

Supplementary Information

Is β -homo-proline a pseudo- γ -turn forming element of β -peptides? An IR and VCD spectroscopic study on Ac- β -HPro-NHMe in cryogenic matrices and solutions

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Table S1. Cartesian geometries of Ac- β^3 -HPro-NHMe conformers as obtained at the B3LYP/6-31++G level of theory.**

conformer	atomic label	x	y	z
A††	N	-0.947397	0.371045	0.196585
	C	-1.822236	0.066985	-0.952759
	C	-0.737730	-0.816960	1.067155
	H	-1.223535	-0.063328	-1.864506
	H	-2.539161	0.873180	-1.125871
	C	-2.498139	-1.248712	-0.548107
	C	-1.409072	-1.952651	0.271001
	H	-1.276760	-0.639788	2.008113
	C	1.693622	-1.009342	0.256259
	H	-2.826965	-1.827276	-1.415781
	H	-3.377402	-1.039766	0.073096
	H	-0.669733	-2.414620	-0.391068
	H	-1.801201	-2.726596	0.937257
	O	1.762542	-1.887982	-0.608013
	C	0.735074	-1.100693	1.439765
	H	1.040410	-0.420752	2.235499
	H	0.786894	-2.126373	1.820294
	N	2.473349	0.105864	0.234801
	H	2.226586	0.856317	0.869160
	C	3.396976	0.376041	-0.855277
	H	3.913283	-0.546874	-1.126399
	H	2.883482	0.750797	-1.750234
	H	4.128395	1.118168	-0.527563
	C	-0.486648	1.606963	0.526220
	O	0.200960	1.802571	1.538977
	C	-0.839120	2.753384	-0.409150
	H	-0.614546	2.517924	-1.454431
	H	-1.906353	2.995142	-0.344804
	H	-0.265575	3.627331	-0.100220

At-	N	-1.068044	0.228411	0.220683
	C	-1.721695	-0.309596	-0.986441
	C	-0.706608	-0.830770	1.195051
	H	-1.366753	0.203937	-1.884027
	H	-2.812200	-0.176637	-0.926246
	C	-1.339745	-1.793355	-0.966954
	C	-1.261309	-2.115530	0.534056
	H	-1.234596	-0.623907	2.133024
	C	1.737177	-0.685933	0.364107
	H	-0.358389	-1.935186	-1.427235
	H	-2.069035	-2.411151	-1.498583
	H	-0.632441	-2.983993	0.741470
	H	-2.262929	-2.322949	0.929167
	O	1.968630	-1.592908	-0.440107
	C	0.802385	-0.861932	1.554347
	H	0.992135	-0.087996	2.299921
	H	1.024262	-1.834384	2.005036
	N	2.304485	0.547518	0.261109
	H	1.946119	1.279616	0.861657
	C	3.180017	0.903131	-0.844176
	H	3.855781	0.070750	-1.050401
	H	2.619434	1.118803	-1.762806
	H	3.764027	1.783980	-0.568321
	C	-0.906077	1.548440	0.507009
	O	-0.336826	1.926254	1.540611
	C	-1.435171	2.547948	-0.509004
	H	-0.864692	2.497784	-1.443469
	H	-2.486191	2.362895	-0.754403
	H	-1.331751	3.546760	-0.085075

Bf-	N	-1.254694	0.172511	0.046761
	C	-2.491022	-0.622492	-0.049101
	C	-0.064229	-0.649781	0.358726
	H	-3.069028	-0.352616	-0.938159
	H	-3.126843	-0.457059	0.832234
	C	-1.974928	-2.068636	-0.092057
	C	-0.687200	-2.004451	0.747197
	H	0.445328	-0.190904	1.210561
	C	2.383710	-0.518563	-0.420649
	H	-1.744124	-2.352993	-1.124941
	H	-2.708558	-2.780894	0.294923
	H	-0.003634	-2.836702	0.562707
	H	-0.937244	-2.006005	1.814705
	O	3.212935	-1.429862	-0.462367
	C	0.927334	-0.725845	-0.840367
	H	0.869095	-1.699351	-1.333064
	H	0.662103	0.041933	-1.573069
	N	2.659627	0.745751	-0.000307
	H	1.885282	1.405671	0.036615
	C	3.969257	1.151151	0.479882
	H	4.355304	1.992821	-0.105781
	H	3.929851	1.447991	1.534628
	H	4.647131	0.302956	0.374373
	C	-1.154756	1.524614	-0.036393
	O	-0.062130	2.100557	0.084736
	C	-2.430730	2.303439	-0.297712
	H	-2.824246	2.083711	-1.296761
	H	-3.213345	2.056311	0.427453
	H	-2.200246	3.366735	-0.234770

