
61	A	1604.7896	8.9247	8.2757	7.9209
62	A	1646.0794	8.6185	87.4224	20.7033
63	A	3029.0735	5.6213	13.9557	288.9150
64	A	3086.4437	6.1459	13.2037	88.9540
65	A	3113.4901	6.3001	11.5483	67.8951
66	A	3157.5996	6.3875	6.4940	61.3000
67	A	3159.0330	6.4097	0.2369	13.0759
68	A	3179.3531	6.5126	19.5865	45.8630
69	A	3181.5749	6.5365	6.8600	262.0310

pyCH3_nC3F7I_s

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.9059	0.0000	0.0027	5.0500
2	A	15.2220	0.0013	0.2175	0.0607
3	A	16.8655	0.0013	0.4213	1.4715
4	A	24.2965	0.0004	0.2274	1.0988
5	A	28.6193	0.0058	0.0052	0.1695
6	A	63.7461	0.0152	0.3087	0.5572
7	A	66.9463	0.0347	0.0129	0.1223
8	A	77.6939	0.0287	7.8654	1.1763
9	A	95.7254	0.0461	0.2359	0.0005
10	A	118.5519	0.1476	1.4437	0.6751
11	A	156.7634	0.3700	7.9386	18.0918
12	A	214.5851	0.4933	2.0232	0.2512
13	A	224.4903	0.1192	0.2706	1.4032
14	A	231.2120	0.5918	0.1017	0.0043
15	A	261.5779	0.8420	7.7742	47.8538
16	A	264.6176	0.7908	0.2133	1.4404
17	A	286.3084	0.8870	4.3313	1.4940
18	A	336.5489	1.2460	1.2160	1.4485
19	A	346.4120	0.1819	0.0010	0.1406
20	A	371.1971	1.5190	0.0371	1.2782
21	A	380.2448	1.5148	0.2661	0.5238
22	A	391.3651	0.2374	0.0059	0.0746
23	A	496.2156	0.4217	19.5868	0.8009
24	A	506.2827	2.6938	1.4742	0.3303
25	A	526.3872	2.9121	6.3714	2.9567
26	A	535.2336	0.9249	18.0419	7.7145
27	A	577.8135	3.4108	5.1773	13.3897
28	A	595.8424	3.7684	0.0953	2.3347
29	A	664.7448	4.4004	45.7186	1.0359
30	A	684.7848	1.9136	0.0171	5.2388
31	A	724.8258	4.9008	97.2820	41.5614
32	A	739.2767	1.0891	2.9813	0.4768
33	A	806.8358	4.9846	110.6326	45.6839
34	A	811.3147	0.5994	30.6888	10.9781
35	A	821.9431	1.1187	14.1785	21.5614
36	A	882.6841	0.5723	0.0054	0.0354
37	A	975.4493	0.7284	0.0731	0.4629
38	A	997.2055	0.8484	0.0000	0.0477
39	A	1007.7524	0.8602	0.0074	0.0725
40	A	1026.1745	4.6193	30.6338	10.8281
41	A	1055.3047	8.3775	29.7995	96.6807
42	A	1060.9595	1.0555	8.1842	1.2417
43	A	1096.0911	1.4094	31.6796	19.2226
44	A	1102.3229	9.2605	61.4271	0.5649
45	A	1108.4088	9.2749	225.0184	0.3386
46	A	1124.0902	1.0590	0.6615	0.0239
47	A	1162.9484	10.3458	98.0947	0.7061

48	A	1180.6499	10.8371	318.9525	16.0410
49	A	1206.4129	11.2709	408.1789	1.0968
50	A	1239.3068	1.7439	53.5591	48.6709
51	A	1246.2768	5.8299	37.7776	1.9109
52	A	1248.7909	1.7814	8.0815	20.8524
53	A	1289.0467	8.8002	0.1918	0.1521
54	A	1301.0997	12.2776	230.1589	7.2400
55	A	1360.9182	1.4500	0.4219	1.6759
56	A	1415.8603	1.4705	3.1858	24.0916
57	A	1447.6566	2.3336	11.7456	1.4688
58	A	1488.1000	1.4825	23.6231	5.7940
59	A	1491.5669	1.3822	8.3831	10.6281
60	A	1531.9532	3.0596	0.3475	3.4979
61	A	1604.8149	8.9302	8.4004	7.9476
62	A	1645.9520	8.6205	87.8427	20.4111
63	A	3029.0175	5.6211	14.1297	289.5257
64	A	3086.3620	6.1457	13.3186	89.1125
65	A	3113.3860	6.2996	11.6126	68.4007
66	A	3157.5148	6.3870	6.5723	60.4154
67	A	3158.9344	6.4092	0.1634	13.2622
68	A	3179.1827	6.5119	19.9132	47.1420
69	A	3181.4165	6.5359	7.2161	263.0742

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.4248	0.0000	0.0284	4.5506
2	A	12.5961	0.0003	1.2319	0.4218
3	A	16.6464	0.0007	1.5590	0.9284
4	A	23.8657	0.0003	0.1912	1.1568
5	A	52.1710	0.0091	0.4998	1.7849
6	A	59.4930	0.0181	2.7548	4.0364
7	A	70.9348	0.0115	0.2470	0.6221
8	A	128.5318	0.0231	0.1901	0.9685
9	A	196.0816	0.0373	0.1387	3.0210
10	A	214.0444	0.0990	0.0177	1.3391
11	A	270.7792	0.0654	0.0945	8.7867
12	A	344.0373	0.1779	0.0102	0.1747
13	A	387.5376	0.2157	0.1320	11.6450
14	A	387.6013	0.2149	0.1875	11.9057
15	A	494.0573	0.4244	16.5320	5.6382
16	A	504.5818	0.4762	1.9382	106.6445
17	A	529.3287	0.9069	10.2725	13.4589
18	A	685.9620	1.9193	0.0038	4.9261
19	A	739.8622	1.1106	3.0195	0.4509
20	A	771.7810	0.4481	10.2729	6.7791
21	A	807.3894	0.5668	28.1525	5.0815
22	A	818.3063	1.1561	15.6638	19.5799
23	A	825.6844	0.5516	3.7172	5.0920
24	A	881.3842	0.5710	0.0104	0.0493
25	A	888.6952	0.9531	3.6318	7.0671
26	A	972.2182	0.7210	0.1070	0.4646
27	A	995.6454	0.8496	0.0002	0.0151
28	A	1005.7737	0.8586	0.0027	0.0615
29	A	1019.6658	4.5136	15.8224	28.4259
30	A	1026.2558	0.8123	1.4387	3.1692
31	A	1048.3926	0.8444	0.2338	2.1741
32	A	1060.0634	1.0404	7.0799	1.0227
33	A	1088.0401	1.4947	2.5345	6.3615
34	A	1096.5031	1.3722	8.9175	12.6501
35	A	1118.1887	1.0506	0.0535	0.0695
36	A	1219.2317	1.2426	6.7403	15.6649
37	A	1227.8078	1.2066	60.4543	21.6970
38	A	1240.5816	1.8383	7.2018	38.7562
39	A	1246.8748	1.4991	9.8006	6.7743
40	A	1285.4857	8.8247	0.0062	0.9423
41	A	1308.6824	1.1540	38.3086	7.0375
42	A	1359.7243	1.4491	0.2443	1.8407
43	A	1375.2982	1.5709	7.8843	1.3298

44	A	1414.7351	1.4730	2.3824	19.2727
45	A	1415.6163	1.4812	11.2633	1.3360
46	A	1444.2186	2.3290	10.4747	1.7327
47	A	1472.9225	1.4024	2.8417	15.7933
48	A	1480.9122	1.3866	3.7060	15.2690
49	A	1488.8682	1.4681	21.5187	5.7595
50	A	1491.2954	1.3798	7.9540	10.3759
51	A	1499.6151	1.3845	8.1677	6.3093
52	A	1507.7464	1.4156	5.7347	3.3128
53	A	1528.7451	3.0547	0.9222	5.4847
54	A	1605.3062	9.0436	10.1690	6.3539
55	A	1641.4753	8.6529	81.1354	22.7314
56	A	2992.4365	5.6411	38.1346	323.6784
57	A	3023.3970	5.5885	25.4042	188.6847
58	A	3026.6070	5.6108	18.9247	268.9457
59	A	3048.2379	5.9643	8.4503	87.4938
60	A	3082.8301	6.1316	16.6929	85.1786
61	A	3082.9604	6.0193	8.1273	146.8788
62	A	3086.9924	6.0833	49.0456	88.3048
63	A	3099.2284	6.2332	30.7033	30.0735
64	A	3109.1492	6.2812	13.6540	66.2789
65	A	3145.6907	6.4684	7.1024	72.3088
66	A	3148.1413	6.3467	11.7980	77.8712
67	A	3149.9174	6.3714	2.8664	18.0311
68	A	3172.2036	6.4811	30.1637	38.2626
69	A	3174.6043	6.5056	5.6075	273.2986

pyCH3-nC3H7I_s

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.8150	0.0000	0.0904	3.4629
2	A	12.9753	0.0003	0.9841	0.4059
3	A	15.7171	0.0006	1.4318	0.5943
4	A	24.4610	0.0004	0.1916	1.1564
5	A	52.8511	0.0097	0.3938	2.1925
6	A	59.2894	0.0175	3.1172	4.1263
7	A	63.4874	0.0068	0.0128	0.3247
8	A	121.2416	0.0251	0.5313	0.6267
9	A	199.8359	0.0847	0.3068	4.3127
10	A	216.4449	0.1061	0.0743	2.9710
11	A	238.9374	0.0364	0.0360	0.0307
12	A	279.1269	0.1683	0.6950	42.5655
13	A	344.0911	0.1780	0.0090	0.1672
14	A	387.6686	0.2307	0.0046	0.1279
15	A	494.2682	0.4237	17.5885	1.4383
16	A	529.4234	0.9080	10.7164	11.4842
17	A	598.1693	0.7713	3.5346	129.7010
18	A	685.9479	1.9176	0.0046	4.9462
19	A	732.1290	0.3461	3.6828	0.1015
20	A	739.7961	1.1103	3.2621	0.6082
21	A	807.4050	0.5662	28.4686	5.4105
22	A	818.3721	1.1612	15.4739	19.6864
23	A	834.9239	0.4872	0.0064	0.7467
24	A	881.2843	0.5709	0.0106	0.0457
25	A	900.3415	0.9294	5.9332	0.4209
26	A	972.1974	0.7212	0.1020	0.4576
27	A	995.4058	0.8492	0.0002	0.0305
28	A	1005.7950	0.8583	0.0002	0.0547
29	A	1019.8096	4.5217	16.1587	27.4446
30	A	1026.7140	0.6871	1.5829	1.0399
31	A	1030.9209	1.7743	0.2765	34.3398
32	A	1060.0119	1.0401	7.0935	1.0365
33	A	1096.5102	1.3723	9.5992	12.7971
34	A	1105.2908	1.4327	2.7800	7.8116
35	A	1118.2803	1.0506	0.0473	0.0681
36	A	1213.9915	1.0897	86.3001	44.2401
37	A	1237.6340	1.3104	0.3161	0.4932
38	A	1240.5360	1.8278	9.0193	38.4141
39	A	1246.8956	1.5045	10.1710	7.5832

40	A	1285.5523	8.8257	0.0034	0.8786
41	A	1322.9069	1.1390	0.2650	7.5297
42	A	1358.6143	1.5131	1.1251	26.1444
43	A	1359.7508	1.4492	0.2353	1.8226
44	A	1410.0807	1.4343	2.3990	0.9687
45	A	1414.7570	1.4729	2.2973	19.9926
46	A	1444.2815	2.3291	10.4942	1.6989
47	A	1479.4857	1.4234	1.6649	11.6483
48	A	1488.8748	1.4684	21.6114	5.8186
49	A	1491.3012	1.3798	7.9516	10.4931
50	A	1493.8633	1.3817	1.9286	13.3882
51	A	1498.6119	1.3750	8.7824	10.7236
52	A	1508.9130	1.4543	7.2476	1.0815
53	A	1528.8200	3.0551	0.8547	5.7514
54	A	1605.3387	9.0437	10.2653	6.4342
55	A	1641.5748	8.6537	81.9630	22.9397
56	A	3018.7429	5.5563	40.1372	216.9776
57	A	3026.6240	5.6109	18.8158	269.5269
58	A	3034.2231	5.7473	8.1421	88.2892
59	A	3059.9791	6.0841	0.0087	106.6999
60	A	3079.9676	5.9269	16.0400	136.8167
61	A	3082.8575	6.1330	15.1635	87.1635
62	A	3085.7864	6.1913	41.9612	13.6508
63	A	3086.4859	6.1528	42.0558	140.1458
64	A	3109.1796	6.2814	13.6547	66.5247
65	A	3141.1794	6.4547	10.2523	50.5911
66	A	3148.3368	6.3475	11.8269	78.3896
67	A	3150.1063	6.3721	2.6921	17.8705
68	A	3172.2963	6.4815	30.1796	38.9452
69	A	3174.7023	6.5061	5.8246	274.6988

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.4600	0.0000	0.5534	0.2851
2	A	20.0527	0.0025	0.5746	2.9984
3	A	22.8776	0.0015	0.0234	3.0966
4	A	38.7161	0.0051	0.2259	2.5132
5	A	40.7204	0.0115	0.0182	0.6181
6	A	45.4600	0.0136	0.1174	2.6191
7	A	76.7891	0.0641	0.1266	0.1068
8	A	88.4679	0.0265	3.8768	7.3597
9	A	115.5290	0.0320	0.0977	0.5610
10	A	142.5231	0.2336	5.9984	3.8436
11	A	142.7839	0.0890	0.0254	0.0136
12	A	159.1550	0.0458	3.7534	2.0759
13	A	179.1926	0.3540	3.0868	3.9146
14	A	191.1674	0.0292	0.2353	0.1166
15	A	212.3046	0.0343	9.5537	8.5559
16	A	237.8749	0.5380	13.5286	65.2678
17	A	254.7828	0.7100	0.6396	0.1088
18	A	280.5145	0.8659	1.2112	4.3917
19	A	297.2283	0.0957	0.0091	0.0018
20	A	298.8552	0.9113	0.4386	0.7586
21	A	322.1091	0.3364	51.6052	7.1100
22	A	326.1691	0.5036	31.2379	2.5835
23	A	343.1195	1.2897	0.1098	1.2254
24	A	391.4232	0.2414	0.0059	0.1253
25	A	415.1658	0.2656	9.7470	1.9689
26	A	462.5590	2.2554	2.3408	3.9558
27	A	474.0895	0.4756	1.2267	2.5232
28	A	529.8799	2.9703	3.3889	0.4282
29	A	532.7107	2.3861	8.2593	17.5761
30	A	536.3067	0.5678	7.5573	1.6959
31	A	556.7045	3.2947	0.2628	0.0452
32	A	565.2968	0.5476	4.3382	0.0690
33	A	606.7400	3.8772	3.5032	1.8837
34	A	684.0670	1.9056	0.4018	4.3259
35	A	701.9039	4.7681	40.1371	0.0189

36	A	740.8116	5.4676	35.5494	30.4559
37	A	743.2102	1.0330	2.7033	1.9399
38	A	760.4984	1.7502	47.5397	18.9244
39	A	819.3772	0.6951	70.2197	2.5762
40	A	835.3166	0.5168	0.2684	0.3316
41	A	883.9062	6.1204	101.5007	113.9508
42	A	948.8890	7.5643	105.2687	0.1376
43	A	957.5210	1.3571	38.5745	2.4574
44	A	963.7222	0.7827	6.2267	1.0272
45	A	992.8812	0.8340	0.0275	0.1387
46	A	1011.3748	4.5004	21.8168	39.5691
47	A	1067.1539	1.0652	13.5332	0.8330
48	A	1098.4099	1.4337	0.2824	5.3261
49	A	1100.1356	8.7139	88.8590	22.0022
50	A	1118.1854	0.9213	0.8700	2.6069
51	A	1130.9891	3.4691	17.1125	1.4000
52	A	1131.4666	1.6777	21.4392	0.7432
53	A	1157.6179	10.3252	7.4689	0.3671
54	A	1165.3751	1.1962	57.6772	22.9548
55	A	1194.0222	1.5713	11.1787	8.5417
56	A	1196.3312	9.1398	365.9560	22.3062
57	A	1209.8011	10.5172	258.2798	12.7405
58	A	1229.1821	2.5122	15.6201	1.6443
59	A	1257.5570	3.8350	463.3706	76.2004
60	A	1258.6028	1.4705	85.7678	38.5138
61	A	1262.8274	11.5779	252.6369	0.5514
62	A	1299.2431	7.8038	0.3995	10.1216
63	A	1355.1298	3.3424	64.8227	41.5850
64	A	1372.5800	1.4951	2.1684	2.4073
65	A	1445.0758	1.6614	0.7272	4.7123
66	A	1455.9060	2.1085	8.9414	3.6282
67	A	1480.2389	1.5267	3.9461	34.8036
68	A	1493.6520	1.3839	4.4404	0.6717
69	A	1503.2214	1.4810	24.8392	13.4826
70	A	1506.7832	1.4134	1.9723	5.1321
71	A	1528.0260	1.4897	31.5673	4.3738
72	A	1536.8736	2.6710	85.5142	5.2399
73	A	1596.5054	10.3629	36.7978	1.9310
74	A	1632.7587	8.1303	251.4213	56.5855
75	A	2996.9196	5.5611	32.4067	63.7907
76	A	3001.5994	5.5912	95.0321	332.8539
77	A	3100.4242	6.1322	3.1852	27.7863
78	A	3102.3027	6.1391	19.5567	85.8246
79	A	3131.6489	6.3805	4.9287	7.8207
80	A	3137.9141	6.3980	17.7818	69.7777
81	A	3147.5469	6.3524	29.6689	115.0935
82	A	3150.5661	6.3861	9.0179	147.8229
83	A	3219.8268	6.6689	2.0776	132.2229
84	A	3219.9454	6.6622	8.0058	8.9047

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-1.2716	0.0000	0.7127	0.2582
2	A	18.8435	0.0022	0.4660	2.8508
3	A	22.4578	0.0015	0.0234	3.0144
4	A	39.1012	0.0051	0.2226	2.6547
5	A	40.9296	0.0120	0.0152	0.5673
6	A	47.8114	0.0160	0.1705	2.5556
7	A	76.9997	0.0671	0.0228	0.0324
8	A	86.9431	0.0243	3.3730	5.9765
9	A	115.0868	0.0313	0.0977	0.5594
10	A	142.2758	0.2702	8.4249	5.8106
11	A	142.4143	0.0911	0.0377	0.0273
12	A	159.1368	0.0457	2.7239	1.8303
13	A	178.3823	0.3042	3.4795	4.7385
14	A	191.1555	0.0292	0.2371	0.1195
15	A	212.1373	0.0345	8.4454	7.5865
16	A	239.1127	0.5363	11.0205	61.3349

17	A	255.0414	0.7114	0.6429	0.1119
18	A	280.4209	0.8655	0.3360	5.1473
19	A	297.3269	0.0955	0.0106	0.0049
20	A	298.8218	0.9238	0.4425	0.7465
21	A	321.4942	0.3449	52.0968	7.3938
22	A	326.5988	0.4872	30.5142	2.3886
23	A	343.2846	1.2909	0.1483	1.3072
24	A	391.7329	0.2416	0.0071	0.1208
25	A	415.0447	0.2655	9.5293	2.0220
26	A	462.6312	2.2687	1.7378	2.5523
27	A	474.1177	0.4756	1.2416	2.5095
28	A	530.0113	2.9721	3.2411	0.4541
29	A	532.7859	2.8947	4.2662	20.7832
30	A	536.1542	0.5440	10.9344	1.5919
31	A	556.7088	3.2937	0.2713	0.0422
32	A	565.2721	0.5478	3.8636	0.1194
33	A	606.8687	3.8952	3.4202	1.9118
34	A	684.0716	1.9056	0.3963	4.2763
35	A	702.0456	4.7683	39.8112	0.0676
36	A	740.9017	5.4841	31.4891	30.9966
37	A	743.4182	1.0311	3.3056	1.5189
38	A	760.4570	1.7490	47.7416	19.3337
39	A	819.5554	0.6960	70.8258	2.7280
40	A	835.3663	0.5167	0.2797	0.3275
41	A	883.8699	6.1156	97.8396	118.4362
42	A	948.7488	7.5646	106.4790	0.1491
43	A	957.5719	1.3774	38.7821	2.5560
44	A	963.9450	0.7767	5.5676	0.9588
45	A	993.4376	0.8353	0.0291	0.1378
46	A	1011.3850	4.5001	21.5056	38.5981
47	A	1067.2242	1.0645	13.4455	0.8723
48	A	1097.7877	6.6253	95.1093	15.2118
49	A	1098.5415	1.5107	13.0105	6.7431
50	A	1118.2031	0.9217	0.8025	2.5647
51	A	1129.3601	8.9688	33.1880	1.9259
52	A	1131.4212	1.2931	6.0484	0.0783
53	A	1161.4663	10.3979	9.7290	0.4433
54	A	1165.1938	1.1987	48.9951	21.9610
55	A	1193.8860	1.6715	4.0501	6.4856
56	A	1196.6281	6.5567	321.2390	18.2543
57	A	1209.9198	11.0124	356.0608	18.3440
58	A	1229.2689	2.5153	15.6712	1.6039
59	A	1257.4931	3.2634	318.3655	77.6350
60	A	1258.7692	1.5735	162.4028	48.1035
61	A	1262.1497	11.5641	249.9165	0.6526
62	A	1299.3048	7.8041	0.3856	9.9225
63	A	1355.3466	3.3450	66.4654	40.9247
64	A	1372.6170	1.4952	2.1728	2.3463
65	A	1445.0621	1.6605	0.7189	4.7284
66	A	1455.9091	2.1094	8.9188	3.6360
67	A	1480.1915	1.5265	3.7394	33.7427
68	A	1493.5220	1.3837	4.4768	0.6774
69	A	1503.1134	1.4804	24.0005	13.9367
70	A	1506.7971	1.4135	2.0418	5.0817
71	A	1527.9845	1.4888	31.5625	4.3919
72	A	1536.8931	2.6771	84.6781	4.8263
73	A	1596.5382	10.3675	36.7124	1.9504
74	A	1632.7778	8.1307	247.7149	56.2974
75	A	2996.8966	5.5609	32.5156	64.7811
76	A	3001.5885	5.5912	96.3174	335.9419
77	A	3100.3464	6.1320	3.1821	27.8947
78	A	3102.2211	6.1389	19.3554	88.2655
79	A	3131.5288	6.3800	4.9123	7.8786
80	A	3137.8026	6.3975	17.9020	71.5528
81	A	3147.5809	6.3525	29.5922	113.3481
82	A	3150.6007	6.3862	8.8130	146.2500
83	A	3219.7846	6.6686	2.1162	130.4227
84	A	3219.9068	6.6621	7.9319	10.2485