Bt+	N	-1.243869	0.141702	-0.163735
	C	-2.523144	-0.588075	-0.108419
	C	-0.078911	-0.747251	0.089602
	C	-2.165360	-1.854034	0.681750
	C	-0.728028	-2.140000	0.225529
	H	0.356521	-0.442230	1.049368
	C	2.426323	-0.491461	-0.435857
	H	-0.741106	-2.637758	-0.751275
	H	-0.167992	-2.780231	0.911839
	O	3.247466	-1.411844	-0.430056
	C	1.018127	-0.662514	-1.009759
	H	1.030759	-1.577626	-1.605712
	H	0.797460	0.175796	-1.675772
	N	2.685471	0.742868	0.065453
	H	1.915434	1.407063	0.095153
	C	3.949228	1.058050	0.710219
	H	4.028618	2.141787	0.819377
	H	4.031255	0.592762	1.700687
	H	4.779909	0.694230	0.100238
	C	-1.099629	1.493050	-0.167506
	O	0.009361	2.029730	-0.021271
	C	-2.347586	2.336464	-0.363770
	H	-2.974640	1.967469	-1.181065
	H	-2.955635	2.344848	0.548527
	H	-2.032441	3.357975	-0.576882
	H	-2.195506	-1.641408	1.756789
	H	-2.854128	-2.679487	0.480886
	H	-2.870342	-0.839818	-1.120599
	H	-3.297617	0.009940	0.376261

Cc-	N	1.857258	-0.003930	-0.072117
	C	2.381633	1.359530	-0.277391
	C	0.485826	-0.011117	0.467492
	H	2.737803	1.488137	-1.303732
	H	3.242695	1.518025	0.382631
	C	1.196699	2.271836	0.078498
	C	0.350931	1.414839	1.038117
	H	0.382975	-0.763417	1.251815
	C	-1.942285	-0.582260	-0.012411
	H	0.622015	2.523814	-0.820369
	H	1.523372	3.213611	0.527857
	H	-0.690905	1.740474	1.112137
	H	0.778610	1.442652	2.046484
	O	-2.076614	-1.279083	0.992437
	C	-0.567330	-0.320759	-0.621261
	H	-0.597885	0.485705	-1.363454
	H	-0.274710	-1.231538	-1.156490
	N	-2.997236	-0.005664	-0.660558
	H	-2.810185	0.530214	-1.495152
	C	-4.382234	-0.210337	-0.261015
	H	-4.378010	-0.762547	0.679349
	H	-4.887914	0.749191	-0.112648
	H	-4.930883	-0.790752	-1.011327
	C	2.711848	-1.068616	-0.160876
	O	3.877467	-0.913950	-0.532275
	C	2.184613	-2.438388	0.238216
	H	2.091053	-2.505883	1.328505
	H	1.203838	-2.666276	-0.188091
	H	2.907556	-3.183508	-0.094369

Cc+	N	1.838660	0.002202	-0.117013
	C	2.447650	1.289958	-0.487531
	C	0.460474	0.172367	0.398173
	H	1.684597	2.291829	0.383736
	H	0.263098	1.709346	0.410472
	C	0.388279	-0.217705	1.418024
	C	-1.984429	-0.460983	0.158498
	H	-0.279882	2.019586	-0.491662
	C	-0.326127	2.028308	1.273504
	H	-2.155837	-0.572648	1.371637
	H	-0.592390	-0.549439	-0.463414
	H	-0.576024	-0.144208	-1.482495
	H	-0.350958	-1.615306	-0.537941
	O	-3.012008	-0.278670	-0.722029
	C	-2.792668	-0.209063	-1.704776
	H	-4.410169	-0.255027	-0.317324
	H	-4.956900	-1.108914	-0.732661
	N	-4.440871	-0.309967	0.771293
	H	-4.893680	0.671388	-0.643933
	C	2.616071	-1.124042	-0.050963
	H	3.779516	-1.124669	-0.460865
	H	2.007772	-2.391729	0.529987
	H	1.233447	-2.216137	1.280432
	C	1.575672	-2.995152	-0.276342
	O	2.820772	-2.969933	0.971905
	C	3.521526	1.245701	-0.301397
	H	2.302449	1.494907	-1.557836
	H	2.113008	2.306848	1.392618
	H	1.718953	3.311152	-0.012099

Df-	N	-0.947747	0.304546	-0.064684
	C	-2.155339	-0.195911	-0.759050
	C	-0.303994	-0.755449	0.752716
	H	-2.045051	-0.125947	-1.846728
	H	-3.026967	0.401709	-0.471289
	C	-2.301603	-1.653686	-0.278749
	C	-1.499643	-1.690045	1.034055
	H	0.071221	-0.292883	1.668895
	C	2.206180	-0.876454	-0.225334
	H	-1.871239	-2.344280	-1.010449
	H	-3.350609	-1.931434	-0.145411
	H	-1.189079	-2.699183	1.317099
	H	-2.097782	-1.278424	1.855282
	O	3.033074	-1.519669	-0.878488
	C	0.829466	-1.507441	0.026562
	H	1.050616	-2.412571	0.606015
	H	0.484930	-1.860879	-0.950928
	N	2.486426	0.325989	0.327711
	H	1.735773	0.902870	0.707111
	C	3.784907	0.949623	0.114858
	H	3.838431	1.853918	0.724179
	H	4.585300	0.265012	0.407446
	H	3.939542	1.213758	-0.938036
	C	-0.676521	1.625315	0.126373
	O	0.240955	2.008014	0.868240
	C	-1.542708	2.629878	-0.611229
	H	-1.657646	2.377528	-1.669660
	H	-2.544762	2.675840	-0.168797
	H	-1.076128	3.610255	-0.517710

Df†	N	0.915658	0.235874	0.203357
	C	2.120603	-0.293685	0.858704
	C	0.265640	-0.846648	-0.584513
	C	2.680677	-1.257783	-0.195000
	C	1.408837	-1.891577	-0.791566
	H	-0.048871	-0.411187	-1.536555
	C	-2.298546	-0.828620	0.269249
	H	1.165078	-2.816276	-0.257838
	H	1.526076	-2.149545	-1.847580
	O	-3.175761	-1.412780	0.912327
	C	-0.929269	-1.506997	0.128228
	H	-1.147148	-2.446075	-0.396313
	H	-0.632455	-1.803512	1.141063
	N	-2.516103	0.346782	-0.364149
	H	-1.729065	0.879729	-0.733387
	C	-3.805368	1.014582	-0.255469
	H	-3.797602	1.890128	-0.907624
	H	-4.608463	0.339265	-0.562309
	H	-4.011173	1.332115	0.773595
	C	0.697916	1.551130	-0.085882
	O	-0.186497	1.905918	-0.879072
	C	1.557483	2.593350	0.609693
	H	1.607615	2.432870	1.690628
	H	2.580816	2.586858	0.217400
	H	1.117278	3.569831	0.408740
	H	3.365177	-1.997870	0.229925
	H	3.227524	-0.688116	-0.954863
	H	1.840530	-0.831129	1.774576
	H	2.809416	0.503366	1.134635

Et-	N	1.507435	0.011770	0.130309
	C	1.586781	1.125644	-0.827480
	C	0.549888	0.241315	1.222051
	H	1.422680	0.772962	-1.849976
	H	2.578039	1.597198	-0.778280
	C	0.478699	2.095861	-0.381124
	C	0.235149	1.747315	1.101389
	H	1.060322	0.022168	2.166167
	C	-1.624093	-0.582682	0.016232
	H	-0.421918	1.913117	-0.969239
	H	0.775129	3.139897	-0.518791
	H	-0.782189	1.985389	1.427488
	H	0.923277	2.310573	1.741994
	O	-1.246009	-0.404370	-1.142018
	C	-0.667486	-0.712643	1.194614
	H	-0.273612	-1.735779	1.190036
	H	-1.209767	-0.585808	2.140243
	N	-2.949147	-0.712487	0.336685
	H	-3.190781	-0.900260	1.298422
	C	-4.006581	-0.749513	-0.661856
	H	-3.562140	-0.495753	-1.624822
	H	-4.455594	-1.747138	-0.731263
	H	-4.789771	-0.022302	-0.424104
	C	2.264210	-1.120252	0.099109
	O	2.161592	-1.991489	0.971321
	C	3.230197	-1.268066	-1.063964
	H	2.685851	-1.339651	-2.012347
	H	3.912901	-0.414585	-1.138323
	H	3.806936	-2.180429	-0.912475

Fc-	N	-1.095588	0.500799	-0.130007
	C	-2.130372	0.051352	-1.084700
	C	-0.709999	-0.574684	0.800824
	H	-1.760537	0.084643	-2.115079
	H	-2.976664	0.743300	-1.031439
	C	-2.494024	-1.375371	-0.623925
	C	-1.982603	-1.444508	0.827956
	H	-0.474780	-0.160919	1.783470
	C	1.817427	-0.588494	0.363597
	H	-1.990973	-2.126112	-1.243107
	H	-3.568152	-1.565084	-0.699813
	H	-1.792603	-2.465482	1.172142
	H	-2.711407	-0.990023	1.508545
	O	2.275349	-0.198903	1.438988
	C	0.517010	-1.379836	0.304461
	H	0.651401	-2.240590	0.969308
	H	0.326090	-1.764687	-0.703525
	N	2.428680	-0.351736	-0.830959
	H	1.955042	-0.639053	-1.674523
	C	3.661470	0.412688	-0.954580
	H	4.084186	0.528498	0.043868
	H	4.375824	-0.118168	-1.591131
	H	3.474357	1.406332	-1.377316
	C	-0.872143	1.849433	0.004195
	O	-1.365462	2.641565	-0.801923
	C	-0.049587	2.336518	1.184948
	H	-0.658324	2.297060	2.097058
	H	0.855201	1.753129	1.366260
	H	0.211184	3.378331	0.996405