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	0.9871	0.0000	0.0267	0.0872
2	A	1.5633	0.0000	0.1083	0.0790
3	A	6.2807	0.0004	0.1708	1.2461
4	A	14.4992	0.0015	0.0472	0.0034
5	A	18.3827	0.0034	0.0235	0.2911
6	A	23.1430	0.0018	0.1056	1.6324
7	A	31.3520	0.0193	0.4656	0.2324
8	A	40.2210	0.0166	0.0245	0.1052
9	A	40.6035	0.0183	0.0088	0.0001
10	A	45.4394	0.0055	0.1808	3.5954
11	A	61.2077	0.0232	0.4336	0.3774
12	A	72.2012	0.0278	5.4132	2.6716
13	A	76.2626	0.0248	0.0074	0.0420
14	A	76.7816	0.0400	2.6256	0.7423
15	A	78.6778	0.0453	1.5748	2.5621
16	A	89.7773	0.0293	0.4177	9.3330
17	A	114.6489	0.0281	0.0407	0.3257
18	A	138.6979	0.1074	0.0793	0.0689
19	A	141.0238	0.2584	13.5932	7.9582
20	A	141.4274	0.1705	0.1435	0.3323
21	A	142.7064	0.2555	5.0729	4.4744
22	A	168.3162	0.0604	8.3889	5.5902
23	A	178.5225	0.3533	2.5036	2.5247
24	A	182.8054	0.1342	2.6605	6.7442
25	A	186.0159	0.0269	0.1796	0.1534
26	A	203.2407	0.0337	12.7815	11.9438
27	A	233.7322	0.6960	25.9035	76.0961
28	A	241.3087	0.6310	6.9262	65.1569
29	A	254.7256	0.6998	0.7823	0.1624
30	A	254.8053	0.7085	0.4091	0.0934
31	A	279.0883	0.8361	1.8987	5.9835
32	A	281.4578	0.8748	1.4511	3.9662
33	A	297.9642	0.1317	0.2113	0.1156
34	A	298.5704	0.8908	0.3259	0.7951
35	A	300.2244	0.3279	0.3659	0.7374
36	A	314.2770	0.2471	86.9385	14.2077
37	A	324.7055	1.0653	2.7816	1.3169
38	A	325.5563	1.1061	0.8362	3.6053
39	A	343.1020	1.2897	0.0946	1.1416
40	A	343.1900	1.2891	0.1625	1.3803
41	A	400.8849	0.2596	0.0065	0.0732
42	A	419.2606	0.2711	6.2540	5.6498
43	A	462.6144	2.2608	2.3199	4.1360
44	A	462.8285	2.2699	1.8299	3.1895
45	A	477.7173	0.4846	1.7658	1.9399
46	A	529.7580	2.9707	3.1667	0.4985
47	A	529.9964	2.9709	3.5034	0.4061
48	A	531.9713	2.6257	2.8254	23.0148
49	A	533.3824	2.8542	7.4198	15.5277
50	A	539.3067	0.5409	17.6248	0.8233
51	A	556.4354	3.2939	0.2287	0.0342
52	A	556.8475	3.2951	0.2616	0.0587
53	A	564.2072	0.5804	0.8687	0.5552
54	A	606.1558	3.8838	4.5446	1.8379
55	A	607.0393	3.8802	3.3032	1.8278
56	A	681.5288	1.8912	0.0814	3.6958
57	A	700.8001	4.7581	36.8039	0.0331
58	A	702.5304	4.7733	41.9177	0.0140
59	A	739.8057	5.3328	36.9393	33.0212
60	A	741.3305	5.4592	35.5478	34.4620
61	A	743.6107	1.0744	1.5319	1.5746
62	A	766.5348	1.7925	50.7246	36.2364
63	A	822.7843	0.6987	72.4255	2.9965
64	A	836.0787	0.5162	0.2691	0.2072
65	A	884.2184	6.1407	121.6788	105.0995
66	A	885.1180	6.1313	94.2428	124.7307
67	A	947.5921	7.5374	97.5407	0.2156
68	A	949.5545	7.5759	112.6024	0.1402

69	A	959.2261	1.5186	36.3564	11.1146
70	A	967.8498	0.7465	1.9145	1.7780
71	A	992.1014	0.8233	0.0418	0.1642
72	A	1021.5776	4.2985	71.4456	25.9085
73	A	1069.8021	1.0694	14.7970	0.5814
74	A	1089.6718	8.1971	90.7670	17.6210
75	A	1098.5936	1.5141	25.3752	36.0216
76	A	1104.2492	9.5051	89.1862	20.2688
77	A	1119.7116	0.9196	1.3799	2.6174
78	A	1122.4409	9.6237	35.4396	2.4087
79	A	1135.3587	9.9073	35.3306	1.9911
80	A	1139.5776	1.2869	1.2685	0.0080
81	A	1153.3667	10.2461	11.0491	0.3906
82	A	1159.9770	10.3655	5.4085	0.4022
83	A	1161.2570	1.1607	102.5785	48.0944
84	A	1189.7670	10.7994	412.9678	37.2589
85	A	1197.0944	1.5739	26.6730	18.8418
86	A	1199.8050	8.9335	297.9738	17.9267
87	A	1205.9093	10.3229	266.7303	7.4561
88	A	1211.3307	10.5549	295.3761	11.5045
89	A	1234.6523	2.4130	14.7670	0.5387
90	A	1251.0918	2.1213	666.6750	102.8077
91	A	1259.4418	6.5431	463.1520	83.7182
92	A	1260.6305	11.5446	235.9849	0.4379
93	A	1261.4383	2.4266	62.3806	37.1302
94	A	1267.1871	11.6242	269.6222	0.9085
95	A	1312.0249	8.0886	0.7203	4.7377
96	A	1368.9820	3.3617	116.0336	85.1264
97	A	1373.0484	1.4973	5.1533	0.9139
98	A	1448.4451	1.4978	0.0256	5.7811
99	A	1464.1315	2.5723	12.1698	2.6030
100	A	1482.1141	1.5352	6.7786	34.1678
101	A	1494.5766	1.3869	4.2040	1.2410
102	A	1504.2485	1.4641	24.7760	15.7447
103	A	1507.5074	1.4297	2.0130	3.7515
104	A	1528.3160	1.5063	42.1637	10.9673
105	A	1544.2835	2.8105	112.0971	8.8138
106	A	1592.7213	10.1886	27.0673	3.2188
107	A	1643.0926	8.1286	367.4542	101.4672
108	A	3001.3125	5.5724	31.8938	65.2587
109	A	3005.8411	5.6028	84.9538	338.9733
110	A	3100.9129	6.1426	3.2494	33.3138
111	A	3102.1535	6.1513	19.6473	71.9329
112	A	3133.3365	6.3860	3.2035	4.3861
113	A	3140.6201	6.4038	18.0284	104.8128
114	A	3162.5108	6.4174	10.6435	39.0872
115	A	3164.9274	6.4477	0.5460	56.5543
116	A	3226.4822	6.6985	6.0407	132.2637
117	A	3226.6690	6.6918	3.4569	27.3493

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-1.2338	0.0000	0.1156	0.0900
2	A	1.4479	0.0000	0.0724	0.0637
3	A	5.9220	0.0003	0.1502	1.1627
4	A	14.4869	0.0015	0.0457	0.0032
5	A	17.6858	0.0031	0.0094	0.1908
6	A	22.8363	0.0017	0.1079	1.6245
7	A	32.7253	0.0222	0.3906	0.1828
8	A	40.4268	0.0171	0.0216	0.0852
9	A	40.6352	0.0183	0.0084	0.0001
10	A	45.7911	0.0055	0.1847	3.6211
11	A	61.6695	0.0238	0.5904	0.4351
12	A	72.1464	0.0305	4.8577	2.3052
13	A	76.2488	0.0248	0.0075	0.0435
14	A	77.2155	0.0413	2.2231	0.8528
15	A	78.5354	0.0357	2.3149	3.2247
16	A	88.6469	0.0295	0.2141	7.0670

17	A	114.2677	0.0275	0.0399	0.3187
18	A	138.4691	0.1084	0.0772	0.0797
19	A	140.6904	0.2617	15.6513	7.0328
20	A	141.3950	0.1752	0.1476	0.3264
21	A	142.7271	0.2690	4.0803	6.8983
22	A	168.2365	0.0614	9.2003	6.0708
23	A	177.9259	0.3063	2.3951	5.2097
24	A	182.5758	0.1201	1.7939	3.6726
25	A	185.8958	0.0269	0.1814	0.1571
26	A	203.1641	0.0345	11.3114	10.3513
27	A	233.7863	0.6968	24.0586	75.8808
28	A	242.1586	0.6404	6.1896	62.2976
29	A	254.7267	0.6985	0.6114	0.1519
30	A	255.0738	0.7113	0.5914	0.1133
31	A	279.0418	0.8319	1.7353	6.3555
32	A	281.3467	0.8713	0.6531	3.6776
33	A	297.8776	0.1282	0.1740	0.1441
34	A	298.5438	0.9321	0.3604	0.6943
35	A	300.1983	0.3465	0.3708	0.7666
36	A	313.7954	0.2512	85.2942	14.4511
37	A	324.8486	1.0170	3.2694	1.1448
38	A	325.5639	1.0935	1.0121	3.4214
39	A	343.1911	1.2891	0.1698	1.3436
40	A	343.2759	1.2909	0.1301	1.3392
41	A	401.1587	0.2598	0.0082	0.0698
42	A	419.0803	0.2712	6.4687	5.5728
43	A	462.6692	2.2695	1.6426	2.6430
44	A	462.8287	2.2700	1.7474	3.1248
45	A	477.7729	0.4848	1.7850	1.9299
46	A	529.7575	2.9707	3.1946	0.4812
47	A	530.1113	2.9726	3.3041	0.4393
48	A	531.9790	2.6511	2.3391	22.8889
49	A	533.3485	2.9539	6.4330	18.9386
50	A	539.2253	0.5356	18.1314	0.9545
51	A	556.4333	3.2939	0.2290	0.0340
52	A	556.8791	3.2945	0.2751	0.0522
53	A	564.0679	0.5806	0.6917	0.5150
54	A	606.1562	3.8827	4.4960	1.9786
55	A	607.1587	3.8978	3.3268	1.9249
56	A	681.5304	1.8912	0.0792	3.6585
57	A	700.7970	4.7580	36.4731	0.0333
58	A	702.6749	4.7734	41.7161	0.0803
59	A	739.8094	5.3498	32.6848	34.1555
60	A	741.4123	5.4914	32.6020	33.4462
61	A	743.6566	1.0728	2.1796	1.2322
62	A	766.4971	1.7918	50.6836	35.9932
63	A	822.8210	0.6986	72.8487	3.0371
64	A	836.0137	0.5161	0.2814	0.1958
65	A	884.2160	6.1420	111.1589	105.8734
66	A	885.1008	6.1275	98.7154	125.6433
67	A	947.5847	7.5374	95.2801	0.2256
68	A	949.3950	7.5760	115.8383	0.1484
69	A	959.2844	1.5208	36.1241	11.3357
70	A	967.9276	0.7462	1.8594	1.8129
71	A	992.5176	0.8243	0.0422	0.1610
72	A	1021.5851	4.2979	71.0958	25.1120
73	A	1069.8820	1.0693	14.7336	0.6155
74	A	1089.6562	8.2128	92.2885	17.8015
75	A	1098.6143	1.5102	26.0717	34.2291
76	A	1101.9833	9.5747	119.0841	14.8763
77	A	1119.7955	0.9198	1.3125	2.5954
78	A	1122.4247	9.6225	35.6849	2.3787
79	A	1133.6824	9.8720	36.4577	1.6852
80	A	1139.5987	1.2863	1.1740	0.0135
81	A	1153.3608	10.2459	11.1822	0.3901
82	A	1161.1201	1.1616	90.9752	46.5394
83	A	1163.9321	10.4412	7.7576	0.5128
84	A	1189.7504	10.8036	423.6652	37.1384
85	A	1196.8640	1.6886	18.8684	16.0346
86	A	1199.8724	6.2332	258.3804	15.0530
87	A	1205.9088	10.4015	268.6318	7.5289

88	A	1211.7323	11.1055	429.5933	16.7268
89	A	1234.7834	2.4166	14.8206	0.5321
90	A	1251.1441	2.0882	498.4249	101.0405
91	A	1259.5356	9.2002	425.6620	101.0685
92	A	1259.8080	11.5280	232.8231	0.6273
93	A	1261.3470	2.2228	134.9696	28.5782
94	A	1267.1908	11.6243	269.3884	0.8360
95	A	1312.0870	8.0817	0.7034	4.5957
96	A	1369.0942	3.3635	117.6576	83.3288
97	A	1373.0733	1.4974	5.1551	0.8826
98	A	1448.5078	1.4984	0.0267	5.8531
99	A	1464.1539	2.5704	12.1219	2.5858
100	A	1482.1253	1.5353	6.4605	32.7671
101	A	1494.4827	1.3868	4.2677	1.2707
102	A	1504.1112	1.4629	23.8882	16.2242
103	A	1507.4756	1.4300	2.0551	3.6904
104	A	1528.2149	1.5056	41.9702	10.9785
105	A	1544.2689	2.8170	110.8709	7.9648
106	A	1592.7366	10.1899	27.0015	3.2253
107	A	1643.1184	8.1302	362.1154	100.6899
108	A	3001.2997	5.5722	32.0272	66.3425
109	A	3005.8428	5.6027	86.1182	343.2283
110	A	3100.7697	6.1423	3.2585	33.5214
111	A	3101.9958	6.1511	19.3985	73.9104
112	A	3133.2028	6.3853	3.1815	4.3724
113	A	3140.5142	6.4031	18.1824	107.5754
114	A	3162.5105	6.4174	10.6041	38.3629
115	A	3164.9286	6.4477	0.5830	56.1852
116	A	3226.4478	6.6984	5.9711	131.6400
117	A	3226.6358	6.6916	3.4520	27.3711

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	0.4742	0.0000	0.0055	0.0566
2	A	1.4032	0.0000	0.2486	0.1442
3	A	6.1085	0.0003	0.1570	1.1845
4	A	14.4582	0.0015	0.0464	0.0045
5	A	18.6909	0.0036	0.0294	0.3310
6	A	23.5819	0.0019	0.1113	1.6131
7	A	32.4416	0.0211	0.5254	0.2865
8	A	40.2197	0.0167	0.0299	0.0981
9	A	40.3534	0.0181	0.0056	0.0004
10	A	45.7761	0.0055	0.1755	3.6292
11	A	58.8944	0.0192	0.3298	0.4097
12	A	72.6976	0.0311	5.3480	2.1484
13	A	76.2819	0.0249	0.0080	0.0421
14	A	76.7538	0.0431	2.3019	0.5561
15	A	78.5980	0.0387	2.3761	3.0316
16	A	91.1547	0.0310	0.4387	10.1448
17	A	115.0938	0.0285	0.0404	0.3264
18	A	138.7870	0.1057	0.0808	0.0702
19	A	140.4887	0.2337	10.2448	5.4228
20	A	141.4111	0.1694	0.1495	0.3315
21	A	142.8399	0.2705	4.3559	4.8417
22	A	168.3502	0.0601	4.7685	2.8119
23	A	178.6253	0.3618	1.7430	4.3458
24	A	182.4663	0.1498	14.4550	12.8378
25	A	186.4267	0.0271	0.1787	0.1513
26	A	203.5727	0.0333	16.0349	9.3589
27	A	234.6495	0.7047	13.7342	76.4914
28	A	241.1326	0.6198	9.7706	60.7890
29	A	254.7882	0.7063	1.1683	0.1070
30	A	254.8264	0.7025	0.0201	0.1535
31	A	279.0595	0.8266	0.0079	7.4700
32	A	281.4540	0.8751	1.4694	4.0549
33	A	298.0249	0.1350	0.2308	0.1563
34	A	298.5736	0.8805	0.3176	0.7468
35	A	300.2578	0.3093	0.3523	0.7252

36	A	314.0303	0.2495	88.5507	16.0118
37	A	324.6630	1.0883	2.0524	2.8047
38	A	325.7688	1.0362	2.7171	1.2411
39	A	343.1166	1.2898	0.1006	1.1502
40	A	343.2322	1.2894	0.1669	1.4240
41	A	400.9403	0.2598	0.0044	0.0694
42	A	419.2738	0.2712	6.3618	5.6009
43	A	462.6259	2.2617	2.5622	3.4917
44	A	462.7920	2.2661	1.6181	4.0214
45	A	477.7831	0.4848	1.7668	1.9412
46	A	529.7815	2.9710	3.0840	0.4807
47	A	529.9932	2.9709	3.5562	0.4197
48	A	532.1240	2.9523	3.7800	21.2086
49	A	533.3730	2.8029	8.0954	15.3221
50	A	539.2187	0.5307	16.3214	2.4587
51	A	556.4342	3.2936	0.2302	0.0331
52	A	556.8503	3.2952	0.2610	0.0587
53	A	564.3258	0.5809	0.8502	0.5450
54	A	606.1910	3.8809	4.3324	2.1726
55	A	607.0373	3.8821	3.2816	1.6675
56	A	681.5318	1.8912	0.0814	3.6924
57	A	700.8274	4.7579	36.3970	0.0480
58	A	702.5328	4.7733	42.2494	0.0139
59	A	739.8500	5.5011	29.7728	32.5416
60	A	741.3296	5.4260	39.5875	33.8952
61	A	743.6444	1.0697	2.8679	2.3266
62	A	766.5326	1.7926	51.4170	35.9800
63	A	822.9090	0.6990	72.3483	2.8088
64	A	836.2119	0.5164	0.2604	0.2238
65	A	884.2988	6.1340	112.4765	104.9810
66	A	885.1434	6.1376	102.4715	124.0971
67	A	947.5513	7.5376	97.4513	0.2271
68	A	949.5634	7.5760	113.0239	0.1340
69	A	959.3455	1.5169	36.3007	11.3171
70	A	967.8430	0.7470	1.7564	1.8175
71	A	992.1974	0.8233	0.0555	0.1431
72	A	1021.5910	4.2983	71.7984	25.9632
73	A	1069.8552	1.0698	14.8016	0.5838
74	A	1088.9905	8.3433	100.2769	17.5510
75	A	1098.5667	1.5097	21.3415	35.2151
76	A	1104.2496	9.4732	89.9798	19.7659
77	A	1119.8449	0.9198	1.4550	2.6886
78	A	1122.0023	9.6018	35.7712	2.2190
79	A	1135.3625	9.9091	35.4575	2.0015
80	A	1139.5906	1.2865	1.2504	0.0177
81	A	1154.4031	10.2654	11.3874	0.4139
82	A	1159.9780	10.3656	5.1632	0.4005
83	A	1161.3581	1.1605	102.7510	47.5395
84	A	1189.9291	10.8225	422.1942	36.1409
85	A	1197.1033	1.5742	30.5874	19.4142
86	A	1199.8210	8.7863	316.6341	18.0262
87	A	1205.8062	10.5743	280.6545	9.6099
88	A	1211.3126	10.4705	264.3499	11.2405
89	A	1234.6953	2.4137	14.7610	0.5318
90	A	1251.2097	2.0972	562.8260	101.0784
91	A	1259.4478	6.2183	435.7612	81.9104
92	A	1260.6425	11.5447	234.3846	0.4555
93	A	1261.5498	2.5088	166.7943	38.9217
94	A	1267.0774	11.6219	270.3675	0.9272
95	A	1312.0582	8.0845	0.7173	4.8491
96	A	1368.9456	3.3618	116.3155	84.2282
97	A	1373.0708	1.4974	5.1530	0.9077
98	A	1448.5444	1.4989	0.0272	5.7938
99	A	1464.1478	2.5703	12.1759	2.6208
100	A	1482.2126	1.5356	6.7367	33.9908
101	A	1494.6455	1.3870	4.2086	1.2323
102	A	1504.2797	1.4641	24.5587	15.9676
103	A	1507.6086	1.4298	2.0035	3.7764
104	A	1528.4016	1.5062	42.2091	10.7596
105	A	1544.2881	2.8104	112.0348	8.6254
106	A	1592.7460	10.1882	27.0649	3.2465

107	A	1643.0966	8.1284	367.0801	101.5284
108	A	3001.3227	5.5725	31.9022	65.6444
109	A	3005.8525	5.6028	85.2995	341.1542
110	A	3100.9121	6.1426	3.2539	33.3157
111	A	3102.1506	6.1513	19.6051	72.0570
112	A	3133.3479	6.3860	3.2019	4.3658
113	A	3140.6305	6.4038	18.0353	104.6712
114	A	3162.5108	6.4174	10.6332	39.1467
115	A	3164.9293	6.4477	0.5802	56.5700
116	A	3226.4900	6.6985	6.0204	132.3683
117	A	3226.6760	6.6918	3.4592	27.4613

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-0.8539	0.0000	0.0617	0.0599
2	A	2.0183	0.0000	0.2277	0.1316
3	A	5.7877	0.0003	0.1385	1.1017
4	A	14.4336	0.0015	0.0454	0.0025
5	A	17.8543	0.0033	0.0103	0.2208
6	A	23.4831	0.0019	0.1168	1.5735
7	A	33.9900	0.0248	0.4668	0.2522
8	A	40.3316	0.0180	0.0161	0.0121
9	A	40.6084	0.0171	0.0176	0.0896
10	A	46.2469	0.0056	0.1751	3.6642
11	A	59.2026	0.0194	0.4207	0.4499
12	A	72.6357	0.0343	4.7865	1.7499
13	A	76.2108	0.0252	0.0218	0.0501
14	A	77.0911	0.0461	1.7789	0.4531
15	A	78.5855	0.0302	3.0966	3.9201
16	A	90.0295	0.0314	0.5313	7.7981
17	A	114.6146	0.0278	0.0396	0.3188
18	A	138.5311	0.1070	0.0778	0.0811
19	A	140.5678	0.2418	9.2080	5.6597
20	A	141.3775	0.1757	0.2843	0.3918
21	A	142.4648	0.2748	6.1939	6.0717
22	A	168.3541	0.0608	5.5337	3.6722
23	A	177.7318	0.3263	5.4361	4.0740
24	A	182.5555	0.1332	9.1521	12.4051
25	A	186.1902	0.0270	0.1831	0.1585
26	A	203.4380	0.0340	14.6221	7.9834
27	A	234.6440	0.7002	14.0338	74.2266
28	A	242.0436	0.6320	7.5150	59.6181
29	A	254.8128	0.6993	0.6347	0.1493
30	A	255.0766	0.7111	0.5663	0.1215
31	A	279.0063	0.8226	0.0274	7.2869
32	A	281.3451	0.8719	0.4457	4.2971
33	A	297.9321	0.1307	0.1880	0.1702
34	A	298.5550	0.9277	0.3552	0.6589
35	A	300.2288	0.3292	0.3595	0.7539
36	A	313.5969	0.2532	86.9756	16.2410
37	A	324.7618	1.0607	2.0865	2.9738
38	A	325.8168	1.0114	3.1470	0.7422
39	A	343.2419	1.2895	0.1764	1.3879
40	A	343.2742	1.2909	0.1348	1.3529
41	A	401.2126	0.2600	0.0059	0.0660
42	A	419.0814	0.2712	6.5935	5.5249
43	A	462.6589	2.2683	1.1067	1.5519
44	A	462.7982	2.2681	2.2943	4.4322
45	A	477.8216	0.4849	1.7874	1.9302
46	A	529.7846	2.9711	3.1287	0.4537
47	A	530.1280	2.9728	3.3380	0.4619
48	A	532.1241	2.9520	3.8237	21.1183
49	A	533.3570	2.9536	6.4549	18.5633
50	A	539.1345	0.5249	16.9419	2.6509
51	A	556.4332	3.2935	0.2299	0.0328
52	A	556.8735	3.2944	0.2746	0.0520
53	A	564.1928	0.5809	0.6757	0.5150
54	A	606.1899	3.8811	4.3389	2.1578

55	A	607.1517	3.8982	3.2794	1.9554
56	A	681.5375	1.8913	0.0792	3.6542
57	A	700.8303	4.7580	35.8547	0.0480
58	A	702.6782	4.7734	42.2367	0.0814
59	A	739.8503	5.5014	25.9724	32.9706
60	A	741.4123	5.4833	35.7546	33.7599
61	A	743.6930	1.0678	3.7874	1.7875
62	A	766.4952	1.7920	51.2945	35.7308
63	A	822.9351	0.6990	72.8038	2.8363
64	A	836.1389	0.5162	0.2739	0.2118
65	A	884.3059	6.1345	102.1570	105.0640
66	A	885.1031	6.1342	106.6855	125.3753
67	A	947.5655	7.5378	94.8301	0.2396
68	A	949.3968	7.5759	116.6251	0.1406
69	A	959.3647	1.5180	36.0787	11.5200
70	A	967.8881	0.7468	1.7180	1.8691
71	A	992.5235	0.8242	0.0560	0.1422
72	A	1021.5989	4.2979	71.5027	25.1514
73	A	1069.9185	1.0695	14.7324	0.6178
74	A	1088.9852	8.3455	100.8709	17.3822
75	A	1098.5974	1.5057	23.1700	33.4082
76	A	1101.9848	9.5666	119.7172	14.8336
77	A	1119.9180	0.9200	1.3946	2.6705
78	A	1121.9937	9.5979	35.9601	2.1802
79	A	1133.6865	9.8725	36.4896	1.6831
80	A	1139.6152	1.2859	1.1575	0.0243
81	A	1154.3836	10.2650	11.1961	0.4267
82	A	1161.1891	1.1613	90.8315	45.8022
83	A	1163.9341	10.4412	8.1229	0.5014
84	A	1189.8863	10.8260	455.4639	36.0871
85	A	1196.8821	1.6844	15.4765	16.7390
86	A	1199.8631	6.2718	290.8993	15.1879
87	A	1205.7296	10.3984	300.1860	9.0738
88	A	1211.8615	11.1587	345.7639	16.4509
89	A	1234.8546	2.4180	14.8259	0.5246
90	A	1251.1292	2.1072	380.0444	99.0757
91	A	1259.5810	6.3703	419.7261	92.6083
92	A	1259.8076	11.5269	231.0626	0.6587
93	A	1261.5050	2.4633	238.2984	37.0989
94	A	1267.0916	11.6222	270.2136	0.8712
95	A	1312.1268	8.0774	0.6997	4.7042
96	A	1369.0880	3.3638	117.8983	82.2246
97	A	1373.0965	1.4976	5.1592	0.8754
98	A	1448.5725	1.4991	0.0275	5.8700
99	A	1464.1781	2.5694	12.1257	2.6054
100	A	1482.2076	1.5357	6.4166	32.5356
101	A	1494.5278	1.3868	4.2769	1.2629
102	A	1504.1455	1.4630	23.6951	16.4594
103	A	1507.5758	1.4300	2.0461	3.7143
104	A	1528.3011	1.5056	41.9564	10.7676
105	A	1544.2805	2.8163	110.7823	7.7787
106	A	1592.7542	10.1899	26.9964	3.2541
107	A	1643.1347	8.1303	361.6186	100.6215
108	A	3001.3058	5.5723	32.0543	66.7877
109	A	3005.8520	5.6027	86.5029	345.6307
110	A	3100.7473	6.1422	3.2639	33.5407
111	A	3101.9712	6.1510	19.3559	74.0398
112	A	3133.1950	6.3852	3.1795	4.3492
113	A	3140.5075	6.4031	18.1943	107.4777
114	A	3162.5046	6.4174	10.5945	38.4114
115	A	3164.9246	6.4476	0.6204	56.2101
116	A	3226.4585	6.6984	5.9513	131.7462
117	A	3226.6460	6.6917	3.4537	27.4869

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-3.1340	0.0000	0.0908	0.4773
2	A	19.0055	0.0011	1.0210	5.4629

3	A	25.0425	0.0014	0.7413	3.8575
4	A	33.1467	0.0050	0.8300	0.6402
5	A	46.2165	0.0053	0.4790	2.8601
6	A	69.0208	0.0156	0.5679	6.8629
7	A	102.6979	0.0166	0.0152	0.1395
8	A	139.7498	0.0391	6.1070	5.1343
9	A	164.0104	0.0191	10.9888	6.4778
10	A	171.3783	0.0221	0.3269	0.1794
11	A	248.8404	0.0812	1.0379	16.3682
12	A	251.0109	0.0416	0.0701	0.3519
13	A	263.8735	0.0977	0.3094	0.9733
14	A	280.2121	0.1556	36.5483	17.7137
15	A	282.7449	0.0965	0.0188	0.0085
16	A	283.3160	0.0626	4.1910	6.6007
17	A	397.9470	0.2547	0.0262	0.1788
18	A	398.1432	0.2066	1.4759	3.4922
19	A	404.3060	0.2761	2.0011	5.1244
20	A	479.7868	0.4911	1.9934	2.8818
21	A	487.3501	0.3979	10.1095	89.3725
22	A	536.1370	0.5007	11.9311	1.7219
23	A	555.4309	0.5586	1.2165	0.8882
24	A	683.6771	1.9085	0.3639	3.9003
25	A	742.3467	1.0529	1.0799	0.6588
26	A	765.0082	1.7189	26.5829	20.7380
27	A	811.9685	0.6966	68.1008	0.5010
28	A	828.2492	0.5056	0.3053	0.5501
29	A	885.3060	1.2516	7.0430	21.5641
30	A	944.0116	0.5997	0.9262	0.2397
31	A	957.7555	0.7121	1.1848	0.1624
32	A	958.3245	0.7717	0.4189	0.5996
33	A	969.1113	1.5908	27.4443	9.4035
34	A	988.3178	0.8208	0.0305	0.2106
35	A	1008.2497	4.3029	38.3962	28.9504
36	A	1039.8504	0.7652	7.4741	4.8830
37	A	1079.1248	1.0437	16.4114	0.0464
38	A	1095.3476	1.4060	0.1544	6.7677
39	A	1125.9445	0.9363	0.2211	3.5484
40	A	1131.3160	1.2323	3.8089	0.1169
41	A	1138.7574	1.7679	0.5409	2.0224
42	A	1151.9543	1.0934	41.1630	4.3842
43	A	1171.9158	1.4334	79.4905	36.8986
44	A	1200.5636	1.4938	8.4820	5.7893
45	A	1233.3442	1.2113	62.9529	34.9675
46	A	1249.3507	2.9858	28.2904	0.6443
47	A	1256.7224	1.1642	25.3771	8.0004
48	A	1312.4495	6.3825	1.0129	10.5760
49	A	1356.9251	1.4470	1.0484	2.2456
50	A	1375.0913	1.5357	4.4853	1.0646
51	A	1386.4240	3.4273	93.5265	13.1623
52	A	1407.8127	1.4740	12.8628	2.5253
53	A	1422.9734	1.4579	4.8307	5.0078
54	A	1446.5931	1.6028	0.2153	7.4779
55	A	1458.9701	2.2916	4.3757	1.4421
56	A	1481.7276	1.3515	3.5999	4.6813
57	A	1483.0440	1.5618	15.9977	13.6770
58	A	1486.9479	1.3609	0.0845	11.0207
59	A	1490.2405	1.3692	3.6628	2.8465
60	A	1494.4806	1.3717	13.0909	13.1610
61	A	1497.9863	1.4220	22.1468	12.8936
62	A	1506.4081	1.3980	5.3602	1.4881
63	A	1508.5888	1.4409	0.9231	1.7137
64	A	1526.5082	1.5892	13.1237	7.6997
65	A	1544.5590	2.7435	118.1929	3.3087
66	A	1587.2673	9.9696	41.3101	1.5460
67	A	1637.6373	8.1230	305.1153	46.2578
68	A	2980.2044	5.5095	56.5156	90.5275
69	A	2986.0911	5.5494	109.7596	348.2157
70	A	3009.5568	5.5722	11.2160	43.2853
71	A	3014.9770	5.5888	65.4421	618.0072
72	A	3077.7388	6.0887	16.0395	148.1110
73	A	3078.9432	6.0622	1.1952	67.2695

74	A	3079.0498	6.0776	8.9548	3.1539
75	A	3080.1081	6.0570	31.8332	52.2485
76	A	3101.2457	6.1787	10.4134	101.5717
77	A	3114.2842	6.2969	10.7374	26.6638
78	A	3122.7903	6.3267	3.2685	2.3086
79	A	3122.8805	6.3114	20.8810	43.4480
80	A	3132.0984	6.3485	25.9061	101.6022
81	A	3139.7706	6.3187	38.3732	117.8533
82	A	3142.8571	6.3516	12.0385	150.0361
83	A	3215.0823	6.6476	3.7691	122.0001
84	A	3215.1317	6.6425	10.7162	21.4333

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-3.2866	0.0000	0.0051	0.7904
2	A	9.2441	0.0002	1.4150	0.1938
3	A	15.4289	0.0006	2.2235	0.2184
4	A	52.0056	0.0099	0.7725	2.9195
5	A	55.0583	0.0134	3.8718	4.9950
6	A	60.9531	0.0125	0.0278	0.5686
7	A	82.6076	0.0101	0.0107	1.1787
8	A	85.3778	0.0091	5.0690	0.3611
9	A	149.5634	0.0225	0.0568	3.9752
10	A	172.7937	0.0214	0.0990	0.1868
11	A	249.2797	0.0812	0.1233	27.8766
12	A	250.8370	0.0398	0.0166	0.2748
13	A	263.6098	0.1013	0.0953	0.5250
14	A	270.2736	0.1104	0.2614	0.9051
15	A	271.5335	0.1350	7.4761	1.3737
16	A	280.7654	0.0588	0.2006	18.2897
17	A	397.4024	0.2843	3.4588	11.1002
18	A	399.0829	0.2103	0.3781	8.9228
19	A	404.9632	0.2676	0.0185	0.2449
20	A	481.9896	0.4989	3.3103	2.6254
21	A	493.2185	0.4061	1.9162	149.8278
22	A	539.2357	0.4724	18.0580	1.4343
23	A	554.6055	0.6100	3.3936	2.8513
24	A	682.0298	1.8993	0.0268	3.3472
25	A	746.2403	1.0288	0.4299	0.2028
26	A	767.3695	1.7241	11.6745	23.3394
27	A	814.3893	0.7141	50.9048	0.7115
28	A	827.9758	0.5023	0.0008	0.3504
29	A	886.7080	1.2434	3.3745	33.5658
30	A	941.1933	0.5977	0.8965	0.2815
31	A	960.2624	0.7149	0.5080	1.0110
32	A	961.6538	0.7747	0.4110	1.0962
33	A	970.0671	1.6138	19.0921	27.1218
34	A	989.1422	0.8187	0.0038	0.2615
35	A	1011.9358	4.2137	77.3037	24.0955
36	A	1036.8790	0.7557	5.8941	5.1267
37	A	1079.9609	1.0410	21.9430	0.2000
38	A	1095.1240	1.4230	6.6489	22.0908
39	A	1132.2191	1.2051	0.9693	0.8086
40	A	1133.6062	0.9726	0.8998	1.6663
41	A	1136.0024	1.7010	0.0429	2.2390
42	A	1143.3115	1.0412	23.5060	3.4272
43	A	1172.4394	1.4648	72.0946	47.7486
44	A	1201.1026	1.4680	6.8263	10.7955
45	A	1231.9473	1.2162	81.6347	39.2332
46	A	1254.5904	1.1623	54.3885	24.4935
47	A	1256.7418	3.1427	35.5253	0.0148
48	A	1323.5605	5.7723	0.8398	10.0652
49	A	1355.2849	1.4354	0.9638	3.2971
50	A	1376.2649	1.5752	11.2340	0.0898
51	A	1396.1181	3.4167	155.5212	35.3721
52	A	1405.6539	1.4672	11.2394	2.5545
53	A	1420.9520	1.4558	5.3269	6.8894
54	A	1447.6739	1.5362	0.4982	11.0801

55	A	1463.1226	2.5174	1.4414	0.5296
56	A	1482.7784	1.3521	3.2638	6.8609
57	A	1485.3349	1.5910	22.1476	5.6220
58	A	1487.1206	1.3621	0.4753	9.7731
59	A	1487.8591	1.3580	2.1958	7.0236
60	A	1495.1986	1.3730	12.9542	13.6388
61	A	1495.8128	1.3927	17.8695	20.3073
62	A	1505.9011	1.3964	5.4134	1.9507
63	A	1514.3581	1.4645	3.9760	1.4777
64	A	1528.4880	1.6118	15.7391	16.0881
65	A	1550.0464	2.8661	144.1815	2.2321
66	A	1584.4850	9.9127	37.3687	2.3641
67	A	1641.8640	8.1086	413.7307	72.8794
68	A	2983.4175	5.5032	71.5571	76.3350
69	A	2989.8227	5.5489	79.9769	313.8833
70	A	3003.0899	5.5532	15.8858	52.8440
71	A	3008.5339	5.5703	99.8376	756.9378
72	A	3056.4712	5.9894	12.5711	112.0225
73	A	3057.5058	6.0035	48.3324	77.1128
74	A	3070.4218	6.0507	11.1115	170.6977
75	A	3072.9662	6.0666	3.7190	12.6114
76	A	3091.5931	6.1328	21.4446	133.8094
77	A	3107.7792	6.2687	13.6548	30.3184
78	A	3115.1841	6.2856	28.3436	49.7486
79	A	3120.7665	6.3017	2.5504	1.4581
80	A	3132.5116	6.3333	37.0359	188.9807
81	A	3144.7108	6.3396	25.0974	58.6172
82	A	3147.5859	6.3719	1.4662	73.4760
83	A	3212.9060	6.6390	8.9979	136.3870
84	A	3212.9925	6.6347	11.7914	51.1779

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.8445	0.0000	0.1342	0.5740
2	A	17.6797	0.0009	1.0655	5.0916
3	A	25.4818	0.0015	0.7980	4.0881
4	A	33.6542	0.0054	0.8420	0.2137
5	A	46.7355	0.0054	0.4860	2.7048
6	A	68.9801	0.0154	0.3357	6.7341
7	A	103.5509	0.0168	0.0159	0.1735
8	A	140.0764	0.0395	5.6898	5.2003
9	A	164.4986	0.0192	10.3542	6.5407
10	A	172.2873	0.0224	0.3881	0.2047
11	A	248.7989	0.0799	0.7433	16.5102
12	A	250.8567	0.0415	0.0741	0.6349
13	A	263.6356	0.0998	0.3760	0.9748
14	A	280.4813	0.1528	35.9349	15.3080
15	A	282.9800	0.0663	2.6084	5.4314
16	A	283.1472	0.0891	0.9595	0.8826
17	A	398.2381	0.2065	1.4834	4.1810
18	A	398.5077	0.2553	0.0271	0.1726
19	A	404.3975	0.2763	2.1534	4.8427
20	A	479.8137	0.4909	2.0709	3.0296
21	A	487.5096	0.3982	9.8841	82.5640
22	A	536.1860	0.5006	11.5790	1.8613
23	A	555.4666	0.5585	1.1142	1.0781
24	A	683.6869	1.9085	0.3582	3.8411
25	A	742.8335	1.0484	0.9782	0.6291
26	A	764.9972	1.7187	24.7331	20.4156
27	A	812.2201	0.6986	67.9941	0.5230
28	A	828.4384	0.5057	0.3283	0.5212
29	A	884.7815	1.2492	7.0900	21.0581
30	A	943.7106	0.5990	0.9539	0.2044
31	A	957.9849	0.7132	1.1534	0.1639
32	A	958.1973	0.7725	0.4124	0.6546
33	A	969.2025	1.5900	28.6050	9.2945
34	A	988.8965	0.8222	0.0290	0.1985
35	A	1008.2399	4.2993	38.2245	27.6968

36	A	1038.5847	0.7616	7.3362	4.4546
37	A	1079.2593	1.0438	16.4732	0.0580
38	A	1095.3094	1.4061	0.1578	6.7085
39	A	1126.0804	0.9369	0.2198	3.7108
40	A	1131.3104	1.2315	3.8696	0.1174
41	A	1138.5107	1.7654	0.6079	2.2870
42	A	1151.9696	1.0926	37.0917	3.8584
43	A	1171.5394	1.4305	76.8996	34.8396
44	A	1200.6485	1.4935	8.0930	5.7701
45	A	1232.6943	1.2155	61.7806	31.8012
46	A	1249.4624	2.9859	28.3836	0.6050
47	A	1256.7039	1.1642	25.2133	7.8462
48	A	1312.5485	6.3720	1.0230	10.1327
49	A	1356.0441	1.4466	0.9332	2.3740
50	A	1375.1204	1.5362	4.5170	1.0585
51	A	1386.6750	3.4260	91.9175	12.3994
52	A	1408.2702	1.4735	12.4165	2.4208
53	A	1423.4364	1.4578	5.6891	4.0345
54	A	1446.7039	1.6060	0.2106	7.4283
55	A	1459.0425	2.2871	4.3394	1.4352
56	A	1481.4485	1.3506	3.1743	5.6996
57	A	1483.1907	1.5620	16.0633	13.6017
58	A	1487.1208	1.3618	0.2977	9.0756
59	A	1490.3654	1.3693	3.1649	3.6625
60	A	1494.4044	1.3712	14.3521	12.4709
61	A	1498.0587	1.4227	21.8098	13.4265
62	A	1506.4831	1.3986	5.3592	1.6655
63	A	1508.8096	1.4410	1.1318	1.7687
64	A	1526.6376	1.5908	12.2484	7.7158
65	A	1544.6743	2.7399	113.8942	2.9874
66	A	1587.1753	9.9608	41.1359	1.5472
67	A	1637.6279	8.1204	294.9325	45.2405
68	A	2980.2887	5.5097	56.7058	92.4569
69	A	2986.1739	5.5496	112.0850	355.8344
70	A	3009.6918	5.5743	11.1143	43.5654
71	A	3015.1355	5.5909	62.5241	601.9493
72	A	3078.8345	6.0895	13.2478	128.7310
73	A	3078.9347	6.0449	8.1542	56.7097
74	A	3080.0744	6.0570	30.6497	56.8738
75	A	3080.5696	6.0988	3.3735	25.0954
76	A	3100.4535	6.1747	11.3907	111.6740
77	A	3114.5802	6.2998	11.1396	27.9057
78	A	3122.8210	6.3267	3.4275	2.4387
79	A	3123.0543	6.3146	21.6396	45.8593
80	A	3132.1352	6.3486	25.6571	104.4783
81	A	3139.6457	6.3181	38.3340	114.5437
82	A	3142.7324	6.3511	11.5532	147.3366
83	A	3215.0665	6.6477	3.4875	124.7766
84	A	3215.1152	6.6423	10.8936	18.6320

pyNR2-iC3H7I_trml

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-2.4148	0.0000	0.0007	0.4049
2	A	0.5844	0.0000	0.0000	0.3925
3	A	7.3653	0.0002	0.1886	1.9952
4	A	9.5607	0.0002	0.9715	0.2829
5	A	19.8108	0.0012	1.1378	0.5782
6	A	25.2364	0.0015	0.8109	3.4930
7	A	28.5648	0.0036	1.5862	1.7011
8	A	47.1248	0.0055	0.4559	2.7255
9	A	55.3457	0.0140	1.0464	3.3953
10	A	57.5244	0.0144	2.6506	3.2883
11	A	61.4582	0.0126	0.0261	0.5826
12	A	69.8690	0.0144	0.3078	9.8981
13	A	103.0352	0.0163	0.0071	0.1399
14	A	146.7432	0.0481	12.3585	7.8756
15	A	161.3639	0.0181	8.4752	6.4217
16	A	171.9869	0.0222	0.1841	0.2178

17	A	248.8541	0.0815	1.1902	14.8661
18	A	249.3959	0.0812	0.0774	30.0623
19	A	250.8068	0.0397	0.0158	0.2648
20	A	251.2476	0.0417	0.0698	0.3335
21	A	263.7781	0.0974	0.3263	0.9278
22	A	265.7070	0.1092	0.0915	1.2906
23	A	280.5633	0.0639	5.0566	23.2803
24	A	281.2748	0.1215	30.1350	16.4614
25	A	283.5099	0.0643	6.3337	6.5184
26	A	283.6054	0.1006	0.0220	0.1196
27	A	398.1178	0.2063	1.4350	3.7404
28	A	399.0322	0.2079	0.7512	5.7430
29	A	400.9127	0.2604	0.0197	0.2064
30	A	406.9374	0.2799	2.7675	12.7012
31	A	480.7476	0.4936	2.5300	2.2346
32	A	487.1956	0.3978	11.3603	88.1947
33	A	493.3677	0.4063	2.0744	162.2044
34	A	536.7200	0.4873	13.3483	4.5899
35	A	556.9586	0.5880	0.2742	2.0103
36	A	682.6404	1.8996	0.0512	3.1313
37	A	742.5036	1.0630	1.2866	0.4253
38	A	766.7506	1.7319	31.8682	26.9178
39	A	812.5033	0.6930	67.0040	0.9490
40	A	828.2090	0.5052	0.3084	0.4167
41	A	885.2326	1.2519	7.3913	21.4259
42	A	886.6931	1.2431	3.2795	36.3637
43	A	941.0909	0.5976	0.8773	0.2988
44	A	944.2106	0.6000	0.9129	0.2479
45	A	958.1418	0.7714	0.4140	0.5784
46	A	959.3202	0.7187	1.3417	0.9632
47	A	961.7297	0.7747	0.3997	1.1138
48	A	969.1998	1.5725	28.4227	18.7210
49	A	987.5917	0.8166	0.0398	0.2320
50	A	1013.2581	4.2817	69.0944	29.3094
51	A	1036.7268	0.7553	6.2339	5.1130
52	A	1040.0893	0.7660	8.1206	4.8292
53	A	1079.7690	1.0462	17.0056	0.0242
54	A	1096.6520	1.4222	7.6471	22.2952
55	A	1127.0949	0.9319	0.4030	3.4925
56	A	1133.2965	1.3040	1.9696	0.6955
57	A	1135.9887	1.6464	0.0005	1.6092
58	A	1138.9629	1.7674	0.5466	1.9708
59	A	1151.1294	1.0868	55.9691	10.2427
60	A	1171.7772	1.4352	111.1822	25.7133
61	A	1172.5637	1.4621	44.2850	66.8074
62	A	1200.9147	1.4876	11.9182	9.4196
63	A	1231.8129	1.2163	90.3605	32.4528
64	A	1233.5048	1.2110	54.7592	50.4415
65	A	1251.1314	2.9416	26.0421	0.2313
66	A	1255.0740	1.1611	48.1398	23.5450
67	A	1318.1806	6.5977	0.8119	7.3383
68	A	1355.2263	1.4348	0.9801	3.3474
69	A	1357.1002	1.4475	1.0709	2.1696
70	A	1374.5370	1.5364	7.1406	0.3012
71	A	1388.5510	3.4050	132.1169	47.8903
72	A	1405.5411	1.4669	11.1525	2.6295
73	A	1407.9003	1.4742	13.0254	2.5919
74	A	1420.8377	1.4555	5.3042	7.6294
75	A	1423.0567	1.4580	4.8033	5.1768
76	A	1447.8089	1.5385	0.0784	8.2759
77	A	1461.8195	2.4732	5.1825	1.0984
78	A	1481.7223	1.3516	3.5674	4.3937
79	A	1482.7916	1.3521	3.2648	6.8252
80	A	1483.5033	1.5652	18.3235	13.1614
81	A	1486.9606	1.3609	0.0850	10.3746
82	A	1487.1265	1.3622	0.4691	9.8868
83	A	1490.4617	1.3690	3.5684	3.1516
84	A	1494.4575	1.3717	12.8102	13.3082
85	A	1495.2059	1.3730	12.1127	14.5981
86	A	1498.2970	1.4175	21.8216	15.7774
87	A	1505.8773	1.3964	5.5023	2.0573