Fc+	N	-1.042981	0.454557	-0.209779
	C	-2.073459	0.030172	-1.165077
	C	-0.670936	-0.684200	0.651085
	C	-2.936293	-0.925439	-0.328144
	C	-1.918534	-1.623410	0.602947
	H	-0.470526	-0.335472	1.665853
	C	1.874038	-0.622701	0.306174
	O	2.295606	-0.334416	1.427625
	C	0.587424	-1.419377	0.131859
	H	0.711713	-2.337327	0.717700
	H	0.427769	-1.713924	-0.912435
	N	2.515401	-0.263254	-0.840998
	H	2.068934	-0.471124	-1.721894
	C	3.739900	0.524122	-0.853199
	H	4.135175	0.543530	0.162886
	H	4.477935	0.068833	-1.520460
	H	3.549648	1.553193	-1.178653
	C	-0.854382	1.794616	0.052074
	O	-1.329772	2.657929	-0.687501
	C	-0.070665	2.179106	1.295861
	H	-0.700867	2.041741	2.183490
	H	0.841012	1.597828	1.445682
	H	0.173443	3.238484	1.213962
	H	-1.634676	-2.602411	0.201890
	H	-2.324307	-1.794452	1.604122
	H	-3.655602	-0.342008	0.256492
	H	-3.501288	-1.634469	-0.940825
	H	-1.617751	-0.489687	-2.019807
	H	-2.595959	0.909559	-1.540934

Gf-	N	0.892681	0.502917	-0.118722
	C	2.125479	0.480678	0.686587
	C	0.623172	-0.781327	-0.781489
	H	1.920956	0.721835	1.735229
	H	2.843938	1.216344	0.302756
	C	2.655544	-0.956403	0.514303
	C	2.019152	-1.431424	-0.806045
	H	0.242338	-0.567100	-1.783330
	C	-1.627498	-0.928227	0.505223
	H	2.321305	-1.583028	1.347385
	H	3.748271	-0.990658	0.496665
	H	1.974899	-2.521258	-0.891441
	H	2.586842	-1.048652	-1.662006
	O	-1.639569	-0.458660	1.642984
	C	-0.404660	-1.671511	-0.025850
	H	-0.701806	-2.484297	-0.700263
	H	0.070818	-2.122146	0.849618
	N	-2.697381	-0.850227	-0.338593
	H	-2.514470	-1.035860	-1.315011
	C	-3.813205	0.040237	-0.045503
	H	-4.073927	-0.057847	1.009118
	H	-3.549833	1.085252	-0.248314
	H	-4.671582	-0.247341	-0.657413
	C	0.134992	1.607047	-0.387606
	O	-0.822259	1.561016	-1.167097
	C	0.521560	2.889631	0.326218
	H	0.440323	2.767750	1.411726
	H	1.551735	3.185817	0.099410
	H	-0.157813	3.677441	0.001459

Gf+	N	0.904497	0.401744	0.101898
	C	2.210284	0.282275	0.757862
	C	0.495258	-0.886893	-0.487992
	C	2.932371	-0.750500	-0.120010
	C	1.805758	-1.726568	-0.515872
	H	0.128014	-0.678681	-1.497820
	C	-1.872312	-0.788081	0.600575
	H	1.740532	-2.542329	0.212642
	H	1.973008	-2.181146	-1.496380
	O	-2.070361	-0.273743	1.700151
	C	-0.608630	-1.603278	0.326588
	H	-0.864365	-2.531649	-0.201247
	H	-0.210959	-1.876666	1.307913
	N	-2.773532	-0.715213	-0.423250
	H	-2.424038	-0.938182	-1.345049
	C	-3.883612	0.227905	-0.367113
	H	-4.333351	0.182579	0.625558
	H	-3.542851	1.253391	-0.553375
	H	-4.630136	-0.052860	-1.114116
	C	0.268210	1.560396	-0.251718
	O	-0.698903	1.552924	-1.018371
	C	0.792251	2.857847	0.341485
	H	0.929175	2.786340	1.424600
	H	1.753158	3.137085	-0.106425
	H	0.066740	3.640193	0.118872
	H	3.758938	-1.244234	0.399661
	H	3.340024	-0.251645	-1.006445
	H	2.722439	1.243869	0.800081
	H	2.092392	-0.084881	1.787297

Hc-	N	-1.178343	0.118780	0.231714
	C	-0.851868	0.622820	1.582822
	C	-0.512236	0.887434	-0.840682
	H	-0.505796	-0.191805	2.225150
	H	-1.762797	1.025968	2.040816
	C	0.213511	1.701982	1.339655
	C	-0.038463	2.161707	-0.108396
	H	-1.244567	1.143394	-1.613279
	C	1.832379	-0.244136	-0.691946
	H	1.220529	1.286906	1.434417
	H	0.129434	2.522821	2.057080
	H	0.848093	2.599043	-0.573825
	H	-0.841592	2.906944	-0.133512
	O	2.851790	0.446742	-0.691770
	C	0.621716	0.102199	-1.554397
	H	0.201980	-0.811560	-1.989445
	H	0.995776	0.718865	-2.376497
	N	1.717499	-1.370821	0.068019
	H	0.815735	-1.822157	0.123383
	C	2.767896	-1.789883	0.985265
	H	3.737422	-1.691030	0.493228
	H	2.785352	-1.178446	1.895935
	H	2.604677	-2.834128	1.259322
	C	-2.243092	-0.731772	0.087496
	O	-2.798936	-1.220622	1.073164
	C	-2.735440	-1.034559	-1.320427
	H	-3.249403	-0.160996	-1.738957
	H	-1.932414	-1.307665	-2.010472
	H	-3.448842	-1.856025	-1.253861