88	A	1506.4575	1.3981	5.3390	1.5811
89	A	1509.2158	1.4489	0.8746	1.2838
90	A	1526.8916	1.5780	22.0799	14.8788
91	A	1547.3538	2.8443	130.3515	3.9375
92	A	1588.0710	10.1192	32.7865	2.2377
93	A	1640.4962	8.1230	393.0078	83.0675
94	A	2982.4735	5.5148	55.6874	94.4845
95	A	2988.2995	5.5547	110.6430	349.5665
96	A	3002.7983	5.5523	15.9599	54.7205
97	A	3008.2420	5.5694	106.4518	786.1272
98	A	3009.8692	5.5732	10.9451	43.6511
99	A	3015.2923	5.5898	65.2463	635.8090
100	A	3070.0761	6.0490	10.9097	168.9561
101	A	3072.6846	6.0653	3.6781	12.5475
102	A	3078.1382	6.0460	6.3217	60.8262
103	A	3078.1419	6.0899	18.4571	141.5067
104	A	3079.2278	6.0602	30.0157	63.1077
105	A	3079.3503	6.0980	3.3912	10.4189
106	A	3091.1757	6.1309	22.1757	136.1878
107	A	3101.8692	6.1818	9.9818	97.7558
108	A	3107.5112	6.2675	13.5861	29.4980
109	A	3114.6842	6.2986	10.4839	26.2366
110	A	3114.8567	6.2844	28.1226	49.1287
111	A	3123.3920	6.3130	20.3109	41.4453
112	A	3123.6994	6.3285	2.7055	1.6697
113	A	3133.3104	6.3515	27.7407	128.8596
114	A	3145.1306	6.3416	24.6622	60.1423
115	A	3148.0375	6.3743	1.6389	73.9488
116	A	3216.9638	6.6566	7.5113	131.2076
117	A	3217.0440	6.6502	9.5617	24.3333

pyNR2-iC3H7I_trm2

NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	-2.4138	0.0000	0.0022	0.3929
2	A	-2.2329	0.0000	0.0026	0.6461
3	A	6.8322	0.0002	0.1632	2.1795
4	A	9.5276	0.0002	0.9498	0.2345
5	A	18.7532	0.0011	1.2584	0.3779
6	A	24.7980	0.0014	0.8408	3.2545
7	A	28.4769	0.0040	1.5954	0.9555
8	A	47.1675	0.0055	0.4562	2.7013
9	A	55.4276	0.0142	1.4503	3.4129
10	A	57.8200	0.0146	1.9983	2.8947
11	A	61.4602	0.0126	0.0264	0.5596
12	A	69.3583	0.0140	0.1597	9.4251
13	A	102.3769	0.0161	0.0067	0.1563
14	A	146.5852	0.0486	12.2080	8.1545
15	A	160.2651	0.0178	7.1876	6.2676
16	A	171.3944	0.0220	0.1848	0.2049
17	A	248.8868	0.0819	0.8613	17.6490
18	A	249.3867	0.0812	0.2396	25.3900
19	A	250.7918	0.0397	0.0159	0.2626
20	A	251.0293	0.0411	0.0669	0.2920
21	A	263.6203	0.0999	0.3152	0.9718
22	A	265.6949	0.1093	0.0941	1.2658
23	A	280.5460	0.0639	4.8215	24.0252
24	A	281.2628	0.1243	30.3257	12.8574
25	A	283.3161	0.0636	3.9338	6.0812
26	A	283.3221	0.1004	0.0465	0.1543
27	A	398.1907	0.2063	1.5964	3.9834
28	A	399.0375	0.2079	0.7581	5.7828
29	A	401.6149	0.2610	0.0226	0.1932
30	A	406.7434	0.2802	3.0925	12.2982
31	A	480.7960	0.4937	2.5599	2.2102
32	A	487.2799	0.3977	10.3736	79.7161
33	A	493.3518	0.4063	2.0831	158.9121
34	A	536.6394	0.4867	12.9393	4.7270
35	A	556.9202	0.5888	0.4418	2.1074

36	A	682.6391	1.8997	0.0491	3.0710
37	A	742.9727	1.0591	1.1456	0.4048
38	A	766.7363	1.7321	29.0595	26.1674
39	A	812.5977	0.6943	66.9113	0.8985
40	A	828.2098	0.5052	0.3452	0.3947
41	A	884.5897	1.2486	7.4678	20.1804
42	A	886.6846	1.2430	3.2595	35.7325
43	A	941.0820	0.5976	0.8736	0.2939
44	A	943.8949	0.5991	0.9489	0.1892
45	A	957.9882	0.7724	0.4367	0.6543
46	A	959.5003	0.7201	1.3132	1.0295
47	A	961.7282	0.7748	0.3967	1.1155
48	A	969.2654	1.5700	29.7438	18.6503
49	A	988.1996	0.8181	0.0374	0.2296
50	A	1013.2544	4.2744	68.6470	27.6732
51	A	1036.6950	0.7553	6.1117	5.2215
52	A	1038.4201	0.7613	7.1419	4.6783
53	A	1079.8158	1.0461	17.0595	0.0306
54	A	1096.6084	1.4223	7.5419	21.7033
55	A	1127.1761	0.9321	0.3989	3.6779
56	A	1133.2942	1.3043	2.0046	0.6698
57	A	1135.9834	1.6456	0.0002	1.6354
58	A	1138.5673	1.7639	0.5566	2.2670
59	A	1150.9713	1.0855	50.5197	9.1870
60	A	1171.3550	1.4292	85.9148	29.2116
61	A	1172.5179	1.4640	63.4985	56.7895
62	A	1200.9284	1.4870	11.3225	9.3645
63	A	1231.7028	1.2168	90.7216	28.5113
64	A	1232.7444	1.2163	51.8200	46.4159
65	A	1251.3188	2.9438	26.1847	0.2190
66	A	1255.0447	1.1611	47.9450	22.8481
67	A	1318.3534	6.5816	0.8127	6.9769
68	A	1355.2082	1.4348	1.0018	3.3082
69	A	1356.0964	1.4466	0.8065	2.3767
70	A	1374.5763	1.5371	7.1987	0.3045
71	A	1388.8501	3.4042	129.9791	44.9364
72	A	1405.5491	1.4669	11.2347	2.6102
73	A	1408.4090	1.4741	12.2672	2.3510
74	A	1420.8464	1.4555	5.2760	7.5499
75	A	1423.5289	1.4577	5.5426	3.4473
76	A	1447.8549	1.5386	0.0697	8.2675
77	A	1461.8807	2.4742	5.1402	1.1187
78	A	1481.3215	1.3500	3.3258	6.4624
79	A	1482.7910	1.3521	3.2435	6.7866
80	A	1483.5697	1.5656	18.1786	12.3645
81	A	1487.1268	1.3622	0.4634	9.4983
82	A	1487.2394	1.3619	0.2810	8.8878
83	A	1490.3511	1.3686	3.2653	4.5552
84	A	1494.3518	1.3710	14.0310	11.8246
85	A	1495.2091	1.3730	12.0514	14.5007
86	A	1498.1714	1.4172	21.2738	16.9452
87	A	1505.8752	1.3964	5.5324	2.0669
88	A	1506.6548	1.3988	5.7139	1.3935
89	A	1509.2845	1.4495	0.8558	1.3416
90	A	1526.8667	1.5778	20.7842	14.8054
91	A	1547.4465	2.8488	124.8604	3.2936
92	A	1587.9696	10.1123	32.6615	2.2298
93	A	1640.5074	8.1211	379.7784	80.2909
94	A	2982.5789	5.5149	56.0001	97.0378
95	A	2988.4112	5.5549	113.4504	359.4280
96	A	3002.8179	5.5524	15.9477	54.3232
97	A	3008.2593	5.5695	105.1794	781.3970
98	A	3010.0042	5.5754	10.9078	43.4879
99	A	3015.4436	5.5919	60.1019	597.6666
100	A	3070.0874	6.0490	10.8435	168.1936
101	A	3072.7056	6.0654	3.6837	12.5188
102	A	3077.8933	6.0455	6.8023	58.2558
103	A	3078.9318	6.0594	39.2939	30.6975
104	A	3079.6398	6.0928	6.4177	169.2738
105	A	3080.9508	6.1004	3.0651	13.4099
106	A	3091.1470	6.1308	22.1194	134.4955

107	A	3100.7408	6.1766	11.0194	116.8467
108	A	3107.5065	6.2675	13.5830	29.3926
109	A	3114.8015	6.3017	11.1072	27.5680
110	A	3114.8477	6.2844	28.0707	48.8503
111	A	3123.4350	6.3158	21.9098	47.4805
112	A	3123.6537	6.3280	2.6709	1.6226
113	A	3133.3022	6.3512	27.5009	133.4518
114	A	3145.0121	6.3411	24.6118	57.9173
115	A	3147.9192	6.3738	1.5028	72.7377
116	A	3216.9469	6.6565	7.3671	130.6976
117	A	3217.0281	6.6502	9.5254	24.7756

pyNR2-iC3H7I_trm3

NM# Symm Wavenumber Force Const IR Intens Raman Activ

pyNR2-iC3H7I_trm4

NM# Symm Wavenumber Force Const IR Intens Raman Activ

1	A	1.7245	0.0000	0.0104	0.3598
2	A	3.8411	0.0000	0.0014	0.5541
3	A	6.8522	0.0001	0.1461	1.5613
4	A	10.3988	0.0003	0.9973	0.6353
5	A	18.5485	0.0010	1.2414	0.6290
6	A	24.8490	0.0014	0.8400	3.6867
7	A	28.4857	0.0039	1.4819	0.7115
8	A	47.0924	0.0056	0.5002	2.4007
9	A	53.2935	0.0115	1.2222	2.0278
10	A	58.3889	0.0148	2.0090	3.0208
11	A	63.4147	0.0150	0.3502	2.0124
12	A	69.3925	0.0141	0.1305	8.8430
13	A	102.2059	0.0160	0.0074	0.1691
14	A	146.5456	0.0484	11.8502	7.5849
15	A	160.5081	0.0179	7.4860	6.1967
16	A	171.4871	0.0221	0.1839	0.2480
17	A	248.8257	0.0798	0.9087	15.1028
18	A	249.3268	0.0802	0.0198	27.1911
19	A	250.3166	0.0398	0.0735	0.2436
20	A	250.8147	0.0416	0.0760	0.7135
21	A	263.4964	0.0992	0.4235	0.8785
22	A	265.0674	0.1091	2.7260	3.1773
23	A	280.7659	0.0602	1.6511	22.4353
24	A	281.8447	0.1215	26.0780	14.4107
25	A	282.8186	0.0988	0.1827	0.2452
26	A	283.2305	0.0693	8.1122	4.2712
27	A	398.1805	0.2063	1.5633	3.9535
28	A	399.4835	0.2087	0.8710	5.7761
29	A	401.6491	0.2610	0.0247	0.2247
30	A	406.7184	0.2801	3.1570	13.0207
31	A	480.7281	0.4927	2.7876	2.9920
32	A	487.3535	0.3981	10.3240	79.2142
33	A	493.4197	0.4066	1.7977	157.7893
34	A	536.6537	0.4872	13.1036	3.5051
35	A	556.9069	0.5885	0.3834	2.2999
36	A	682.6376	1.8995	0.0572	3.1219
37	A	742.8750	1.0605	1.1272	0.4203
38	A	766.7384	1.7320	28.7285	25.8338
39	A	812.6267	0.6938	66.7467	0.9009
40	A	828.4032	0.5054	0.3517	0.3913
41	A	884.6206	1.2489	7.4642	19.8206
42	A	886.7968	1.2435	3.3241	35.6480
43	A	940.9756	0.5971	0.9002	0.2783
44	A	943.7861	0.5990	0.9624	0.1944
45	A	957.9970	0.7724	0.4219	0.6289
46	A	959.4723	0.7200	1.3494	0.9283
47	A	961.6641	0.7752	0.3979	1.0535
48	A	969.2476	1.5694	29.7664	18.6281
49	A	988.4165	0.8184	0.0333	0.1947
50	A	1013.2510	4.2775	68.6755	28.0060

51	A	1036.7531	0.7555	6.1198	4.4458
52	A	1038.5906	0.7617	7.1213	4.7465
53	A	1079.7422	1.0460	17.0913	0.0281
54	A	1096.6188	1.4224	7.4804	21.6818
55	A	1127.1953	0.9315	0.4233	3.8156
56	A	1133.8216	1.2293	1.7085	0.0763
57	A	1135.4488	1.7823	0.3510	2.3282
58	A	1138.6214	1.7638	0.6252	2.3685
59	A	1150.9626	1.0855	50.2280	9.2240
60	A	1171.3319	1.4296	80.9762	29.4660
61	A	1172.5843	1.4640	67.2743	55.2658
62	A	1200.8923	1.4870	11.2336	9.4190
63	A	1231.6518	1.2166	88.0152	30.4127
64	A	1232.7376	1.2157	53.4896	43.5585
65	A	1251.3363	2.9442	26.2750	0.2358
66	A	1255.0619	1.1612	47.9112	22.9160
67	A	1318.3339	6.5803	0.8163	7.0179
68	A	1354.7123	1.4356	1.0626	3.3338
69	A	1356.0143	1.4473	0.9281	2.4151
70	A	1374.6045	1.5372	7.1613	0.3037
71	A	1388.8208	3.4048	129.9224	44.2821
72	A	1405.5951	1.4659	10.8759	2.7125
73	A	1408.3999	1.4736	12.3177	2.3885
74	A	1420.9995	1.4557	5.4112	7.4848
75	A	1423.5799	1.4579	5.6034	3.5712
76	A	1447.7996	1.5371	0.0754	8.2179
77	A	1461.8925	2.4777	5.1836	1.2098
78	A	1481.3476	1.3504	3.1769	5.9320
79	A	1482.8037	1.3520	3.1087	7.4831
80	A	1483.5542	1.5652	18.0340	13.0289
81	A	1487.0378	1.3621	0.6231	9.1151
82	A	1487.1360	1.3619	0.3046	9.4631
83	A	1490.2956	1.3685	3.1281	3.9137
84	A	1494.3623	1.3711	14.4137	12.2443
85	A	1495.2531	1.3731	12.3173	14.2366
86	A	1498.1513	1.4170	21.1571	16.6242
87	A	1505.7892	1.3962	5.3820	1.9802
88	A	1506.5099	1.3987	5.4657	1.5427
89	A	1509.3809	1.4494	1.0940	1.3484
90	A	1526.9322	1.5779	20.7128	14.6202
91	A	1547.4206	2.8483	125.1365	3.1243
92	A	1587.9840	10.1121	32.9546	2.2662
93	A	1640.5058	8.1207	379.5121	80.6435
94	A	2982.6001	5.5149	56.1245	97.6746
95	A	2988.4351	5.5549	114.0139	361.1671
96	A	3002.7130	5.5523	15.7484	54.1627
97	A	3008.1833	5.5695	104.3014	776.3529
98	A	3009.9537	5.5754	10.8094	43.3377
99	A	3015.4004	5.5919	60.5834	596.3288
100	A	3069.8500	6.0481	10.8690	164.6725
101	A	3072.5587	6.0651	3.5356	12.6442
102	A	3077.7586	6.0454	7.4741	58.3793
103	A	3078.8408	6.0602	40.4835	22.9532
104	A	3079.2623	6.0909	3.7811	159.7929
105	A	3081.0513	6.1003	3.8312	28.6494
106	A	3091.2591	6.1304	22.6535	137.9346
107	A	3100.8597	6.1766	11.1649	114.8048
108	A	3107.9273	6.2684	13.7343	29.9030
109	A	3114.9523	6.3014	9.3551	27.6967
110	A	3114.9988	6.2856	29.2401	51.5141
111	A	3123.4838	6.3164	21.8686	46.4560
112	A	3123.6287	6.3278	2.3278	1.4934
113	A	3133.2925	6.3511	27.5256	132.7649
114	A	3145.0524	6.3413	24.6790	58.6235
115	A	3147.9530	6.3739	1.5845	73.9558
116	A	3216.9310	6.6564	7.3795	131.1188
117	A	3217.0151	6.6502	9.5142	25.3464

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.3682	0.0000	0.8807	0.2084
2	A	11.6577	0.0011	0.2237	0.6150
3	A	16.7026	0.0017	0.2380	1.4703
4	A	26.0651	0.0021	0.0417	4.2034
5	A	43.5242	0.0073	0.2139	2.9815
6	A	45.4001	0.0100	0.1181	2.1850
7	A	79.3272	0.0503	0.5507	0.6496
8	A	83.8211	0.0256	1.5440	4.1100
9	A	114.7017	0.0454	2.9036	2.2738
10	A	122.2005	0.0444	1.7173	0.9743
11	A	156.4819	0.0476	2.9475	2.6561
12	A	160.6543	0.1693	0.4131	2.0518
13	A	187.8732	0.0279	0.3614	0.2119
14	A	205.9015	0.0320	8.3734	6.4923
15	A	220.1986	0.5092	1.3572	1.2030
16	A	239.1653	0.6478	4.1812	46.0950
17	A	258.1148	0.7598	3.4497	6.1306
18	A	275.6307	0.8271	6.6164	5.5238
19	A	295.5367	0.0954	0.0229	0.0065
20	A	302.9663	1.0038	2.6148	0.8454
21	A	316.8546	0.2394	72.1411	7.8608
22	A	324.3634	1.1342	1.1406	2.6517
23	A	347.5916	1.3091	0.0660	1.2438
24	A	392.3050	0.2431	0.0110	0.1277
25	A	395.4979	1.6556	0.5382	2.4144
26	A	413.5831	0.2668	7.7522	2.4307
27	A	460.7614	2.2093	2.6308	4.2524
28	A	474.8916	0.4787	1.3108	2.6525
29	A	527.8266	2.9340	8.9497	0.7016
30	A	535.8802	0.5381	10.4416	1.6734
31	A	563.5882	0.5457	2.7869	0.1607
32	A	578.6860	3.5091	0.6349	9.2721
33	A	614.2755	3.8601	5.9258	1.1612
34	A	645.3377	4.2877	8.1390	11.3565
35	A	684.0713	1.9062	0.3883	4.1350
36	A	741.1293	5.4489	39.8624	14.8075
37	A	743.5098	1.0358	2.9732	1.2334
38	A	760.9622	1.7469	45.7582	18.1041
39	A	818.2863	0.6955	75.7068	2.2641
40	A	834.3692	0.5150	0.3362	0.3364
41	A	873.8526	5.9635	189.1608	54.2279
42	A	958.6965	1.1659	30.4791	2.3588
43	A	963.4809	0.8620	11.5308	1.8827
44	A	992.8389	0.8337	0.0224	0.1325
45	A	1010.9261	4.4833	18.9224	34.3925
46	A	1018.5213	8.3253	230.4672	34.3053
47	A	1069.2394	1.0593	14.7294	0.7222
48	A	1098.1566	1.4112	0.4877	4.4731
49	A	1102.7306	9.4845	70.9274	10.0953
50	A	1108.2091	9.5678	28.4191	0.8550
51	A	1119.0834	0.9217	0.9612	2.7673
52	A	1131.4964	1.2721	3.3824	0.0132
53	A	1155.0397	10.2488	130.0620	8.2303
54	A	1163.4288	1.1826	59.7291	14.7799
55	A	1190.6332	8.6241	461.6735	8.0130
56	A	1195.4055	1.5880	16.4885	7.4967
57	A	1202.9176	10.4771	326.4980	3.5821
58	A	1232.2878	2.7817	18.4236	3.0613
59	A	1232.6148	8.4895	158.6303	18.3870
60	A	1258.2818	1.1705	17.9244	9.1025
61	A	1300.8043	7.6246	0.7084	9.2330
62	A	1318.0134	12.7621	59.4761	13.6546
63	A	1359.6071	3.3834	67.8678	31.3546
64	A	1372.9509	1.4988	2.3141	2.1352
65	A	1445.4058	1.6614	0.6023	5.0442
66	A	1456.3800	2.1192	8.5891	3.1629
67	A	1480.8266	1.5311	4.7939	26.9386
68	A	1493.5614	1.3823	4.6688	1.0461
69	A	1502.5874	1.4733	23.6504	14.0418

70	A	1507.0595	1.4166	1.6422	4.7709
71	A	1527.9478	1.5092	24.2145	4.5349
72	A	1537.6511	2.6530	88.4173	4.6905
73	A	1595.3736	10.3215	37.1448	1.8896
74	A	1633.3165	8.1294	244.0571	52.7418
75	A	2994.2164	5.5529	35.4861	68.0001
76	A	2999.0672	5.5842	98.4322	340.7148
77	A	3097.2305	6.1171	4.1173	32.0701
78	A	3098.9276	6.1252	20.7280	80.8151
79	A	3129.1862	6.3696	4.7048	6.9595
80	A	3135.9081	6.3870	19.0186	78.9168
81	A	3146.7422	6.3488	30.3372	111.2210
82	A	3149.7753	6.3824	8.8801	143.6289
83	A	3219.0584	6.6655	2.1345	132.9725
84	A	3219.1665	6.6588	8.4423	9.0977

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.7636	0.0000	0.0298	3.7704
2	A	12.6899	0.0012	0.1401	0.1181
3	A	14.2336	0.0008	0.7797	1.3793
4	A	20.3622	0.0019	0.3920	0.3476
5	A	30.9961	0.0014	2.0419	0.7564
6	A	61.1848	0.0114	0.9988	0.0906
7	A	71.9030	0.0247	0.3286	0.1898
8	A	74.4893	0.0274	7.4307	1.3213
9	A	79.3589	0.0082	0.0020	1.2588
10	A	91.0618	0.0530	0.8278	0.2352
11	A	120.7539	0.1302	4.6570	1.3838
12	A	153.5891	0.0498	0.0978	0.7118
13	A	166.0448	0.0643	2.1644	5.8080
14	A	180.8873	0.0226	0.0303	0.1287
15	A	219.9993	0.5289	0.4630	4.4704
16	A	234.0955	0.7249	11.9877	60.0721
17	A	253.5598	0.1875	0.7634	1.3459
18	A	258.7710	0.2264	3.6939	2.7803
19	A	276.3152	0.3545	7.1471	5.5661
20	A	278.6112	0.1777	4.8817	0.4090
21	A	302.0816	0.9873	1.8777	1.0420
22	A	324.6352	1.1342	0.8753	2.9720
23	A	347.6964	1.3080	0.0967	1.4033
24	A	394.1694	0.3199	8.7906	14.8310
25	A	396.1921	1.3375	0.7488	0.6504
26	A	411.9994	0.2826	0.0027	0.1372
27	A	460.2530	2.2319	1.6505	4.8152
28	A	484.9971	0.5093	3.5710	2.4442
29	A	527.3931	2.9179	10.8802	0.8211
30	A	540.0165	0.4457	16.9922	0.4585
31	A	556.8832	0.6793	8.2900	1.2323
32	A	577.3112	3.5024	0.9949	10.8715
33	A	610.6942	3.8109	5.5388	1.2841
34	A	644.0030	4.2792	7.7666	12.3337
35	A	680.1679	1.8930	0.0146	3.6034
36	A	740.3916	5.4764	41.2027	18.5349
37	A	747.0728	1.0274	0.0782	0.1255
38	A	770.0438	1.7621	8.3277	35.6491
39	A	817.5446	0.7240	52.3026	0.8834
40	A	828.9891	0.5019	0.0002	0.2149
41	A	875.0831	6.0388	191.7632	56.9590
42	A	964.1136	0.7190	0.2747	1.0847
43	A	969.7947	1.6466	9.6190	32.3081
44	A	989.1008	0.8120	0.0024	0.2647
45	A	1015.4595	5.9530	228.1567	12.4409
46	A	1019.9668	5.2399	90.7226	37.1794
47	A	1080.0050	1.0476	23.1643	0.6618
48	A	1088.5117	7.1995	96.2435	2.7930
49	A	1092.7211	1.8254	21.6333	17.4614
50	A	1099.6290	4.8274	16.1502	30.3968

51	A	1137.8291	1.0821	0.4692	0.8588
52	A	1138.1854	1.0558	0.6848	0.9893
53	A	1139.6041	1.0122	4.0213	0.9950
54	A	1148.8076	10.1006	146.0990	12.4861
55	A	1183.7327	10.6799	522.5698	7.4925
56	A	1199.6324	10.9769	324.5576	3.2696
57	A	1202.4198	1.4513	9.1908	10.3113
58	A	1229.9535	9.7045	172.9319	24.8948
59	A	1253.5761	1.1722	59.3495	18.1147
60	A	1260.8577	2.9571	35.8354	0.2133
61	A	1318.5320	12.7355	73.9973	15.8506
62	A	1331.0211	5.6298	1.2300	8.2742
63	A	1377.7717	1.6039	13.2414	0.0014
64	A	1404.8469	3.2553	178.6244	29.1937
65	A	1449.5528	1.4766	0.1487	12.1102
66	A	1469.8867	2.7822	2.0015	0.3383
67	A	1486.6153	1.6031	22.1400	6.7105
68	A	1487.3620	1.3530	0.3157	7.4253
69	A	1496.2367	1.3780	17.4654	20.2473
70	A	1516.3597	1.4904	4.2981	0.5903
71	A	1529.4505	1.5934	21.3391	16.4255
72	A	1557.7710	3.1536	168.1690	2.1760
73	A	1580.7667	9.5110	33.7399	3.1453
74	A	1648.6642	8.1295	463.9063	63.5873
75	A	2998.5578	5.5095	77.6364	57.9517
76	A	3004.8703	5.5515	50.8119	345.5897
77	A	3048.8833	6.0238	2.6178	141.7774
78	A	3049.8767	6.0432	58.4766	43.4613
79	A	3128.7124	6.3281	1.9539	0.9920
80	A	3141.5874	6.3650	31.0430	196.0194
81	A	3155.8204	6.3877	15.1539	41.0167
82	A	3158.2464	6.4169	0.0710	59.0007
83	A	3217.7232	6.6619	8.1128	150.5647
84	A	3217.8414	6.6561	7.4191	43.1774

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.3743	0.0000	0.8806	0.2082
2	A	11.6577	0.0011	0.2239	0.6148
3	A	16.6985	0.0017	0.2380	1.4706
4	A	26.0641	0.0021	0.0417	4.2052
5	A	43.5246	0.0073	0.2139	2.9792
6	A	45.3945	0.0100	0.1182	2.1849
7	A	79.3288	0.0504	0.5503	0.6490
8	A	83.8217	0.0256	1.5442	4.1104
9	A	114.7183	0.0454	2.9090	2.2770
10	A	122.1931	0.0444	1.7129	0.9722
11	A	156.4841	0.0476	2.9479	2.6564
12	A	160.6548	0.1691	0.4125	2.0510
13	A	187.8797	0.0279	0.3608	0.2114
14	A	205.9059	0.0320	8.3734	6.4933
15	A	220.1980	0.5092	1.3574	1.2028
16	A	239.1653	0.6478	4.1809	46.0940
17	A	258.1153	0.7598	3.4496	6.1306
18	A	275.6310	0.8271	6.6162	5.5233
19	A	295.5393	0.0954	0.0228	0.0065
20	A	302.9662	1.0038	2.6142	0.8453
21	A	316.8538	0.2394	72.1410	7.8608
22	A	324.3631	1.1342	1.1406	2.6516
23	A	347.5914	1.3091	0.0660	1.2438
24	A	392.3028	0.2431	0.0110	0.1277
25	A	395.4986	1.6556	0.5381	2.4138
26	A	413.5841	0.2668	7.7520	2.4306
27	A	460.7610	2.2093	2.6305	4.2527
28	A	474.8916	0.4787	1.3110	2.6527
29	A	527.8268	2.9340	8.9486	0.7016
30	A	535.8793	0.5381	10.4424	1.6733
31	A	563.5875	0.5457	2.7867	0.1606

32	A	578.6859	3.5091	0.6348	9.2715
33	A	614.2754	3.8601	5.9254	1.1612
34	A	645.3384	4.2877	8.1394	11.3566
35	A	684.0713	1.9062	0.3883	4.1350
36	A	741.1294	5.4489	39.8629	14.8079
37	A	743.5075	1.0357	2.9723	1.2332
38	A	760.9620	1.7469	45.7577	18.1041
39	A	818.2864	0.6955	75.7065	2.2641
40	A	834.3664	0.5150	0.3364	0.3364
41	A	873.8520	5.9635	189.1579	54.2287
42	A	958.6969	1.1659	30.4772	2.3586
43	A	963.4809	0.8620	11.5330	1.8829
44	A	992.8408	0.8337	0.0224	0.1325
45	A	1010.9261	4.4833	18.9214	34.3916
46	A	1018.5212	8.3253	230.4650	34.3059
47	A	1069.2402	1.0593	14.7292	0.7222
48	A	1098.1571	1.4112	0.4879	4.4730
49	A	1102.7303	9.4845	70.9540	10.0954
50	A	1108.2083	9.5677	28.4065	0.8543
51	A	1119.0842	0.9217	0.9613	2.7673
52	A	1131.4963	1.2721	3.3829	0.0132
53	A	1155.0424	10.2488	130.0590	8.2303
54	A	1163.4296	1.1826	59.7256	14.7795
55	A	1190.6338	8.6228	461.5853	8.0147
56	A	1195.4064	1.5880	16.5080	7.4955
57	A	1202.9173	10.4767	326.5669	3.5798
58	A	1232.2881	2.7821	18.4477	3.0644
59	A	1232.6145	8.4864	158.6006	18.3871
60	A	1258.2818	1.1705	17.9246	9.1025
61	A	1300.8043	7.6246	0.7083	9.2328
62	A	1318.0133	12.7621	59.4748	13.6544
63	A	1359.6071	3.3834	67.8668	31.3535
64	A	1372.9509	1.4988	2.3141	2.1351
65	A	1445.4064	1.6615	0.6024	5.0442
66	A	1456.3805	2.1192	8.5892	3.1629
67	A	1480.8276	1.5311	4.7939	26.9376
68	A	1493.5631	1.3823	4.6689	1.0461
69	A	1502.5888	1.4733	23.6516	14.0417
70	A	1507.0599	1.4166	1.6420	4.7709
71	A	1527.9483	1.5092	24.2123	4.5348
72	A	1537.6514	2.6529	88.4162	4.6904
73	A	1595.3738	10.3215	37.1446	1.8897
74	A	1633.3165	8.1294	244.0534	52.7410
75	A	2994.2153	5.5529	35.4938	68.0316
76	A	2999.0671	5.5842	98.4262	340.6888
77	A	3097.2312	6.1171	4.1192	32.0744
78	A	3098.9288	6.1252	20.7260	80.8123
79	A	3129.1870	6.3696	4.7051	6.9600
80	A	3135.9087	6.3870	19.0184	78.9155
81	A	3146.7420	6.3488	30.3373	111.2184
82	A	3149.7749	6.3824	8.8797	143.6298
83	A	3219.0584	6.6655	2.1352	132.9617
84	A	3219.1665	6.6588	8.4416	9.1083

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.7350	0.0000	0.0309	3.7679
2	A	12.6805	0.0012	0.1419	0.1233
3	A	14.2593	0.0008	0.7666	1.3545
4	A	20.3225	0.0019	0.3996	0.3585
5	A	31.1000	0.0014	2.0512	0.7589
6	A	61.2741	0.0115	1.0145	0.0907
7	A	71.7811	0.0244	0.3114	0.1858
8	A	74.5139	0.0274	7.4257	1.3263
9	A	79.3818	0.0082	0.0020	1.2589
10	A	90.9721	0.0529	0.8422	0.2411
11	A	120.8575	0.1313	4.6485	1.3796
12	A	153.5718	0.0496	0.0980	0.7137

13	A	166.0168	0.0644	2.1615	5.8040
14	A	180.8375	0.0226	0.0311	0.1292
15	A	220.0021	0.5289	0.4639	4.4739
16	A	234.0948	0.7248	11.9876	60.0628
17	A	253.6089	0.1882	0.7668	1.3691
18	A	258.7288	0.2249	3.6612	2.7427
19	A	276.2558	0.3462	7.1835	5.5842
20	A	278.6595	0.1800	4.8809	0.4170
21	A	302.0800	0.9872	1.8760	1.0416
22	A	324.6369	1.1343	0.8738	2.9713
23	A	347.6971	1.3080	0.0965	1.4039
24	A	394.1746	0.3200	8.7824	14.8327
25	A	396.1908	1.3341	0.7542	0.6444
26	A	411.9597	0.2826	0.0027	0.1370
27	A	460.2499	2.2319	1.6510	4.8135
28	A	484.9944	0.5093	3.5682	2.4454
29	A	527.3918	2.9183	10.8698	0.8210
30	A	540.0175	0.4457	16.9953	0.4592
31	A	556.8837	0.6792	8.2870	1.2315
32	A	577.3116	3.5025	0.9956	10.8694
33	A	610.6979	3.8112	5.5485	1.2845
34	A	644.0029	4.2792	7.7694	12.3341
35	A	680.1680	1.8930	0.0145	3.6048
36	A	740.3908	5.4765	41.1971	18.5327
37	A	747.0718	1.0274	0.0784	0.1231
38	A	770.0452	1.7621	8.3322	35.6530
39	A	817.5459	0.7240	52.3036	0.8829
40	A	828.9825	0.5019	0.0001	0.2150
41	A	875.0846	6.0389	191.7225	56.9609
42	A	964.1137	0.7190	0.2740	1.0853
43	A	969.7936	1.6465	9.6259	32.3080
44	A	989.0910	0.8119	0.0024	0.2652
45	A	1015.4581	5.9540	228.2121	12.4467
46	A	1019.9670	5.2390	90.6450	37.1670
47	A	1080.0063	1.0476	23.1889	0.6610
48	A	1088.5074	7.2010	96.2485	2.7894
49	A	1092.7189	1.8256	21.6181	17.4516
50	A	1099.6299	4.8247	16.1461	30.3918
51	A	1137.8237	1.0763	0.4527	0.8937
52	A	1138.1749	1.0613	0.7105	0.9564
53	A	1139.6058	1.0122	4.0534	0.9995
54	A	1148.8146	10.1009	146.0766	12.4876
55	A	1183.7263	10.6797	522.8513	7.4787
56	A	1199.6246	10.9713	324.2724	3.2879
57	A	1202.4192	1.4514	9.2852	10.3040
58	A	1229.9563	9.7056	172.9676	24.8875
59	A	1253.5823	1.1722	59.3645	18.1238
60	A	1260.8528	2.9570	35.8181	0.2136
61	A	1318.5319	12.7354	73.9898	15.8512
62	A	1331.0174	5.6308	1.2308	8.2729
63	A	1377.7746	1.6039	13.2378	0.0014
64	A	1404.8455	3.2553	178.6108	29.1940
65	A	1449.5514	1.4765	0.1487	12.1113
66	A	1469.8873	2.7822	2.0021	0.3373
67	A	1486.6113	1.6030	22.1446	6.7092
68	A	1487.3634	1.3530	0.3180	7.4243
69	A	1496.2368	1.3780	17.4654	20.2470
70	A	1516.3506	1.4904	4.2974	0.5912
71	A	1529.4481	1.5934	21.3394	16.4216
72	A	1557.7691	3.1535	168.1625	2.1754
73	A	1580.7655	9.5112	33.7397	3.1468
74	A	1648.6639	8.1294	463.8791	63.5856
75	A	2998.5462	5.5095	77.6114	57.9859
76	A	3004.8580	5.5515	50.8437	345.5278
77	A	3048.9028	6.0237	2.6344	141.7252
78	A	3049.8965	6.0432	58.4498	43.5273
79	A	3128.7083	6.3281	1.9541	0.9923
80	A	3141.5819	6.3650	31.0449	196.0204
81	A	3155.8188	6.3877	15.1534	41.0325
82	A	3158.2444	6.4169	0.0715	58.9979
83	A	3217.7180	6.6621	8.1668	154.7226

84 A 3217.8284 6.6558 7.3662 39.0228

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.7282	0.0000	0.6118	0.1639
2	A	15.9034	0.0015	0.4210	2.1832
3	A	19.1611	0.0018	0.1598	0.5518
4	A	29.6916	0.0031	0.0579	4.0527
5	A	43.4548	0.0123	0.2783	3.0228
6	A	44.2055	0.0070	0.0988	1.7713
7	A	71.6602	0.0487	0.0617	0.0349
8	A	82.3257	0.0212	2.5017	5.5637
9	A	113.2517	0.1566	2.6880	0.9744
10	A	120.1949	0.0263	0.0026	0.1747
11	A	155.3379	0.0665	6.5784	10.8860
12	A	159.1653	0.0903	1.7645	10.9943
13	A	187.3870	0.0277	0.2002	0.1211
14	A	206.1273	0.0319	8.0376	4.0034
15	A	213.8536	0.4789	2.3256	0.2150
16	A	231.1476	0.5912	0.1068	0.0020
17	A	263.4759	0.8345	6.8861	50.4684
18	A	264.7075	0.7928	0.0664	1.1876
19	A	286.6374	0.8848	5.0008	1.1263
20	A	295.5502	0.0956	0.0195	0.0056
21	A	316.0909	0.2377	76.8534	8.7988
22	A	336.8577	1.2326	0.3068	1.3783
23	A	371.2928	1.5193	0.0655	0.9389
24	A	379.5742	1.5369	0.3560	0.5591
25	A	392.4737	0.2433	0.0080	0.1200
26	A	413.6128	0.2668	8.0198	2.5316
27	A	474.9315	0.4778	1.4778	2.5727
28	A	506.5509	2.6859	1.2001	0.3160
29	A	526.6217	2.9088	6.4656	2.8007
30	A	536.0637	0.5393	10.5572	1.5649
31	A	563.6481	0.5450	3.1295	0.3031
32	A	580.6290	3.4095	7.9588	13.8413
33	A	596.3070	3.7715	0.1058	2.1779
34	A	666.3482	4.4182	47.4469	0.7231
35	A	684.0640	1.9062	0.3867	4.1931
36	A	725.4497	4.9257	107.8133	44.0862
37	A	743.9085	1.0298	3.2262	1.3625
38	A	761.0955	1.7414	45.7498	18.3077
39	A	806.0231	5.0317	136.6891	50.4150
40	A	819.0885	0.7082	46.2935	0.2068
41	A	834.6746	0.5155	0.2821	0.3445
42	A	958.9384	1.2051	32.4151	2.5227
43	A	963.8614	0.8436	10.6709	1.8370
44	A	992.9416	0.8337	0.0224	0.1430
45	A	1010.8683	4.4772	23.7713	36.3660
46	A	1052.9131	8.5485	41.7145	87.8981
47	A	1069.3324	1.0590	14.6761	0.6922
48	A	1098.1039	1.4113	0.4320	4.4679
49	A	1114.4727	9.9357	256.7406	0.9761
50	A	1116.1966	9.7251	52.8866	0.3517
51	A	1119.0141	0.9217	0.8660	2.7765
52	A	1131.5057	1.2722	3.4235	0.0136
53	A	1163.2444	1.1801	42.5564	16.0289
54	A	1168.9619	10.4545	84.5750	0.7445
55	A	1184.7881	10.3145	278.5251	20.4443
56	A	1195.4328	1.5245	24.7926	7.7984
57	A	1208.1776	11.3139	416.6528	1.0494
58	A	1232.5040	2.5939	20.1248	1.3727
59	A	1247.2570	11.1433	81.0618	25.6813
60	A	1258.2912	1.1711	17.3848	9.5729
61	A	1299.4456	12.3686	228.3325	4.2974
62	A	1300.9434	7.6134	0.7328	9.7123
63	A	1360.0952	3.3867	67.6404	33.3675
64	A	1372.9616	1.4992	2.3489	2.1778

65	A	1445.3910	1.6580	0.5871	5.1155
66	A	1456.3912	2.1252	8.5215	3.3159
67	A	1480.7707	1.5312	4.8090	31.3361
68	A	1493.4050	1.3823	4.5452	0.9882
69	A	1502.4983	1.4729	24.1158	14.0591
70	A	1507.0165	1.4164	1.6286	4.7625
71	A	1527.9056	1.5094	24.5123	4.6551
72	A	1537.7326	2.6564	90.4782	5.4209
73	A	1595.1725	10.3123	37.3762	1.8948
74	A	1633.3835	8.1294	249.5709	55.4120
75	A	2993.7223	5.5517	35.5909	68.3433
76	A	2998.5750	5.5831	99.9611	338.0911
77	A	3097.2012	6.1161	3.9040	31.1596
78	A	3098.8832	6.1241	21.1342	83.4591
79	A	3129.1903	6.3696	4.7369	7.0006
80	A	3135.8780	6.3869	19.0910	78.2043
81	A	3146.6525	6.3484	30.6348	112.5237
82	A	3149.6770	6.3820	9.1040	144.9329
83	A	3219.0617	6.6655	2.1581	133.9532
84	A	3219.1675	6.6588	8.5750	8.9142

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.8863	0.0000	0.0261	3.4959
2	A	13.5242	0.0007	1.0715	1.8634
3	A	14.0827	0.0012	0.2741	0.0807
4	A	27.9250	0.0059	0.0000	0.0831
5	A	30.3671	0.0013	2.3063	0.9093
6	A	59.7809	0.0091	0.6062	0.0631
7	A	65.9000	0.0331	0.0000	0.0539
8	A	72.4283	0.0235	8.2975	1.2033
9	A	79.3896	0.0082	0.0016	1.2757
10	A	93.2497	0.0509	0.4167	0.0375
11	A	116.1727	0.0827	1.5738	0.1854
12	A	154.2212	0.1264	7.3784	16.7329
13	A	162.8712	0.0397	4.1116	8.5784
14	A	180.7702	0.0226	0.0280	0.1184
15	A	214.6259	0.4788	1.9208	0.2798
16	A	231.1893	0.5912	0.1000	0.0050
17	A	253.9475	0.1437	0.0282	0.1163
18	A	258.8723	0.7193	10.6441	54.9273
19	A	267.2777	0.3636	0.2723	1.6415
20	A	278.3083	0.1439	6.1880	3.5569
21	A	286.1172	0.8405	4.3542	1.6303
22	A	336.3870	1.2443	1.5471	1.7944
23	A	371.0844	1.5174	0.0313	1.2717
24	A	380.2249	1.5416	0.2193	0.4847
25	A	394.2940	0.3051	9.5003	13.4513
26	A	413.1999	0.2834	0.0037	0.1465
27	A	484.8885	0.5097	3.7376	2.5225
28	A	506.1260	2.6722	1.3114	0.2989
29	A	526.1446	2.8912	7.4338	3.6368
30	A	540.0379	0.4463	17.1073	0.5068
31	A	556.8151	0.6784	8.1850	1.3224
32	A	576.5567	3.3868	4.0985	17.0246
33	A	595.6340	3.7667	0.0901	2.3458
34	A	663.9800	4.3865	47.3734	1.0459
35	A	680.2062	1.8930	0.0141	3.5835
36	A	724.2335	4.9030	95.4069	47.7134
37	A	747.2894	1.0259	0.2039	0.1924
38	A	769.9805	1.7627	8.4975	38.0062
39	A	806.3670	5.4618	104.9537	47.6062
40	A	817.5884	0.7254	56.3297	1.0149
41	A	829.0628	0.5021	0.0000	0.2157
42	A	964.1446	0.7202	0.2584	1.0592
43	A	969.8133	1.6451	9.4145	33.2061
44	A	989.5231	0.8137	0.0001	0.2605
45	A	1017.7572	4.2074	104.9649	4.7402

46	A	1055.0309	8.4140	31.1881	111.1276
47	A	1079.9970	1.0473	22.8854	0.6566
48	A	1093.6145	1.4941	40.7200	37.5343
49	A	1096.8288	9.3221	65.8691	0.5741
50	A	1106.2165	8.9671	226.7168	0.5716
51	A	1137.7582	1.1172	0.1509	0.6311
52	A	1138.1323	1.0236	0.2199	1.1712
53	A	1139.6357	1.0124	3.5402	1.0025
54	A	1161.1297	10.2941	98.8488	0.6867
55	A	1178.8867	10.8001	322.4500	19.5466
56	A	1202.3694	1.4493	7.7958	10.8500
57	A	1205.2694	11.2459	402.9907	1.1069
58	A	1244.3401	6.0250	109.8651	34.2195
59	A	1253.9030	1.2714	68.0235	10.7221
60	A	1260.8217	2.9630	36.4534	0.2210
61	A	1301.3320	12.0178	239.7989	6.0554
62	A	1330.8934	5.6300	1.2701	8.1243
63	A	1377.7621	1.6036	13.2275	0.0015
64	A	1404.6742	3.2597	178.8543	32.6266
65	A	1449.5045	1.4773	0.1587	12.0681
66	A	1469.7182	2.7775	2.0166	0.3865
67	A	1486.5881	1.6030	22.1880	6.6980
68	A	1487.3608	1.3531	0.3348	7.4484
69	A	1496.2204	1.3782	17.4704	20.3506
70	A	1516.3216	1.4898	4.3163	0.6092
71	A	1529.4263	1.5938	21.5836	16.9813
72	A	1557.5916	3.1472	168.1468	2.1116
73	A	1580.8553	9.5224	34.0421	3.2218
74	A	1648.4814	8.1282	467.3664	65.3384
75	A	2998.2927	5.5094	77.7159	58.8387
76	A	3004.6112	5.5515	51.6677	345.4047
77	A	3048.8666	6.0226	2.7968	141.6151
78	A	3049.8611	6.0420	58.4163	44.4498
79	A	3128.5336	6.3274	1.9664	1.0015
80	A	3141.4061	6.3643	31.2911	196.8454
81	A	3155.7252	6.3872	15.3770	39.8897
82	A	3158.1481	6.4165	0.0709	58.8485
83	A	3217.5718	6.6616	8.4796	157.6800
84	A	3217.6786	6.6551	7.4514	37.7798

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	2.1881	0.0000	0.4313	0.2269
2	A	16.7051	0.0019	0.4403	1.4399
3	A	20.6354	0.0016	0.2283	1.6674
4	A	28.6176	0.0041	0.1741	3.0448
5	A	39.4914	0.0050	0.1976	4.0864
6	A	45.7768	0.0122	0.0741	1.6158
7	A	72.3086	0.0526	0.0666	0.0838
8	A	84.1497	0.0233	3.4910	7.2749
9	A	108.1020	0.0475	0.5742	0.4266
10	A	125.4631	0.0395	0.1186	0.1654
11	A	156.6813	0.0477	0.7347	2.4005
12	A	158.8966	0.2048	9.4500	18.3163
13	A	187.8592	0.0279	0.3358	0.1764
14	A	206.6398	0.0318	8.4380	4.2935
15	A	213.6855	0.4834	2.2678	0.2032
16	A	231.3180	0.5922	0.0977	0.0045
17	A	262.6076	0.8194	6.8488	50.8759
18	A	264.3213	0.7988	0.5493	6.4223
19	A	286.6873	0.8831	6.4761	0.9740
20	A	295.7448	0.0954	0.0547	0.0128
21	A	316.5321	0.2383	79.3821	8.3376
22	A	336.9555	1.2260	0.2154	1.7585
23	A	371.4111	1.5208	0.0737	1.1455
24	A	379.5226	1.5379	0.3744	0.6425
25	A	392.5428	0.2434	0.0080	0.1335
26	A	413.8051	0.2664	8.3067	2.3936