Hc+	N	-1.006571	0.475298	-0.179727
	C	-1.370443	-0.169535	-1.458205
	C	-0.720445	-0.530113	0.877796
	H	-0.492965	-0.245619	-2.114273
	H	-2.116997	0.441251	-1.967345
	C	-1.859471	-1.554701	-1.024269
	C	-0.943727	-1.884734	0.163060
	H	-1.461557	-0.417691	1.679860
	C	1.881183	-0.652550	0.619013
	H	0.012200	-2.280593	-0.196971
	H	-1.365002	-2.627861	0.845890
	O	2.672149	-1.572979	0.825477
	C	0.675231	-0.411777	1.531037
	H	0.782317	0.566187	2.012208
	H	0.744119	-1.167047	2.318622
	N	2.047122	0.228367	-0.406867
	H	1.303986	0.885171	-0.600023
	C	3.148962	0.103276	-1.351617
	H	4.089779	-0.015830	-0.809371
	H	3.025521	-0.766134	-2.007988
	H	3.194212	1.008670	-1.959926
	C	-1.301123	1.805546	0.009044
	O	-1.629617	2.524756	-0.936238
	C	-1.178855	2.384909	1.409860
	H	-1.483018	1.694304	2.200576
	H	-0.144074	2.688450	1.603913
	H	-1.801003	3.279851	1.446583
	H	-2.905826	-1.494939	-0.702285
	H	-1.796088	-2.293934	-1.827833

Ic-	N	-1.794111	0.050775	-0.066943
	C	-2.629559	-1.106971	-0.443834
	C	-0.454281	-0.347926	0.404666
	H	-3.012936	-0.989933	-1.461651
	H	-3.498085	-1.155297	0.223417
	C	-1.690999	-2.312039	-0.274189
	C	-0.658525	-1.833426	0.761711
	H	-0.181945	0.234845	1.289756
	C	2.045752	-0.241026	-0.159121
	H	-1.199634	-2.554296	-1.223538
	H	-2.227715	-3.208090	0.048858
	H	0.282507	-2.385019	0.747143
	H	-1.080950	-1.901513	1.771060
	O	2.425698	-1.221179	0.480734
	C	0.620620	-0.120596	-0.692087
	H	0.496202	-0.870623	-1.482065
	H	0.459016	0.857133	-1.157757
	N	2.864812	0.817940	-0.433960
	H	2.505146	1.567427	-1.005968
	C	4.269110	0.850285	-0.051426
	H	4.924668	0.668080	-0.911094
	H	4.519628	1.819548	0.389672
	H	4.433199	0.064276	0.686351
	C	-2.368412	1.287070	0.030474
	O	-3.540445	1.472683	-0.304212
	C	-1.524888	2.422069	0.595066
	H	-1.406546	2.305245	1.678875
	H	-0.524379	2.474207	0.156402
	H	-2.052947	3.356350	0.403660

Jc-	N	1.359117	0.523966	0.135607
	C	2.610121	0.071217	0.777233
	C	0.620599	-0.586973	-0.477678
	H	2.596951	0.291442	1.849127
	H	3.448523	0.627819	0.345979
	C	2.677197	-1.436427	0.470918
	C	1.748566	-1.607542	-0.744725
	H	0.158466	-0.256509	-1.412476
	C	-1.666813	-0.296010	0.713520
	H	2.309248	-2.023168	1.319451
	H	3.699248	-1.767597	0.267923
	H	1.377728	-2.629597	-0.868316
	H	2.273750	-1.325480	-1.664410
	O	-1.655596	0.533198	1.620157
	C	-0.479573	-1.207299	0.432275
	H	-0.819567	-2.133690	-0.047736
	H	-0.046261	-1.470456	1.400585
	N	-2.733715	-0.452144	-0.131380
	H	-2.689976	-1.176242	-0.833047
	C	-3.954360	0.332941	-0.022169
	H	-4.823128	-0.315765	0.132231
	H	-3.846568	0.993725	0.838758
	H	-4.117494	0.939561	-0.919812
	C	1.159689	1.872969	-0.015903
	O	1.961555	2.675210	0.465665
	C	-0.064435	2.354088	-0.775665
	H	-0.241747	1.802982	-1.704588
	H	-0.951536	2.257745	-0.143259
	H	0.090009	3.408038	-1.008268