27	A	474.8760	0.4776	1.3585	2.5782
28	A	506.3961	2.6836	1.1602	0.2598
29	A	526.7100	2.9035	7.9416	3.0033
30	A	536.1330	0.5388	10.4359	1.4881
31	A	563.6088	0.5469	4.2217	0.2897
32	A	580.7621	3.3710	7.6143	15.2381
33	A	596.2363	3.7701	0.1563	2.0930
34	A	666.2596	4.4141	51.2427	0.9500
35	A	684.0366	1.9060	0.3912	4.2771
36	A	725.4362	4.9287	116.2776	42.2876
37	A	743.5654	1.0298	3.0589	1.4641
38	A	761.1655	1.7444	47.3823	17.9841
39	A	806.1048	5.0881	143.0684	45.3410
40	A	818.9569	0.7071	46.8438	0.2608
41	A	834.4851	0.5154	0.2380	0.3540
42	A	958.7864	1.2141	32.6363	2.4313
43	A	963.7303	0.8382	10.6593	1.7535
44	A	992.8100	0.8333	0.0271	0.1472
45	A	1010.8059	4.4771	24.1140	38.4974
46	A	1053.4183	8.5557	27.9921	94.3409
47	A	1069.2116	1.0597	14.5210	0.6914
48	A	1098.0257	1.4115	0.5103	4.4324
49	A	1113.6870	9.8975	229.6661	0.7923
50	A	1117.9851	9.5949	56.7260	0.4273
51	A	1119.0775	0.9232	0.8428	2.7609
52	A	1131.4288	1.2727	3.1340	0.0183
53	A	1163.4490	1.1829	49.0261	18.0890
54	A	1166.5737	10.0106	99.3802	0.7224
55	A	1184.2644	10.7529	300.0677	19.2191
56	A	1195.4441	1.5188	13.4028	8.6003
57	A	1209.7144	11.3329	412.5001	1.1176
58	A	1232.3006	2.5858	19.2972	1.4778
59	A	1247.3338	11.2123	56.9653	17.9525
60	A	1258.2298	1.1707	20.3632	9.6426
61	A	1299.5850	12.3839	242.3614	5.6635
62	A	1300.9142	7.6396	1.2575	10.0191
63	A	1360.1429	3.3832	71.1343	34.9827
64	A	1372.8894	1.4988	2.3518	2.2495
65	A	1445.3640	1.6593	0.5961	5.1306
66	A	1456.4019	2.1234	8.4635	3.2725
67	A	1480.8346	1.5313	4.9661	32.9952
68	A	1493.5836	1.3826	4.4496	1.0147
69	A	1502.7074	1.4747	25.3059	13.3359
70	A	1506.9580	1.4164	1.6036	4.8424
71	A	1527.9094	1.5115	25.2231	4.7242
72	A	1537.8227	2.6473	95.6372	6.2515
73	A	1595.0508	10.3063	37.6495	1.8467
74	A	1633.4016	8.1279	262.7793	56.8740
75	A	2993.8722	5.5523	35.6508	67.4043
76	A	2998.7437	5.5836	96.8811	331.5860
77	A	3097.3533	6.1168	4.2519	32.9850
78	A	3099.0982	6.1252	20.9018	77.1968
79	A	3129.4566	6.3707	4.7492	7.0108
80	A	3136.1677	6.3880	18.9426	75.7589
81	A	3146.5396	6.3480	30.8741	116.2854
82	A	3149.5707	6.3815	9.5465	148.0558
83	A	3219.0121	6.6650	2.4902	129.4678
84	A	3219.1275	6.6589	8.3504	13.5540

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.8875	0.0000	0.0260	3.4959
2	A	13.5219	0.0007	1.0723	1.8642
3	A	14.0826	0.0012	0.2741	0.0807
4	A	27.9257	0.0059	0.0000	0.0831
5	A	30.3518	0.0013	2.3049	0.9085
6	A	59.7799	0.0091	0.6056	0.0631
7	A	65.9004	0.0331	0.0000	0.0539

8	A	72.4297	0.0235	8.2981	1.2031
9	A	79.3892	0.0082	0.0016	1.2758
10	A	93.2513	0.0509	0.4167	0.0375
11	A	116.1726	0.0827	1.5738	0.1854
12	A	154.2213	0.1264	7.3787	16.7337
13	A	162.8720	0.0397	4.1111	8.5770
14	A	180.7749	0.0226	0.0280	0.1185
15	A	214.6255	0.4788	1.9208	0.2798
16	A	231.1892	0.5912	0.1000	0.0050
17	A	253.9457	0.1437	0.0282	0.1163
18	A	258.8725	0.7193	10.6447	54.9280
19	A	267.2774	0.3637	0.2723	1.6416
20	A	278.3092	0.1439	6.1872	3.5559
21	A	286.1173	0.8405	4.3540	1.6304
22	A	336.3871	1.2443	1.5471	1.7944
23	A	371.0843	1.5174	0.0313	1.2717
24	A	380.2249	1.5416	0.2193	0.4847
25	A	394.2928	0.3051	9.5006	13.4519
26	A	413.2001	0.2834	0.0037	0.1465
27	A	484.8891	0.5097	3.7376	2.5225
28	A	506.1260	2.6722	1.3114	0.2988
29	A	526.1446	2.8912	7.4337	3.6368
30	A	540.0381	0.4463	17.1068	0.5067
31	A	556.8149	0.6784	8.1855	1.3225
32	A	576.5568	3.3868	4.0985	17.0246
33	A	595.6342	3.7667	0.0901	2.3458
34	A	663.9800	4.3865	47.3736	1.0459
35	A	680.2061	1.8930	0.0141	3.5835
36	A	724.2338	4.9030	95.4069	47.7133
37	A	747.2895	1.0259	0.2038	0.1923
38	A	769.9807	1.7627	8.4970	38.0064
39	A	806.3669	5.4617	104.9536	47.6060
40	A	817.5882	0.7254	56.3301	1.0148
41	A	829.0626	0.5021	0.0000	0.2157
42	A	964.1445	0.7202	0.2582	1.0589
43	A	969.8135	1.6451	9.4136	33.2069
44	A	989.5230	0.8137	0.0001	0.2605
45	A	1017.7572	4.2074	104.9642	4.7400
46	A	1055.0312	8.4140	31.1887	111.1279
47	A	1079.9970	1.0473	22.8857	0.6567
48	A	1093.6145	1.4941	40.7199	37.5341
49	A	1096.8298	9.3221	65.8698	0.5741
50	A	1106.2167	8.9671	226.7136	0.5716
51	A	1137.7592	1.1173	0.1511	0.6304
52	A	1138.1335	1.0235	0.2196	1.1717
53	A	1139.6350	1.0124	3.5367	1.0020
54	A	1161.1317	10.2941	98.8479	0.6867
55	A	1178.8859	10.8001	322.4548	19.5455
56	A	1202.3696	1.4493	7.7961	10.8504
57	A	1205.2710	11.2459	402.9911	1.1069
58	A	1244.3395	6.0270	109.8477	34.2159
59	A	1253.9054	1.2713	68.0424	10.7256
60	A	1260.8223	2.9630	36.4542	0.2210
61	A	1301.3326	12.0177	239.7974	6.0553
62	A	1330.8942	5.6301	1.2699	8.1245
63	A	1377.7645	1.6036	13.2278	0.0015
64	A	1404.6751	3.2597	178.8530	32.6263
65	A	1449.5048	1.4773	0.1587	12.0681
66	A	1469.7191	2.7775	2.0167	0.3865
67	A	1486.5884	1.6030	22.1879	6.6981
68	A	1487.3606	1.3531	0.3344	7.4485
69	A	1496.2203	1.3782	17.4700	20.3505
70	A	1516.3222	1.4898	4.3165	0.6090
71	A	1529.4267	1.5938	21.5844	16.9815
72	A	1557.5923	3.1472	168.1500	2.1116
73	A	1580.8553	9.5223	34.0420	3.2218
74	A	1648.4817	8.1282	467.3660	65.3382
75	A	2998.2941	5.5094	77.7195	58.8324
76	A	3004.6127	5.5515	51.6622	345.4105
77	A	3048.8634	6.0226	2.7944	141.6242
78	A	3049.8578	6.0420	58.4205	44.4406

79	A	3128.5343	6.3274	1.9664	1.0014
80	A	3141.4071	6.3643	31.2910	196.8459
81	A	3155.7252	6.3872	15.3770	39.8899
82	A	3158.1480	6.4165	0.0709	58.8484
83	A	3217.5714	6.6616	8.4796	157.6815
84	A	3217.6781	6.6551	7.4513	37.7783

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	0.7007	0.0000	0.0167	0.0378
2	A	1.6093	0.0000	0.0132	0.0089
3	A	5.2860	0.0003	0.1175	0.8846
4	A	12.7220	0.0013	0.0958	0.0042
5	A	15.3092	0.0025	0.1064	0.4142
6	A	18.8403	0.0017	0.2250	0.4921
7	A	25.7485	0.0120	0.3670	0.3404
8	A	27.2457	0.0057	0.0108	0.1522
9	A	30.9517	0.0044	0.0160	2.4582
10	A	47.4324	0.0069	0.1139	2.5850
11	A	59.2101	0.0196	0.3994	0.3538
12	A	65.2814	0.0311	0.0015	0.0298
13	A	71.6743	0.0500	0.0425	0.0263
14	A	72.4712	0.0224	7.4158	2.5577
15	A	81.6862	0.0207	1.7020	11.3492
16	A	89.7537	0.0497	0.2444	0.0830
17	A	112.0561	0.1452	0.2931	0.4727
18	A	117.6253	0.0243	0.0211	0.0473
19	A	117.7527	0.1262	2.9569	1.0702
20	A	155.9801	0.2917	14.1338	25.0139
21	A	158.7643	0.2968	4.6132	17.7031
22	A	170.7806	0.0490	5.0239	6.2475
23	A	181.2475	0.0252	0.1770	0.0741
24	A	197.7273	0.0315	12.4749	7.1208
25	A	213.5627	0.4825	2.6485	0.1997
26	A	214.6505	0.4715	1.6517	0.3235
27	A	231.2272	0.5916	0.1054	0.0042
28	A	231.3158	0.5920	0.0895	0.0044
29	A	260.4631	0.8271	14.7759	61.1420
30	A	263.9953	0.6526	0.2893	1.1991
31	A	264.0705	0.8431	3.8840	59.9140
32	A	264.9041	0.7755	0.0254	1.7029
33	A	286.1522	0.8729	9.8940	1.4839
34	A	286.8774	0.8815	5.2354	1.1366
35	A	296.8836	0.1051	0.0002	0.0658
36	A	308.6856	0.2356	85.0578	11.9944
37	A	336.5489	1.2419	0.8552	2.1249
38	A	337.0040	1.2378	0.2994	1.7842
39	A	371.1838	1.5186	0.0242	1.1982
40	A	371.5085	1.5219	0.0594	1.1137
41	A	379.5245	1.5376	0.3881	0.5448
42	A	380.2151	1.5389	0.2287	0.5093
43	A	401.5456	0.2603	0.0057	0.1043
44	A	417.8087	0.2722	5.5309	6.8220
45	A	478.1151	0.4863	2.1340	2.0557
46	A	506.2623	2.6855	1.2133	0.2721
47	A	506.6638	2.6869	1.2204	0.2401
48	A	526.3128	2.9140	7.4336	3.5541
49	A	526.8418	2.9167	8.3193	3.2688
50	A	538.6478	0.5199	16.8850	2.7239
51	A	563.0265	0.5813	0.7236	1.0411
52	A	577.5409	3.3780	4.4723	17.5771
53	A	581.8747	3.4022	9.1835	13.9078
54	A	595.7936	3.7680	0.1006	2.2783
55	A	596.4486	3.7723	0.1762	2.0333
56	A	664.5190	4.3927	55.3823	0.8963
57	A	666.9048	4.4169	51.3068	1.1736
58	A	681.8328	1.8929	0.0356	3.6287
59	A	724.6217	4.8900	150.9749	35.5807

60	A	725.8996	4.9341	88.2879	53.4373
61	A	744.4214	1.0586	2.2557	1.1563
62	A	766.5505	1.7852	54.8180	34.7270
63	A	806.1664	5.2367	214.3920	35.1649
64	A	807.0705	5.4477	58.2112	54.3645
65	A	822.1056	0.7087	51.5172	0.5920
66	A	835.4231	0.5152	0.2030	0.2560
67	A	960.4589	1.4675	35.7694	12.5482
68	A	967.3129	0.7594	3.1610	2.3916
69	A	992.1402	0.8239	0.0423	0.1585
70	A	1020.0930	4.3161	77.7020	18.4372
71	A	1053.1197	8.5516	16.6059	78.1452
72	A	1055.3689	8.4550	33.7154	129.5699
73	A	1071.4287	1.0644	15.1055	0.4703
74	A	1098.1027	1.5005	43.8243	30.5912
75	A	1101.2495	9.3994	61.4224	0.5758
76	A	1107.8428	8.5841	215.6058	0.4058
77	A	1116.2066	9.9387	238.2020	0.4769
78	A	1120.3639	0.9198	1.0561	2.7372
79	A	1124.2441	9.8600	46.1428	0.4130
80	A	1138.8414	1.2799	0.3192	0.0058
81	A	1159.9552	1.1483	81.9495	37.9255
82	A	1162.2641	10.3197	95.9312	0.6620
83	A	1168.1595	10.4394	95.2121	0.6682
84	A	1180.1583	10.8050	311.8565	19.7212
85	A	1186.0050	10.8365	303.2239	18.4197
86	A	1198.1305	1.5019	20.5890	16.1073
87	A	1206.3303	11.2674	376.7484	1.0445
88	A	1211.3573	11.3692	442.5584	1.1675
89	A	1237.1253	2.4832	19.9651	0.4700
90	A	1245.1628	7.6404	73.2666	31.0981
91	A	1248.0932	11.2994	64.4279	11.5865
92	A	1256.6668	1.2226	58.6379	15.1835
93	A	1298.9902	12.3219	331.2438	7.2826
94	A	1301.2875	12.0943	170.9286	8.0043
95	A	1312.5582	7.9063	0.5100	5.1788
96	A	1372.4340	3.3747	123.4712	80.8416
97	A	1373.4227	1.5023	5.5452	0.8813
98	A	1448.4414	1.5044	0.0148	6.1058
99	A	1463.8303	2.5530	11.0005	2.2636
100	A	1482.3952	1.5394	7.9688	31.6674
101	A	1494.0101	1.3840	4.2678	1.5698
102	A	1503.4130	1.4570	24.7652	15.7425
103	A	1507.5750	1.4321	1.5192	3.5177
104	A	1528.1218	1.5173	38.6960	11.8432
105	A	1544.8770	2.8154	119.4723	9.5921
106	A	1591.7745	10.1454	27.8718	3.0090
107	A	1642.6754	8.1239	379.2846	99.5819
108	A	2998.5512	5.5643	34.5937	68.0260
109	A	3003.2403	5.5958	87.2357	337.7162
110	A	3097.9441	6.1287	3.7200	36.2046
111	A	3099.0929	6.1380	21.5608	66.3868
112	A	3131.5636	6.3770	3.2303	4.0139
113	A	3139.1399	6.3950	19.2692	108.7405
114	A	3159.5795	6.4046	12.6803	42.9624
115	A	3162.0685	6.4353	0.1897	60.7809
116	A	3225.1057	6.6923	6.2896	133.7559
117	A	3225.2833	6.6857	4.2240	26.6438

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.2411	0.0000	0.0028	0.0101
2	A	1.7975	0.0000	0.1103	0.0475
3	A	4.8044	0.0002	0.0801	0.8338
4	A	12.8456	0.0013	0.0931	0.0075
5	A	14.2979	0.0021	0.0477	0.2162
6	A	18.5153	0.0016	0.2227	0.5308
7	A	27.3325	0.0058	0.0124	0.1689

8	A	27.9220	0.0149	0.2395	0.2185
9	A	30.5566	0.0044	0.0200	2.4348
10	A	47.7803	0.0071	0.1194	2.5101
11	A	60.4024	0.0209	0.5713	0.4366
12	A	65.2854	0.0311	0.0015	0.0319
13	A	71.6294	0.0498	0.0429	0.0157
14	A	73.2309	0.0235	7.1628	2.2545
15	A	79.6275	0.0187	1.0305	9.1080
16	A	89.7828	0.0496	0.2424	0.0794
17	A	111.9579	0.1539	3.1324	0.8327
18	A	116.9927	0.0239	0.0028	0.0444
19	A	117.9391	0.1266	1.8681	1.1368
20	A	155.7354	0.2856	14.7728	22.2372
21	A	158.3604	0.3544	3.1857	23.1322
22	A	170.7057	0.0471	2.5155	3.3915
23	A	181.7891	0.0254	0.1698	0.0888
24	A	197.7642	0.0318	11.6840	6.0742
25	A	213.6289	0.4823	2.6343	0.1970
26	A	214.6485	0.4708	1.6316	0.3182
27	A	231.1590	0.5913	0.1071	0.0017
28	A	231.2183	0.5915	0.0997	0.0042
29	A	260.5395	0.8333	14.5267	61.7029
30	A	264.0022	0.6489	0.2753	1.4711
31	A	264.8636	0.8567	4.0869	51.0948
32	A	265.0877	0.7808	0.0191	1.2529
33	A	286.1550	0.8740	7.6956	2.0794
34	A	286.8055	0.8849	4.2422	0.9043
35	A	296.8229	0.1049	0.0003	0.0664
36	A	308.3990	0.2346	80.5608	13.0223
37	A	336.5400	1.2416	0.9326	1.9559
38	A	336.9555	1.2425	0.2928	1.2052
39	A	371.1800	1.5186	0.0249	1.2184
40	A	371.4047	1.5205	0.0667	1.0300
41	A	379.4810	1.5370	0.3821	0.5657
42	A	380.2251	1.5390	0.2316	0.4877
43	A	401.6651	0.2602	0.0059	0.0946
44	A	417.5938	0.2724	5.9419	6.6083
45	A	478.1903	0.4865	2.1612	2.0165
46	A	506.2613	2.6853	1.2221	0.3018
47	A	506.7282	2.6878	1.2669	0.3042
48	A	526.3107	2.9140	6.8867	3.8910
49	A	526.7810	2.9191	6.4990	2.2640
50	A	538.6583	0.5204	16.4430	2.8753
51	A	563.0010	0.5799	0.2688	0.9309
52	A	577.5362	3.3771	4.5953	17.1301
53	A	581.8683	3.4415	10.0811	12.2676
54	A	595.7905	3.7679	0.1018	2.2706
55	A	596.4938	3.7729	0.1126	2.2186
56	A	664.5140	4.3927	51.2506	0.9169
57	A	667.0666	4.4239	47.6206	0.7488
58	A	681.8618	1.8931	0.0345	3.5501
59	A	724.6426	4.8961	115.9227	38.6236
60	A	725.8879	4.9281	103.8826	51.1000
61	A	744.7751	1.0584	2.5084	1.0623
62	A	766.5126	1.7824	51.2561	34.0864
63	A	806.2421	5.2276	154.4249	41.0838
64	A	807.0298	5.4558	99.2743	51.8897
65	A	822.1516	0.7086	53.5870	0.4950
66	A	835.5327	0.5152	0.2710	0.2251
67	A	960.6686	1.4664	35.7683	12.8948
68	A	967.5615	0.7607	2.9801	2.4468
69	A	992.8894	0.8257	0.0377	0.1427
70	A	1020.1795	4.3171	78.4827	16.7414
71	A	1052.6505	8.5483	49.9954	71.5328
72	A	1055.3749	8.4534	28.2581	120.8954
73	A	1071.6076	1.0639	15.2881	0.4667
74	A	1098.2004	1.5001	44.2104	29.4518
75	A	1101.2569	9.4000	61.1580	0.5787
76	A	1107.7995	8.5763	228.2422	0.4169
77	A	1116.9138	9.9908	270.5712	0.8479
78	A	1120.5164	0.9225	0.5429	2.7590

79	A	1122.2129	9.5565	48.9568	0.3510
80	A	1138.9485	1.2789	0.6023	0.0044
81	A	1159.8021	1.1498	66.2129	35.0502
82	A	1162.2206	10.3183	95.1307	0.6676
83	A	1170.5811	10.4836	82.0845	0.8120
84	A	1180.0987	10.8116	315.3902	20.1688
85	A	1186.8719	10.4536	269.0625	16.1537
86	A	1198.1149	1.5074	36.1733	15.5310
87	A	1206.3339	11.2672	347.9350	1.1344
88	A	1209.4428	11.3415	476.6478	1.0389
89	A	1237.3770	2.4921	19.8980	0.4451
90	A	1245.1471	7.6604	93.6805	29.2833
91	A	1248.0569	11.2064	84.7977	19.8380
92	A	1256.7317	1.2228	49.0777	14.8279
93	A	1298.9457	12.2750	243.7432	5.7530
94	A	1301.2607	12.0913	224.3348	7.0120
95	A	1312.6194	7.8905	0.4639	4.8071
96	A	1372.3155	3.3805	117.5301	77.2855
97	A	1373.5176	1.5028	5.5478	0.8569
98	A	1448.5016	1.5045	0.0150	6.2160
99	A	1463.8515	2.5542	10.9890	2.2882
100	A	1482.4520	1.5396	7.4170	29.2253
101	A	1494.1344	1.3840	4.4096	1.5824
102	A	1503.3480	1.4561	23.6692	16.3431
103	A	1507.8026	1.4324	1.5977	3.4482
104	A	1528.2311	1.5171	36.7994	11.6558
105	A	1544.8206	2.8156	112.1373	7.8809
106	A	1591.9615	10.1530	27.5489	3.0392
107	A	1642.6820	8.1250	359.6369	97.2528
108	A	2998.4175	5.5637	34.9138	70.1386
109	A	3003.1200	5.5953	90.2537	346.3842
110	A	3097.5423	6.1272	3.8637	36.4394
111	A	3098.6894	6.1366	21.2539	71.3114
112	A	3131.1964	6.3753	3.1979	4.0093
113	A	3138.7981	6.3935	19.5092	112.9615
114	A	3159.6889	6.4051	12.5385	41.0546
115	A	3162.1790	6.4357	0.2294	59.7828
116	A	3225.1085	6.6924	6.1302	133.2809
117	A	3225.2873	6.6857	4.1992	27.2426

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.4459	0.0001	0.3174	0.4497
2	A	13.7113	0.0005	0.9899	3.2283
3	A	31.5693	0.0018	0.6310	5.2821
4	A	32.9502	0.0049	0.5715	1.2790
5	A	49.8275	0.0057	1.0009	1.1261
6	A	69.5599	0.0158	0.1491	5.5424
7	A	101.8815	0.0162	0.0286	0.2022
8	A	126.2774	0.0214	0.4818	0.7186
9	A	139.6832	0.0397	5.1601	4.9579
10	A	163.8048	0.0190	9.1836	5.8847
11	A	172.1055	0.0224	0.3866	0.1889
12	A	196.8176	0.0371	0.4573	2.4283
13	A	270.5145	0.0645	0.0772	5.9357
14	A	280.9811	0.1744	35.5151	9.8588
15	A	282.7186	0.0966	0.3095	0.0695
16	A	387.3400	0.2042	0.6860	14.3691
17	A	398.7886	0.2554	0.0232	0.1494
18	A	404.0549	0.2761	2.0865	4.5187
19	A	479.7407	0.4910	2.0593	2.8411
20	A	502.7669	0.4760	4.4863	70.8957
21	A	536.1519	0.5026	11.2822	2.1446
22	A	555.5088	0.5576	1.1973	0.5924
23	A	683.6830	1.9085	0.3490	3.7644
24	A	743.0545	1.0462	0.9508	0.5417
25	A	764.7737	1.6785	23.1200	17.7004
26	A	771.9444	0.4478	9.3124	7.3253