Jc+	N	1.343680	0.512514	0.261046
	C	2.643690	0.101516	0.808801
	C	0.610105	-0.657148	-0.254478
	C	3.045070	-1.054514	-0.112622
	C	1.704978	-1.764556	-0.374123
	H	0.199394	-0.423307	-1.242079
	C	-1.761111	-0.250314	0.755853
	O	-1.867249	0.628587	1.607759
	C	-0.536964	-1.153448	0.667296
	H	-0.835283	-2.148190	0.310476
	H	-0.147765	-1.266170	1.682993
	N	-2.721324	-0.478961	-0.193950
	H	-2.590699	-1.248547	-0.833938
	C	-3.957797	0.284528	-0.274303
	H	-4.829613	-0.364060	-0.135922
	H	-3.939539	1.028156	0.523191
	H	-4.043675	0.796162	-1.239100
	C	1.100073	1.846480	0.021552
	O	1.883652	2.713127	0.411911
	C	-0.165396	2.243764	-0.716580
	H	-0.518174	1.505121	-1.440500
	H	-0.961333	2.407741	0.015526
	H	0.038191	3.186195	-1.226984
	H	3.320044	0.955738	0.797486
	H	2.534033	-0.235064	1.849475
	H	3.792219	-1.718159	0.332934
	H	3.461290	-0.652372	-1.043093
	H	1.533887	-2.532372	0.389101
	H	1.665615	-2.262447	-1.347729

Kc-	N	1.559559	0.230179	-0.208477
	C	1.272946	1.512717	-0.877550
	C	0.669294	-0.040709	0.925376
	H	1.040523	1.344242	-1.931966
	H	2.166174	2.145580	-0.829824
	C	0.086638	2.098463	-0.091996
	C	0.126266	1.364951	1.263373
	H	1.257842	-0.429724	1.763370
	C	-1.459426	-0.756840	-0.414820
	H	-0.851058	1.894229	-0.614740
	H	0.170366	3.182646	0.024803
	H	-0.846751	1.330848	1.763464
	H	0.828898	1.862218	1.941420
	O	-1.154627	-0.658306	-1.600848
	C	-0.434166	-1.105799	0.659195
	H	0.042815	-2.037048	0.339680
	H	-0.926750	-1.309229	1.618584
	N	-2.738783	-0.565042	0.035824
	H	-2.929124	-0.704750	1.016757
	C	-3.855213	-0.277558	-0.852646
	H	-3.453743	-0.154707	-1.859165
	H	-4.579613	-1.099693	-0.857529
	H	-4.364543	0.644373	-0.553118
	C	2.673788	-0.474018	-0.570758
	O	3.398240	-0.086259	-1.489289
	C	3.004370	-1.739595	0.208404
	H	3.182832	-1.525532	1.268541
	H	2.202220	-2.481499	0.146419
	H	3.911026	-2.164137	-0.222485

Kc+	N	1.399981	-0.018055	-0.242565
	C	1.534652	1.051883	-1.244410
	C	0.617052	0.413990	0.931492
	C	1.293937	2.325273	-0.429110
	C	0.235473	1.874349	0.585793
	H	1.266673	0.413076	1.818869
	C	-1.503601	-0.862897	0.125591
	H	-0.753613	1.895415	0.113573
	H	0.190239	2.498047	1.484065
	O	-1.213072	-1.806730	-0.605176
	C	-0.618412	-0.455410	1.299530
	H	-0.293388	-1.384356	1.771471
	H	-1.188489	0.104571	2.052011
	N	-2.629981	-0.113198	-0.075857
	H	-2.895335	0.563836	0.623263
	C	-3.586050	-0.442581	-1.125313
	H	-3.048418	-0.655678	-2.051221
	H	-4.183040	-1.325627	-0.868594
	H	-4.251564	0.409291	-1.280360
	C	2.132014	-1.169583	-0.389778
	O	2.821036	-1.357849	-1.393612
	C	2.060070	-2.212338	0.710315
	H	2.064052	-1.781355	1.716754
	H	1.145482	-2.801007	0.585099
	H	2.920058	-2.872981	0.596736
	H	2.520003	0.989407	-1.708292
	H	0.784504	0.930990	-2.038246
	H	2.217032	2.622588	0.082381
	H	0.962706	3.166926	-1.044407

Table S2. Calculated vibrational frequencies, intensities, rotator strengths and angles between electric and magnetic dipole derivatives.

$A_{\text{t}}+$	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	$A_{\text{t}}-$	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	42.9	4	-5	111.1		39.1	3	17	30.7
	57.4	2	22	40.2		47.3	3	-1	95.6
	59.1	4	8	60.4		57.5	6	-7	95.2
	65.9	14	-43	160.7		68.5	12	-29	129.7
	107.1	8	-2	92.6		95.9	7	-8	110.0
	117.2	1	22	22.3		119.0	1	16	18.2
	143.4	0	1	84.3		139.3	1	22	33.7
	159.7	0	-3	114.9		156.2	1	-1	103.4
	203.1	3	8	58.7		195.2	2	5	62.7
	225.3	6	8	66.0		215.9	6	9	69.9
	245.4	4	-1	93.5		246.8	4	-12	149.9
	278.2	7	-10	101.9		265.5	6	-6	98.1
	309.2	3	-7	110.2		320.1	5	-13	119.4
	397.1	5	5	81.7		401.2	5	20	59.2
	423.1	16	46	31.5		419.6	16	21	68.2
	483.1	9	-49	138.6		470.6	10	-35	116.7
	528.5	11	25	62.5		521.3	3	16	30.7
	536.9	55	-62	106.5		529.5	88	-42	101.8
	569.6	34	-14	103.8		597.5	4	-7	99.2
	598.5	9	6	86.6		605.7	26	69	18.7
	615.0	11	25	68.2		614.1	9	-19	131.9
	630.4	36	50	56.7		622.2	14	13	74.0
	711.8	0	6	43.1		739.3	0	-3	110.7
	794.7	3	-5	112.7		776.5	2	1	80.3
	832.9	4	3	80.5		828.3	2	-8	116.2
	862.4	3	-4	119.8		865.8	2	-7	132.3
	876.7	2	15	48.9		879.2	2	-11	121.9
	906.2	4	20	31.0		892.0	2	-5	111.0
	911.2	2	13	50.7		917.5	0	1	36.5
	936.6	1	5	84.9		937.5	9	2	88.5
	981.6	6	7	80.0		971.1	1	4	83.4
	990.1	13	9	73.9		989.3	13	47	48.0
	1013.3	3	2	76.9		1017.4	12	-12	86.5
	1034.6	4	-1	94.8		1035.9	4	0	100.5
	1061.8	0	-5	167.6		1056.7	1	-4	124.2
	1074.3	5	-3	66.3		1081.6	1	-1	101.5
	1100.0	6	19	63.0		1109.5	1	0	82.4
	1124.5	7	17	66.7		1125.6	7	14	70.5
	1146.7	7	19	28.8		1158.0	10	8	103.6
	1164.0	2	15	29.2		1160.0	2	-14	72.8
	1188.2	6	-15	102.8		1174.1	12	-40	112.6
	1194.7	50	-140	146.3		1192.1	26	-16	131.5
	1208.8	12	-48	120.1		1202.3	31	-75	131.8
	1249.4	4	-7	92.6		1248.1	9	-3	95.5
	1258.8	35	-15	100.1		1257.9	28	-29	107.4
	1282.2	15	-15	101.1		1293.6	31	-40	98.2
	1303.4	22	-45	116.4		1303.1	3	-12	127.1

1331.4	6	-3	102.5	1324.3	8	15	36.2
1344.9	4	11	67.7	1340.8	1	-14	151.3
1346.3	3	-14	146.5	1345.1	5	11	23.2
1354.6	26	26	61.9	1356.0	25	1	84.7
1371.4	20	74	20.6	1372.7	16	51	24.6
1413.4	126	-35	98.6	1409.0	247	-13	91.8
1415.3	139	25	80.7	1415.6	35	28	66.4
1437.9	18	-1	90.9	1438.1	15	-5	95.0
1447.9	27	-15	121.6	1448.2	26	-19	130.6
1452.1	10	2	138.0	1453.2	10	8	86.1
1454.6	22	-15	84.4	1455.4	12	-1	64.7
1465.1	3	0	95.9	1465.6	16	-11	134.5
1472.5	6	5	21.8	1473.2	9	6	118.9
1475.7	8	8	91.6	1474.0	13	-9	85.4
1495.2	0	-1	132.0	1492.4	0	2	64.5
1535.5	191	58	83.3	1533.9	190	57	83.4
1643.0	227	-74	94.5	1646.0	235	-81	95.0
1680.7	337	-64	94.7	1682.3	321	-75	95.5
2894.6	42	-9	115.5	2877.0	59	-8	96.5
2897.9	19	19	79.4	2904.0	50	28	83.8
2902.7	54	21	85.4	2915.6	7	2	84.8
2919.5	9	16	66.1	2919.9	7	6	81.0
2922.1	31	-21	106.6	2930.3	49	5	84.5
2940.0	6	-11	125.1	2948.4	27	-10	122.4
2945.4	25	-11	117.0	2949.1	24	-17	124.8
2975.1	33	-67	159.3	2968.3	23	36	70.4
2977.9	26	-7	93.9	2978.4	31	-11	95.3
2980.1	19	30	65.5	2979.3	8	3	85.9
2981.2	18	61	43.5	2991.8	12	-21	110.8
2992.0	21	-21	105.8	3001.6	19	6	84.8
3012.9	6	0	91.0	3005.8	7	6	80.5
3019.7	8	-3	93.7	3019.4	8	-3	93.9
3033.6	7	-1	92.3	3034.3	7	0	90.7
3420.3	64	7	88.8	3431.4	51	1	89.7

Bt-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Bt+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	12.1	1	1	85.5		22.3	1	-3	106.5
	52.3	5	9	41.8		54.4	4	-21	113.4
	61.5	5	-1	95.0		61.6	3	27	19.8
	77.8	6	-3	104.1		71.2	7	10	64.2
	100.6	1	3	78.1		98.6	2	7	7.6
	118.6	1	-4	128.2		124.3	2	-14	146.2
	132.3	1	0	88.0		140.3	1	4	81.9
	144.9	1	5	43.9		156.8	1	-1	102.0
	188.7	2	1	85.9		198.5	4	2	79.1
	206.1	7	-7	97.9		209.4	6	-12	105.3
	234.6	4	-6	129.3		252.0	4	-3	100.4
	289.3	8	-9	101.5		275.3	5	2	86.3
	328.4	2	16	50.7		313.0	1	6	49.4
	379.5	6	-3	95.1		391.7	5	13	42.7