27	A	812.4248	0.6990	67.6630	0.5758
28	A	827.9580	0.5559	3.9866	3.4977
29	A	828.9267	0.5150	0.6723	1.4754
30	A	888.5074	0.9353	4.2434	5.2064
31	A	958.2363	0.7149	1.2158	0.2666
32	A	969.0001	1.5830	29.4239	9.2354
33	A	989.9345	0.8244	0.0231	0.1694
34	A	1008.3249	4.3084	37.3479	26.1311
35	A	1027.8357	0.8137	1.3955	2.8928
36	A	1047.2393	0.8479	0.7755	2.3823
37	A	1079.0464	1.0439	16.5412	0.0705
38	A	1089.2079	1.4771	2.6104	4.9897
39	A	1095.3661	1.4062	0.1305	6.3645
40	A	1126.1807	0.9374	0.2319	3.6896
41	A	1131.3364	1.2308	3.9696	0.1148
42	A	1151.9591	1.0925	34.0374	3.8684
43	A	1200.4574	1.4925	7.7653	5.7332
44	A	1218.0925	1.2429	5.5188	9.1403
45	A	1228.5884	1.1927	50.3587	18.4271
46	A	1249.3714	2.9862	28.4212	0.5338
47	A	1256.6841	1.1643	24.5821	7.7541
48	A	1307.6087	1.1548	38.2654	7.4052
49	A	1312.4286	6.3773	0.9514	9.5257
50	A	1375.1264	1.5357	4.5807	1.0323
51	A	1376.5971	1.5771	5.3540	0.8425
52	A	1386.2774	3.4150	86.8452	11.0327
53	A	1418.7460	1.4825	8.8059	0.5988
54	A	1446.6832	1.6058	0.2140	7.3769
55	A	1459.0318	2.2882	4.3150	1.3961
56	A	1472.7518	1.4047	3.3487	12.5519
57	A	1478.9747	1.3841	4.2503	12.5272
58	A	1483.1895	1.5618	14.0477	10.9069
59	A	1490.3857	1.3693	3.8398	4.0502
60	A	1498.0203	1.4226	18.6535	14.0716
61	A	1500.4077	1.3864	9.7695	4.9711
62	A	1507.5569	1.4133	5.0427	2.9710
63	A	1509.0866	1.4413	1.0874	1.9885
64	A	1526.8249	1.5919	11.3954	7.3268
65	A	1544.5073	2.7316	109.5553	2.2804
66	A	1587.3457	9.9704	40.4903	1.5598
67	A	1637.5811	8.1195	282.8963	42.3966
68	A	2980.8719	5.5110	56.6341	92.1946
69	A	2986.7628	5.5509	110.7977	357.0440
70	A	2994.9265	5.6511	28.4774	309.7108
71	A	3025.9863	5.6002	19.4392	165.9570
72	A	3053.2370	5.9848	7.5077	78.9434
73	A	3078.6715	6.0438	7.2826	58.0118
74	A	3079.7642	6.0569	32.4853	48.0697
75	A	3088.5807	6.1208	12.4820	100.3867
76	A	3092.9172	6.0224	32.6854	107.4497
77	A	3102.5179	6.2483	26.4795	31.3773
78	A	3122.6333	6.3259	3.1781	2.2223
79	A	3132.0101	6.3481	25.5875	107.5706
80	A	3139.7983	6.3188	37.8661	111.4200
81	A	3142.8837	6.3518	11.0346	144.7001
82	A	3155.4260	6.5127	4.7331	65.9250
83	A	3215.1446	6.6462	5.8335	89.2472
84	A	3215.3075	6.6451	8.1894	54.1877

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.1374	0.0000	0.0523	3.0979
2	A	12.6538	0.0003	1.4209	0.3033
3	A	15.0448	0.0006	1.9404	0.8515
4	A	48.5154	0.0079	1.3177	1.6537
5	A	57.0101	0.0171	3.0445	4.5350
6	A	70.5001	0.0111	0.2038	0.9665
7	A	82.6041	0.0101	0.0244	1.1952

8	A	83.7597	0.0087	5.1494	0.3023
9	A	128.8607	0.0232	0.1880	1.1577
10	A	149.8481	0.0226	0.0470	3.8443
11	A	173.0716	0.0215	0.0883	0.2075
12	A	197.0319	0.0373	0.2089	3.4646
13	A	267.1008	0.0938	0.0216	0.9301
14	A	270.3226	0.0848	2.4553	1.7280
15	A	272.4608	0.0987	5.6321	11.1827
16	A	387.4877	0.2017	0.5657	30.5595
17	A	397.3849	0.2892	2.7350	13.6517
18	A	404.9514	0.2681	0.0135	0.2947
19	A	482.0600	0.4991	3.3397	2.7071
20	A	504.3163	0.4752	0.4959	141.0835
21	A	539.3686	0.4719	17.2180	2.8739
22	A	554.7072	0.6117	3.7201	2.1965
23	A	681.9791	1.8980	0.0254	3.4140
24	A	746.6950	1.0237	0.3911	0.0948
25	A	767.4599	1.6932	13.0568	23.9642
26	A	771.5951	0.4511	8.4121	5.4594
27	A	814.8287	0.7167	50.9703	0.7391
28	A	825.1324	0.5476	3.9268	6.1010
29	A	828.1890	0.5025	0.0016	0.3360
30	A	888.5470	0.9571	3.4536	7.7714
31	A	960.4777	0.7156	0.5188	0.8541
32	A	970.0451	1.6138	18.4641	26.1219
33	A	989.5416	0.8186	0.0044	0.2782
34	A	1012.1649	4.2126	75.8087	25.1260
35	A	1025.3454	0.8088	1.3573	3.0212
36	A	1048.2575	0.8419	0.1753	2.0192
37	A	1079.9717	1.0412	21.9993	0.2049
38	A	1087.5125	1.5009	2.5585	7.0157
39	A	1095.1165	1.4243	5.7119	23.2343
40	A	1132.6361	1.1485	0.6145	0.7664
41	A	1133.8181	0.9860	0.9749	1.6898
42	A	1143.1865	1.0403	21.7464	3.4832
43	A	1201.1716	1.4675	6.8749	10.1980
44	A	1218.9447	1.2397	8.9932	18.7936
45	A	1227.2533	1.2141	63.2647	22.4096
46	A	1254.5049	1.1619	62.5672	19.4436
47	A	1256.8639	3.1379	35.6855	0.0143
48	A	1308.5862	1.1537	39.7862	7.1570
49	A	1323.7113	5.7639	0.8519	10.2114
50	A	1374.8296	1.5702	10.3581	2.1079
51	A	1376.3730	1.5765	11.3235	0.0763
52	A	1396.4560	3.4104	151.6614	31.4860
53	A	1415.0676	1.4806	11.1226	1.1192
54	A	1447.7263	1.5331	0.4997	11.0254
55	A	1463.3176	2.5273	1.5066	0.4395
56	A	1472.7889	1.4016	2.6125	16.7655
57	A	1481.2118	1.3871	3.6311	15.8081
58	A	1485.3618	1.5912	22.0318	5.6588
59	A	1487.8252	1.3578	2.1660	7.1151
60	A	1495.8101	1.3924	18.5285	19.1179
61	A	1499.4050	1.3841	7.8370	6.4967
62	A	1507.8720	1.4160	5.5388	3.2888
63	A	1514.4440	1.4652	4.0212	1.3759
64	A	1528.5396	1.6111	15.5602	15.6785
65	A	1550.2950	2.8747	144.5793	2.3645
66	A	1584.3412	9.8949	37.6449	2.3239
67	A	1642.1218	8.1103	410.7145	70.3781
68	A	2983.7951	5.5037	71.7073	73.7217
69	A	2990.1932	5.5498	80.9417	289.7714
70	A	2991.1472	5.6362	36.9288	373.4793
71	A	3022.6420	5.5860	26.6943	200.4431
72	A	3046.9540	5.9582	8.6371	87.2471
73	A	3056.2384	5.9897	12.3702	113.6339
74	A	3057.2723	6.0039	48.8829	77.4151
75	A	3081.2093	5.9898	11.1177	163.8349
76	A	3085.5239	6.1001	51.4911	88.2741
77	A	3098.8403	6.2310	31.5668	28.1697
78	A	3120.9936	6.3024	2.5273	1.4769

79	A	3132.7751	6.3342	36.6992	187.8033
80	A	3143.0559	6.4566	8.0180	75.4391
81	A	3145.0949	6.3413	24.5192	59.1645
82	A	3147.9567	6.3735	1.6409	75.3755
83	A	3212.9971	6.6396	8.6582	139.5586
84	A	3213.0768	6.6350	11.7128	46.9946

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	6.4356	0.0001	0.3173	0.4493
2	A	13.7082	0.0005	0.9899	3.2286
3	A	31.5778	0.0018	0.6319	5.2736
4	A	32.9523	0.0049	0.5718	1.2854
5	A	49.8408	0.0057	0.9998	1.1295
6	A	69.5598	0.0158	0.1493	5.5405
7	A	101.8762	0.0162	0.0285	0.2022
8	A	126.2786	0.0214	0.4819	0.7188
9	A	139.6804	0.0397	5.1569	4.9583
10	A	163.8024	0.0190	9.1858	5.8852
11	A	172.1002	0.0224	0.3877	0.1893
12	A	196.8150	0.0371	0.4574	2.4279
13	A	270.5153	0.0645	0.0771	5.9355
14	A	280.9799	0.1744	35.5117	9.8585
15	A	282.7183	0.0966	0.3138	0.0706
16	A	387.3409	0.2042	0.6860	14.3696
17	A	398.7905	0.2554	0.0232	0.1494
18	A	404.0544	0.2761	2.0864	4.5188
19	A	479.7416	0.4910	2.0593	2.8411
20	A	502.7681	0.4760	4.4861	70.8975
21	A	536.1533	0.5026	11.2815	2.1446
22	A	555.5090	0.5576	1.1976	0.5924
23	A	683.6832	1.9085	0.3490	3.7644
24	A	743.0568	1.0462	0.9513	0.5418
25	A	764.7737	1.6785	23.1192	17.7004
26	A	771.9444	0.4478	9.3123	7.3252
27	A	812.4282	0.6990	67.6643	0.5758
28	A	827.9599	0.5559	3.9912	3.5039
29	A	828.9320	0.5149	0.6676	1.4692
30	A	888.5074	0.9353	4.2435	5.2064
31	A	958.2377	0.7149	1.2158	0.2666
32	A	969.0002	1.5830	29.4238	9.2353
33	A	989.9363	0.8244	0.0231	0.1694
34	A	1008.3251	4.3085	37.3476	26.1315
35	A	1027.8368	0.8137	1.3956	2.8927
36	A	1047.2396	0.8479	0.7755	2.3823
37	A	1079.0459	1.0439	16.5415	0.0705
38	A	1089.2089	1.4771	2.6103	4.9898
39	A	1095.3679	1.4062	0.1306	6.3645
40	A	1126.1809	0.9374	0.2319	3.6896
41	A	1131.3375	1.2308	3.9694	0.1147
42	A	1151.9593	1.0925	34.0377	3.8683
43	A	1200.4572	1.4925	7.7656	5.7331
44	A	1218.0924	1.2429	5.5200	9.1411
45	A	1228.5890	1.1928	50.3571	18.4263
46	A	1249.3722	2.9862	28.4212	0.5338
47	A	1256.6849	1.1642	24.5823	7.7542
48	A	1307.6092	1.1548	38.2659	7.4052
49	A	1312.4289	6.3774	0.9515	9.5258
50	A	1375.1272	1.5357	4.5807	1.0323
51	A	1376.5976	1.5771	5.3540	0.8426
52	A	1386.2777	3.4150	86.8454	11.0330
53	A	1418.7464	1.4825	8.8059	0.5988
54	A	1446.6830	1.6058	0.2140	7.3767
55	A	1459.0322	2.2882	4.3149	1.3961
56	A	1472.7518	1.4047	3.3487	12.5521
57	A	1478.9749	1.3841	4.2502	12.5271
58	A	1483.1898	1.5618	14.0468	10.9073
59	A	1490.3831	1.3693	3.8398	4.0500

60	A	1498.0181	1.4225	18.6541	14.0708
61	A	1500.4077	1.3864	9.7675	4.9720
62	A	1507.5571	1.4133	5.0426	2.9710
63	A	1509.0873	1.4413	1.0874	1.9886
64	A	1526.8255	1.5919	11.3972	7.3269
65	A	1544.5072	2.7317	109.5564	2.2802
66	A	1587.3463	9.9704	40.4903	1.5598
67	A	1637.5813	8.1194	282.8986	42.3967
68	A	2980.8745	5.5110	56.6338	92.1925
69	A	2986.7657	5.5509	110.7963	357.0383
70	A	2994.9286	5.6511	28.4775	309.7132
71	A	3025.9855	5.6002	19.4397	165.9611
72	A	3053.2365	5.9848	7.5077	78.9448
73	A	3078.6724	6.0438	7.2797	58.0133
74	A	3079.7649	6.0569	32.4883	48.0671
75	A	3088.5796	6.1208	12.4877	100.3794
76	A	3092.9167	6.0224	32.6807	107.4663
77	A	3102.5181	6.2483	26.4790	31.3679
78	A	3122.6340	6.3259	3.1781	2.2221
79	A	3132.0107	6.3481	25.5872	107.5692
80	A	3139.7986	6.3188	37.8661	111.4204
81	A	3142.8841	6.3518	11.0346	144.7003
82	A	3155.4259	6.5127	4.7331	65.9254
83	A	3215.1448	6.6462	5.8335	89.2477
84	A	3215.3077	6.6451	8.1894	54.1871

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.2819	0.0000	0.1552	2.8085
2	A	12.7123	0.0003	1.3802	0.3261
3	A	15.1435	0.0006	1.9895	0.6039
4	A	48.3343	0.0078	0.2574	1.5307
5	A	57.0154	0.0166	4.4642	4.8458
6	A	70.4190	0.0110	0.1529	0.9853
7	A	82.6450	0.0101	0.0133	1.2022
8	A	84.6673	0.0089	4.7208	0.5337
9	A	128.8541	0.0232	0.2385	0.8572
10	A	149.8122	0.0226	0.0688	3.4985
11	A	173.0879	0.0215	0.0848	0.2106
12	A	197.0867	0.0373	0.1558	4.4090
13	A	267.2170	0.0939	0.1064	1.4976
14	A	270.2342	0.0837	3.3504	11.2284
15	A	272.6879	0.1004	4.3922	0.7133
16	A	387.4724	0.2016	0.4689	29.8185
17	A	397.4492	0.2892	2.8837	14.5072
18	A	405.3494	0.2684	0.0257	0.3340
19	A	482.0601	0.4991	3.3311	2.7004
20	A	504.3142	0.4751	0.4818	142.4826
21	A	539.4040	0.4724	18.0302	1.2286
22	A	554.6988	0.6111	3.3259	2.7603
23	A	681.9871	1.8980	0.0251	3.4220
24	A	746.7367	1.0233	0.4984	0.3497
25	A	767.4764	1.7068	12.2435	23.4302
26	A	771.5720	0.4501	8.8943	5.6949
27	A	814.8790	0.7167	50.8523	0.7368
28	A	825.1210	0.5476	3.8941	6.1245
29	A	828.2495	0.5026	0.0014	0.3270
30	A	888.5465	0.9571	3.4723	7.7957
31	A	960.5605	0.7161	0.5102	0.7654
32	A	970.0483	1.6124	18.6981	26.4443
33	A	989.5953	0.8189	0.0055	0.2216
34	A	1012.1636	4.2128	76.1198	25.1733
35	A	1025.3290	0.8087	1.3544	3.0375
36	A	1048.2381	0.8418	0.1791	2.0105
37	A	1079.9645	1.0412	21.9815	0.2060
38	A	1087.4509	1.5007	2.5422	7.0647
39	A	1095.1274	1.4244	5.6513	23.3057
40	A	1132.6418	1.1445	0.5942	0.7660

41	A	1133.7840	0.9890	0.9979	1.7434
42	A	1143.2483	1.0406	21.8620	3.4102
43	A	1201.1615	1.4677	6.8992	10.2079
44	A	1218.9139	1.2395	9.0700	19.0470
45	A	1227.2347	1.2143	63.3372	22.4811
46	A	1254.5114	1.1619	62.8330	19.7621
47	A	1256.8173	3.1362	35.6383	0.0171
48	A	1308.5773	1.1536	39.8909	7.0317
49	A	1323.6717	5.7698	0.8546	10.1715
50	A	1374.8100	1.5702	10.4408	2.1287
51	A	1376.3569	1.5761	11.3064	0.0844
52	A	1396.4139	3.4106	151.9374	31.3103
53	A	1415.0651	1.4807	11.1400	1.1289
54	A	1447.7375	1.5336	0.5029	11.0396
55	A	1463.3156	2.5260	1.5109	0.5179
56	A	1472.7764	1.4016	2.6370	16.7117
57	A	1481.2132	1.3871	3.6233	15.8752
58	A	1485.3739	1.5911	22.0553	5.6754
59	A	1487.8653	1.3579	2.1895	7.1087
60	A	1495.8383	1.3925	18.2761	19.6750
61	A	1499.4087	1.3842	7.8244	6.5010
62	A	1507.8764	1.4160	5.7107	3.3203
63	A	1514.3945	1.4650	4.0100	1.4590
64	A	1528.5085	1.6107	15.4498	15.5521
65	A	1550.2735	2.8749	144.5128	2.2896
66	A	1584.3557	9.8952	37.6445	2.3215
67	A	1642.1152	8.1105	411.1267	70.7881
68	A	2983.7850	5.5038	71.6215	75.9980
69	A	2990.1804	5.5498	83.1033	291.6760
70	A	2991.1299	5.6361	36.6769	379.4435
71	A	3022.6497	5.5861	26.6141	201.4456
72	A	3047.0102	5.9584	8.6210	87.3134
73	A	3056.3485	5.9900	12.4125	112.3213
74	A	3057.3795	6.0042	48.3235	75.6190
75	A	3081.2067	5.9889	11.1525	163.8142
76	A	3085.5375	6.1010	51.4870	87.7486
77	A	3098.8859	6.2312	31.5641	28.4473
78	A	3120.9645	6.3023	2.5331	1.4119
79	A	3132.7354	6.3341	36.6943	187.2765
80	A	3143.0390	6.4565	8.0229	74.6978
81	A	3145.0975	6.3413	24.5243	59.2053
82	A	3147.9608	6.3735	1.6226	75.3182
83	A	3213.0496	6.6407	8.0613	155.7853
84	A	3213.1084	6.6343	12.3063	30.8295

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	4.9144	0.0000	0.3030	0.5671
2	A	15.6617	0.0007	0.9810	4.1090
3	A	30.3380	0.0013	0.4231	5.1383
4	A	32.3335	0.0055	0.5083	0.6099
5	A	47.3515	0.0045	0.5311	1.5947
6	A	70.2496	0.0160	0.2866	6.7146
7	A	102.0870	0.0161	0.0360	0.0774
8	A	114.4404	0.0206	0.7147	0.3079
9	A	140.7778	0.0392	5.0728	5.0976
10	A	167.0422	0.0199	10.2178	6.8169
11	A	172.8522	0.0226	0.4025	0.1811
12	A	198.0356	0.0821	0.9419	4.3148
13	A	237.5833	0.0360	0.0388	0.0378
14	A	278.6140	0.1702	7.8060	36.6732
15	A	283.0916	0.1796	31.6960	3.2591
16	A	284.1076	0.0963	0.0165	0.0010
17	A	397.9337	0.2545	0.0206	0.1528
18	A	405.0570	0.2752	2.2377	4.6967
19	A	479.5185	0.4901	2.0016	2.8491
20	A	536.0289	0.5034	11.9944	2.0180
21	A	555.7647	0.5559	1.1220	0.5973

22	A	594.8439	0.7827	10.8011	90.9146
23	A	683.7241	1.9084	0.3556	3.8652
24	A	734.6712	0.3474	3.2360	0.1445
25	A	742.6543	1.0515	1.0579	0.5661
26	A	764.8304	1.7203	24.3336	20.0572
27	A	812.2891	0.6969	67.3432	0.6020
28	A	828.6035	0.5059	0.2846	0.4681
29	A	837.5305	0.4895	0.1132	0.6306
30	A	901.1440	0.9244	7.0478	0.4186
31	A	957.9360	0.7147	1.3459	0.1793
32	A	968.6735	1.5792	29.5610	8.9160
33	A	988.7836	0.8221	0.0266	0.1939
34	A	1008.3535	4.3162	37.2791	27.7451
35	A	1029.1073	0.6890	0.9817	1.2089
36	A	1029.2844	1.8170	0.8045	32.9202
37	A	1078.7409	1.0440	16.4285	0.0833
38	A	1095.4846	1.4061	0.1665	6.5337
39	A	1106.4233	1.4353	1.8155	4.4547
40	A	1125.3743	0.9336	0.3324	3.6692
41	A	1131.3454	1.2378	3.8949	0.0846
42	A	1152.7461	1.0979	37.4658	4.2340
43	A	1200.2997	1.4907	10.6908	5.9448
44	A	1216.7053	1.0836	77.9559	34.3636
45	A	1236.8685	1.3091	0.3436	0.4857
46	A	1248.4174	2.9593	27.8224	0.5958
47	A	1256.8371	1.1644	24.6919	7.9329
48	A	1311.7174	6.4702	1.0339	9.9496
49	A	1323.8017	1.1408	0.3741	6.5931
50	A	1359.9006	1.5069	2.4172	19.8190
51	A	1374.9340	1.5325	4.4286	1.1207
52	A	1385.2727	3.4294	89.5445	12.2331
53	A	1411.4900	1.4333	2.1152	0.8995
54	A	1446.5936	1.6084	0.2491	7.3266
55	A	1458.8805	2.2790	4.3656	1.4720
56	A	1479.6845	1.4273	1.6477	8.7396
57	A	1483.0396	1.5604	14.8065	12.7585
58	A	1490.6034	1.3703	3.6415	3.5431
59	A	1494.3773	1.3798	2.3976	13.0452
60	A	1498.3395	1.4262	22.3947	13.1401
61	A	1498.9742	1.3753	9.1197	10.1336
62	A	1508.6017	1.4390	1.0918	2.1532
63	A	1509.4147	1.4580	7.6004	0.8429
64	A	1526.6976	1.5873	12.4628	7.3777
65	A	1544.2330	2.7285	111.7885	2.8672
66	A	1587.5201	9.9800	40.9753	1.5749
67	A	1637.4253	8.1212	289.3945	44.4682
68	A	2980.6365	5.5113	55.4021	90.8399
69	A	2986.4788	5.5507	111.3746	362.9722
70	A	3021.2939	5.5669	34.3129	201.6016
71	A	3039.8173	5.7687	6.2277	72.3741
72	A	3065.5293	6.1071	0.3449	98.6935
73	A	3080.4426	6.0480	7.0732	56.6240
74	A	3081.5687	6.0610	33.1518	49.3017
75	A	3087.1100	5.9802	9.0986	133.6807
76	A	3089.7800	6.2093	37.4782	10.8974
77	A	3091.6376	6.1453	34.5612	113.6473
78	A	3123.0076	6.3291	3.3649	2.6707
79	A	3132.1406	6.3504	25.3430	104.6923
80	A	3139.9902	6.3196	37.9862	113.9473
81	A	3143.0742	6.3526	11.3214	146.9761
82	A	3150.8724	6.4975	6.8556	46.0522
83	A	3215.3682	6.6494	2.8158	135.1209
84	A	3215.4130	6.6430	11.4093	9.8622

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.6872	0.0000	0.2340	2.0746
2	A	13.1978	0.0003	1.1507	0.2856

3	A	14.1493	0.0005	1.8252	0.3991
4	A	48.3653	0.0082	0.2769	1.9805
5	A	56.7190	0.0160	4.7504	4.8178
6	A	62.8907	0.0065	0.0006	0.6054
7	A	82.6538	0.0101	0.0118	1.2181
8	A	84.5887	0.0088	4.7403	0.4947
9	A	122.1971	0.0256	0.4674	0.7930
10	A	149.7654	0.0228	0.0548	2.9564
11	A	173.0821	0.0215	0.0761	0.2208
12	A	203.3735	0.0876	0.4406	8.4310
13	A	239.1869	0.0365	0.0343	0.0320
14	A	267.6602	0.1013	0.0000	0.1420
15	A	272.2559	0.1376	7.7575	2.4130
16	A	278.9128	0.1677	1.3247	53.1205
17	A	397.5015	0.2893	3.0306	14.9177
18	A	405.5897	0.2686	0.0258	0.3435
19	A	482.0959	0.4992	3.3089	2.6567
20	A	539.3938	0.4716	17.8031	2.5311
21	A	554.7118	0.6123	3.3851	1.5297
22	A	598.2904	0.7664	2.3841	161.0150
23	A	681.9746	1.8965	0.0237	3.4321
24	A	731.3177	0.3456	3.6429	0.1016
25	A	746.9871	1.0228	0.3971	0.2323
26	A	767.5620	1.7257	11.4267	22.7416
27	A	814.8745	0.7171	51.0322	0.7156
28	A	828.1971	0.5025	0.0005	0.3353
29	A	834.0948	0.4865	0.0058	0.8241
30	A	900.0160	0.9303	5.7994	0.5726
31	A	960.7052	0.7172	0.5236	0.8964
32	A	970.0586	1.6122	18.5962	27.1050
33	A	989.4265	0.8189	0.0051	0.2401
34	A	1012.3235	4.2150	76.9556	24.0473
35	A	1025.4898	0.6851	1.5233	1.0491
36	A	1031.1738	1.7632	0.1884	36.0331
37	A	1079.9710	1.0413	21.9932	0.2113
38	A	1095.1400	1.4245	6.4376	22.9569
39	A	1104.8035	1.4313	3.0110	10.7316
40	A	1132.7255	1.1337	0.5473	0.8717
41	A	1133.8399	0.9972	1.0622	1.6364
42	A	1143.2279	1.0404	22.1074	3.4393
43	A	1201.1751	1.4674	7.3918	10.2101
44	A	1212.6525	1.0913	92.8160	49.0564
45	A	1237.5285	1.3110	0.3005	0.5123
46	A	1254.5480	1.1611	62.2939	20.1995
47	A	1256.8643	3.1342	35.7330	0.0122
48	A	1322.7778	1.1395	0.2696	7.1053
49	A	1323.7645	5.7515	0.8353	10.5633
50	A	1358.4109	1.5139	1.0406	30.5112
51	A	1376.3762	1.5764	11.2061	0.0832
52	A	1396.4620	3.4123	155.9422	33.0916
53	A	1409.5329	1.4342	2.5359	1.0526
54	A	1447.7632	1.5323	0.5012	11.0505
55	A	1463.4005	2.5303	1.5275	0.5272
56	A	1479.2866	1.4224	1.5316	12.4231
57	A	1485.3915	1.5911	22.0655	5.8402
58	A	1487.8589	1.3579	2.1813	7.1251
59	A	1493.6853	1.3822	1.9619	13.5515
60	A	1495.8547	1.3924	18.2755	19.6988
61	A	1498.4682	1.3749	8.5689	10.9721
62	A	1508.7461	1.4533	7.2612	1.1975
63	A	1514.4091	1.4652	4.0188	1.4515
64	A	1528.5321	1.6101	15.8649	16.0210
65	A	1550.3673	2.8789	144.8116	2.3232
66	A	1584.3626	9.8933	37.8775	2.3666
67	A	1642.2352	8.1116	415.4320	72.0876
68	A	2983.8724	5.5039	71.7443	76.1007
69	A	2990.2697	5.5496	78.2216	320.0517
70	A	3017.8886	5.5528	42.3958	230.3018
71	A	3033.1645	5.7434	7.9111	90.3466
72	A	3056.3222	5.9901	12.3531	112.5826
73	A	3057.3535	6.0044	48.4818	76.1933

74	A	3058.7169	6.0787	0.0160	107.0924
75	A	3077.8702	5.9149	18.8491	146.6599
76	A	3084.7250	6.1868	42.4529	14.3348
77	A	3085.0852	6.1514	43.5509	150.6659
78	A	3121.0129	6.3025	2.5318	1.4227
79	A	3132.7907	6.3343	36.8318	188.5222
80	A	3138.5242	6.4431	11.4407	52.9248
81	A	3145.3213	6.3422	24.7054	59.3646
82	A	3148.1814	6.3745	1.4207	74.9019
83	A	3213.1421	6.6411	8.2359	156.6088
84	A	3213.2000	6.6346	12.2858	31.4487

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	1.1769	0.0000	0.0027	0.3776
2	A	17.3118	0.0009	0.8497	4.1702
3	A	29.8548	0.0016	0.4597	4.2430
4	A	31.1668	0.0028	0.4919	2.1714
5	A	47.5271	0.0045	0.5453	1.4861
6	A	70.4074	0.0165	0.6202	7.1019
7	A	101.8614	0.0160	0.0282	0.0720
8	A	114.5820	0.0205	0.7040	0.2926
9	A	140.8583	0.0386	5.6215	4.6863
10	A	166.9965	0.0200	11.2005	6.4410
11	A	171.8782	0.0223	0.4025	0.1724
12	A	198.1236	0.0821	0.8698	4.6627
13	A	237.5081	0.0360	0.0396	0.0323
14	A	278.4234	0.1717	6.9314	41.1226
15	A	283.3312	0.1795	35.0596	2.7728
16	A	284.0929	0.0967	0.0534	0.0046
17	A	397.6093	0.2542	0.0217	0.1678
18	A	405.1977	0.2752	2.2062	4.8709
19	A	479.4474	0.4899	1.9551	2.9162
20	A	536.2752	0.5049	12.0685	1.8857
21	A	555.8873	0.5538	1.7007	1.4089
22	A	595.2590	0.7830	10.7315	98.1691
23	A	683.7170	1.9083	0.3631	3.9562
24	A	734.8682	0.3476	3.2913	0.1346
25	A	742.8114	1.0440	1.1147	0.5653
26	A	764.8407	1.7199	27.3078	20.4455
27	A	812.7933	0.7012	67.0003	0.6814
28	A	828.6510	0.5062	0.2433	0.4956
29	A	837.7362	0.4892	0.0894	0.7425
30	A	901.3566	0.9241	8.0021	0.2895
31	A	957.9989	0.7154	1.4386	0.1789
32	A	968.6014	1.5769	27.8365	8.9511
33	A	988.5404	0.8215	0.0285	0.2051
34	A	1008.3596	4.3188	37.6372	29.7050
35	A	1029.3771	1.8100	0.9106	35.1596
36	A	1029.8936	0.6913	1.0244	1.2578
37	A	1078.6106	1.0439	16.3392	0.0749
38	A	1095.5287	1.4061	0.1831	6.7494
39	A	1106.9880	1.4365	1.9164	4.2762
40	A	1125.2036	0.9327	0.3464	3.5369
41	A	1131.3438	1.2393	3.8068	0.0765
42	A	1152.8977	1.0991	40.3659	4.9139
43	A	1200.1862	1.4904	13.1392	6.1337
44	A	1218.1173	1.0862	80.3574	38.7261
45	A	1237.6333	1.3091	0.2431	0.4694
46	A	1248.2064	2.9565	27.6297	0.6805
47	A	1256.8694	1.1645	25.1350	8.1952
48	A	1311.5176	6.4897	1.0360	10.6221
49	A	1322.7799	1.1392	0.3747	6.9762
50	A	1358.5456	1.5087	3.4926	21.5859
51	A	1374.8821	1.5318	4.3862	1.1406
52	A	1384.9419	3.4285	93.4490	13.5325
53	A	1411.7000	1.4335	2.3819	0.9598
54	A	1446.5120	1.6076	0.2796	7.3854

55	A	1458.8119	2.2782	4.3773	1.4700
56	A	1479.9629	1.4278	1.8383	9.6591
57	A	1482.9646	1.5599	16.2847	14.4475
58	A	1490.4705	1.3702	3.5101	3.5531
59	A	1494.4303	1.3806	2.9620	14.3000
60	A	1498.3519	1.4263	21.7823	11.5774
61	A	1498.8075	1.3749	9.1941	10.6127
62	A	1508.3424	1.4385	1.0034	2.1600
63	A	1509.4267	1.4574	6.6951	0.9989
64	A	1526.5479	1.5843	13.7201	7.3069
65	A	1544.1128	2.7330	117.3119	3.4312
66	A	1587.6451	9.9880	41.3972	1.5609
67	A	1637.4173	8.1225	304.1525	46.1447
68	A	2980.4674	5.5111	55.0841	88.0698
69	A	2986.3081	5.5504	108.3523	351.1578
70	A	3021.7035	5.5679	33.9282	213.1408
71	A	3037.3446	5.7585	9.0823	76.3059
72	A	3064.1686	6.1027	0.0200	97.9658
73	A	3080.7859	6.0485	6.7295	55.3861
74	A	3081.9279	6.0614	32.7699	44.7513
75	A	3087.4744	6.0100	10.1518	147.8287
76	A	3089.6111	6.2074	39.6107	14.1703
77	A	3091.3437	6.1159	34.9074	115.9407
78	A	3122.9466	6.3294	3.4242	2.7984
79	A	3132.0162	6.3504	25.7305	100.0629
80	A	3140.1422	6.3203	38.0518	118.5846
81	A	3143.2297	6.3533	11.9910	151.0153
82	A	3151.4398	6.4997	6.2300	40.0819
83	A	3215.3326	6.6478	4.8419	107.4618
84	A	3215.4109	6.6445	9.5851	37.6261

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NM#	Symm	Wavenumber	Force Const	IR Intens	Raman Activ
1	A	3.6827	0.0000	0.2338	2.0748
2	A	13.1893	0.0003	1.1510	0.2855
3	A	14.1496	0.0005	1.8251	0.3991
4	A	48.3651	0.0082	0.2769	1.9805
5	A	56.7176	0.0160	4.7504	4.8178
6	A	62.8885	0.0065	0.0006	0.6054
7	A	82.6535	0.0101	0.0118	1.2181
8	A	84.5839	0.0088	4.7399	0.4947
9	A	122.1961	0.0256	0.4674	0.7930
10	A	149.7652	0.0228	0.0548	2.9563
11	A	173.0823	0.0215	0.0761	0.2208
12	A	203.3748	0.0876	0.4406	8.4307
13	A	239.1836	0.0365	0.0343	0.0320
14	A	267.6587	0.1013	0.0000	0.1420
15	A	272.2555	0.1376	7.7570	2.4130
16	A	278.9078	0.1677	1.3246	53.1198
17	A	397.5008	0.2893	3.0306	14.9179
18	A	405.5898	0.2686	0.0258	0.3435
19	A	482.0959	0.4992	3.3089	2.6567
20	A	539.3939	0.4716	17.8031	2.5309
21	A	554.7117	0.6123	3.3851	1.5298
22	A	598.2886	0.7664	2.3841	161.0147
23	A	681.9746	1.8965	0.0237	3.4321
24	A	731.3167	0.3456	3.6429	0.1016
25	A	746.9871	1.0228	0.3971	0.2323
26	A	767.5619	1.7257	11.4265	22.7415
27	A	814.8743	0.7171	51.0324	0.7156
28	A	828.1971	0.5025	0.0005	0.3353
29	A	834.0917	0.4865	0.0058	0.8241
30	A	900.0161	0.9303	5.7993	0.5727
31	A	960.7051	0.7172	0.5236	0.8964
32	A	970.0588	1.6122	18.5958	27.1053
33	A	989.4264	0.8189	0.0051	0.2401
34	A	1012.3235	4.2150	76.9557	24.0470
35	A	1025.4872	0.6851	1.5233	1.0491

36	A	1031.1728	1.7632	0.1885	36.0324
37	A	1079.9712	1.0413	21.9934	0.2113
38	A	1095.1398	1.4245	6.4377	22.9571
39	A	1104.8029	1.4313	3.0109	10.7322
40	A	1132.7252	1.1339	0.5480	0.8706
41	A	1133.8402	0.9971	1.0614	1.6375
42	A	1143.2274	1.0404	22.1057	3.4390
43	A	1201.1750	1.4674	7.3914	10.2100
44	A	1212.6507	1.0913	92.8159	49.0575
45	A	1237.5274	1.3110	0.3005	0.5123
46	A	1254.5463	1.1611	62.2936	20.1995
47	A	1256.8648	3.1342	35.7334	0.0122
48	A	1322.7783	1.1395	0.2696	7.1055
49	A	1323.7650	5.7513	0.8353	10.5633
50	A	1358.4114	1.5139	1.0405	30.5106
51	A	1376.3750	1.5764	11.2062	0.0832
52	A	1396.4623	3.4123	155.9434	33.0917
53	A	1409.5305	1.4341	2.5359	1.0527
54	A	1447.7631	1.5323	0.5012	11.0504
55	A	1463.4001	2.5303	1.5273	0.5273
56	A	1479.2865	1.4224	1.5317	12.4232
57	A	1485.3916	1.5911	22.0657	5.8401
58	A	1487.8588	1.3579	2.1811	7.1252
59	A	1493.6854	1.3822	1.9619	13.5514
60	A	1495.8546	1.3924	18.2753	19.6989
61	A	1498.4663	1.3749	8.5689	10.9721
62	A	1508.7462	1.4533	7.2612	1.1975
63	A	1514.4094	1.4652	4.0188	1.4514
64	A	1528.5321	1.6101	15.8642	16.0213
65	A	1550.3673	2.8789	144.8122	2.3232
66	A	1584.3625	9.8934	37.8778	2.3666
67	A	1642.2352	8.1117	415.4348	72.0874
68	A	2983.8728	5.5039	71.7454	76.1002
69	A	2990.2701	5.5496	78.2202	320.0526
70	A	3017.8885	5.5528	42.3956	230.2995
71	A	3033.1648	5.7435	7.9110	90.3466
72	A	3056.3206	5.9901	12.3528	112.5855
73	A	3057.3519	6.0044	48.4828	76.1916
74	A	3058.7169	6.0787	0.0160	107.0929
75	A	3077.8702	5.9149	18.8491	146.6596
76	A	3084.7248	6.1868	42.4529	14.3344
77	A	3085.0852	6.1514	43.5508	150.6648
78	A	3121.0128	6.3025	2.5318	1.4226
79	A	3132.7908	6.3343	36.8318	188.5227
80	A	3138.5243	6.4431	11.4406	52.9248
81	A	3145.3213	6.3422	24.7055	59.3646
82	A	3148.1813	6.3745	1.4207	74.9019
83	A	3213.1419	6.6411	8.2360	156.6066
84	A	3213.1998	6.6346	12.2858	31.4510

C. Experimental Spectra and Images

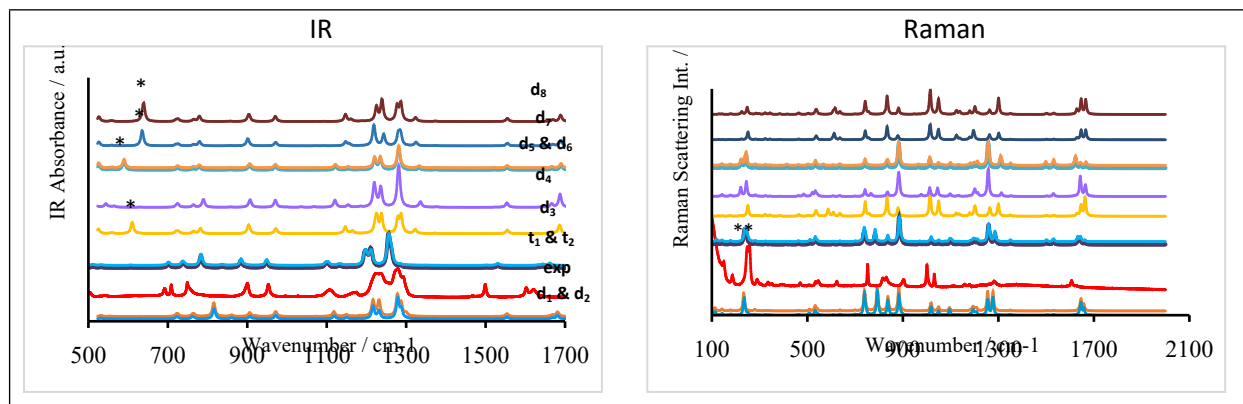


Figure S1. IR (left panel) and Raman spectra (right panel) of the mixture of ANL and iso-C₃F₇I at molar fraction of 1:1 along with the calculated ones for dimers and trimers.

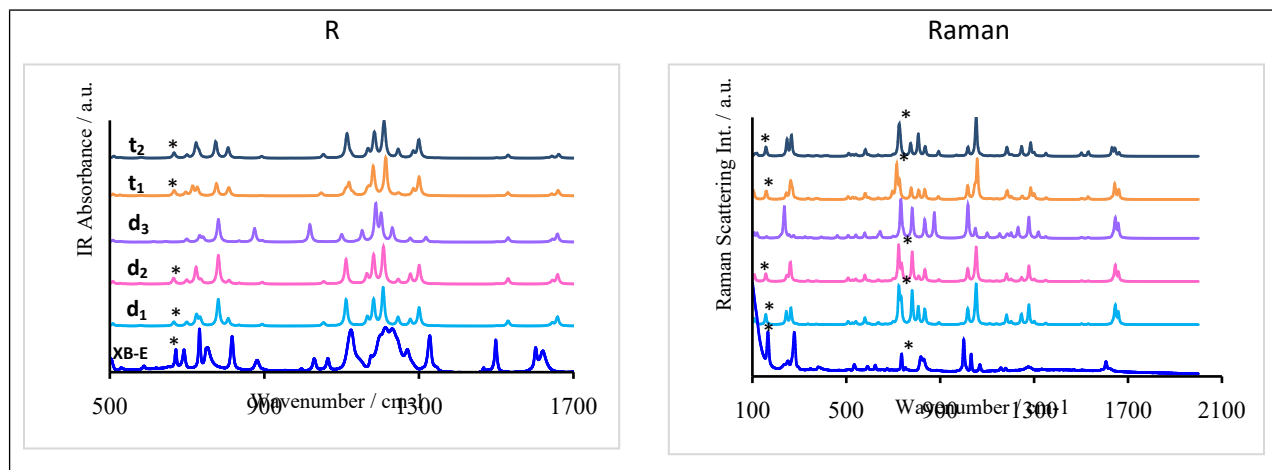
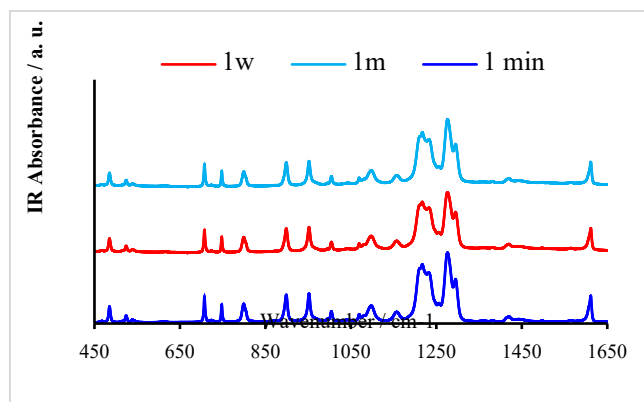
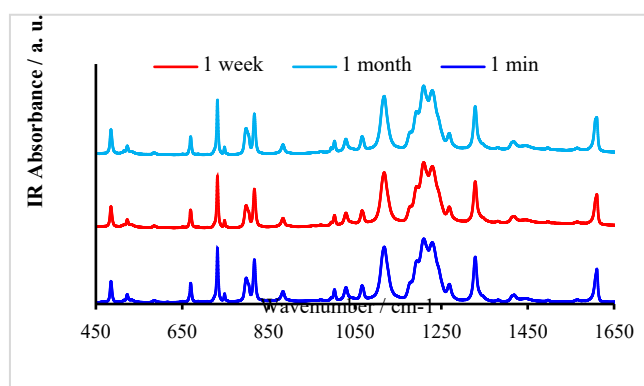


Figure S2. FT-IR (left panel) and Raman spectra (right panel) of mixtures of ANL and n-C₃F₇I at molar fraction of 1:1, along with the calculated Raman spectra of dimers and trimers.



(a)



(b)

Figure S3. FT-IR spectra for [MePy · iso-C3F7I] (a) and [MePy · n-C3F7I] (b) after 1 minute (dark blue), 1 week (red) and 1 month (light blue) after mixing

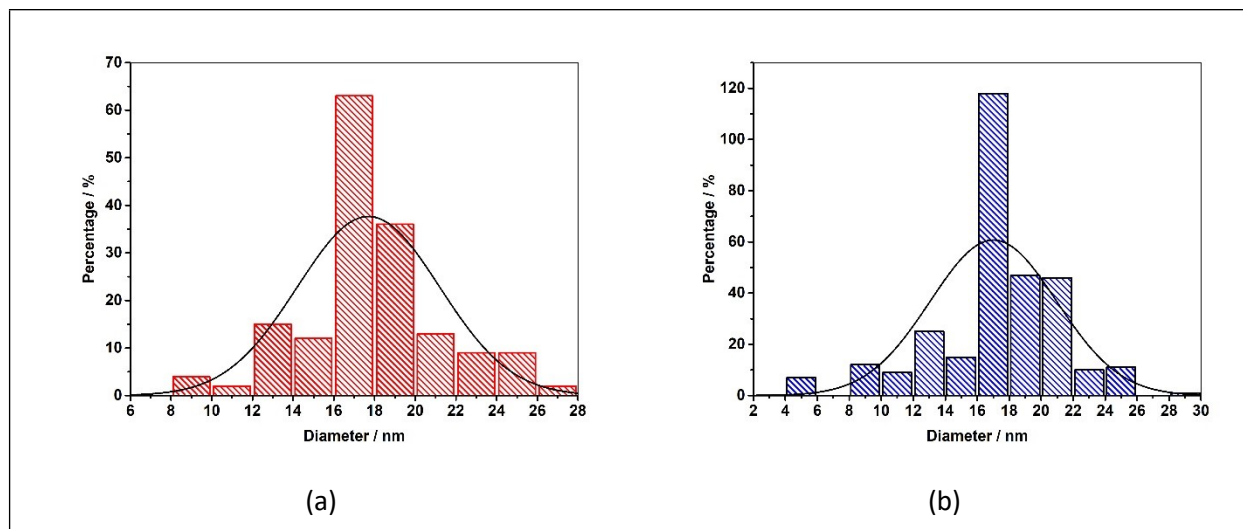


Figure S4. The size distribution (TEM histograms and Gaussian fit) for [MePy · iso-C₃F₇I] (a) and [MePy · n-C₃F₇I] at 72 h after mixing.

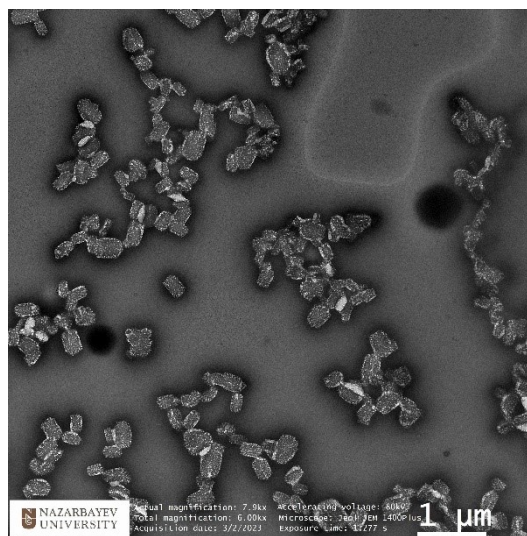
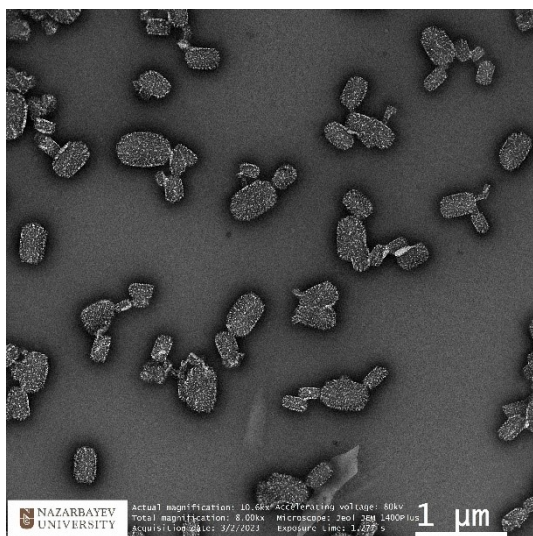


Figure S5: TEM images for [MePy · iso-C₃F₇I] 6 weeks after mixing.