419.9	20	-30	145.2	410.6	20	-32	146.0
434.2	4	-16	114.1	422.1	5	-29	130.8
525.6	11	23	38.3	525.6	9	6	60.7
590.0	6	-4	94.3	561.7	7	19	74.5
598.7	3	7	76.7	601.7	4	-20	112.3
616.8	10	3	83.6	615.1	8	-10	110.3
641.0	11	42	65.4	635.3	30	62	61.1
686.0	15	-48	116.1	685.8	15	-52	116.4
734.4	54	8	86.8	705.5	32	-29	106.3
798.1	5	-6	170.2	775.1	3	10	67.5
839.9	4	-14	114.7	841.7	6	23	34.6
864.1	6	-19	138.9	865.7	2	11	49.0
868.5	2	4	65.3	878.9	3	8	42.2
893.1	0	-2	84.6	901.1	1	-3	104.7
929.6	1	11	52.8	913.0	2	1	83.6
935.1	7	0	103.3	930.8	3	21	21.6
961.4	8	-5	127.3	986.2	15	-1	94.8
985.7	3	11	51.2	989.4	1	-2	68.9
1016.3	11	14	71.7	1032.3	6	13	90.8
1036.5	3	-3	95.3	1036.0	3	-3	38.8
1056.2	1	-3	82.1	1046.8	3	-3	88.0
1066.6	2	0	106.5	1066.7	6	2	87.3
1115.6	5	10	75.4	1105.6	8	11	69.1
1127.2	1	-3	107.9	1129.5	3	-14	124.1
1155.8	8	-9	84.4	1143.8	6	3	63.4
1157.4	29	33	104.7	1169.3	4	5	80.7
1161.4	2	-7	82.0	1182.8	1	16	86.0
1187.5	14	0	92.8	1193.2	47	-43	110.1
1205.7	36	-22	106.7	1205.5	3	52	13.7
1247.1	12	36	34.1	1243.0	10	7	77.7
1264.6	23	57	54.5	1271.2	8	39	42.8
1284.3	26	26	78.3	1290.2	38	0	86.3
1300.2	6	-25	114.9	1299.1	1	-11	122.7
1317.3	2	-7	108.2	1327.5	0	2	54.4
1330.9	0	1	61.4	1337.1	3	22	22.1
1345.3	6	20	29.9	1343.9	5	-20	159.4
1357.6	19	0	97.4	1358.4	19	18	57.1
1369.8	12	47	56.0	1365.7	28	86	54.6
1410.0	52	-1	89.6	1416.7	266	-98	102.0
1414.2	268	-27	92.0	1418.1	6	9	50.2
1437.9	22	1	84.2	1439.5	21	-1	83.8
1444.5	12	9	78.5	1445.5	10	16	57.8
1452.1	16	5	83.0	1447.8	17	18	65.2
1464.5	1	-1	129.5	1453.1	17	-13	105.3
1465.3	29	4	79.0	1463.1	4	-1	99.0
1466.5	6	-5	96.5	1472.8	3	3	72.6
1474.7	4	-8	154.2	1475.8	1	-1	93.9
1493.5	1	-1	95.4	1493.8	2	2	79.3
1570.4	199	13	85.9	1556.6	243	3	89.0
1639.5	362	-38	91.6	1640.0	369	-33	91.3

1688.7	353	10	89.3	1687.2	349	7	89.5
2887.6	51	-9	94.8	2888.9	49	4	88.3
2905.6	77	-4	90.8	2905.0	63	-19	94.3
2920.2	7	2	87.3	2912.5	7	11	12.6
2924.4	17	14	64.6	2920.8	8	4	83.1
2932.2	20	-16	101.6	2924.5	12	-23	144.0
2946.0	3	-2	98.3	2929.8	31	11	83.5
2955.7	34	1	89.9	2953.6	12	-1	91.5
2958.3	30	21	50.8	2973.1	28	7	87.3
2959.6	21	23	77.2	2980.5	24	-42	135.1
2979.1	10	-1	90.9	2982.9	18	6	86.7
2985.4	27	-32	109.9	2987.2	22	34	67.7
2992.8	15	16	79.4	2992.4	22	-18	100.9
2999.0	17	3	58.7	3004.0	9	9	70.6
3024.1	3	1	86.1	3012.5	15	4	87.6
3036.7	6	0	89.6	3034.9	6	0	90.8
3342.9	251	-4	90.2	3353.2	287	1	90.0

Cc-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Cc+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	27.3	4	3	82.3		23.1	4	7	74.1
	37.6	3	29	40.4		30.1	2	9	80.1
	40.3	1	-3	98.3		40.4	3	20	13.5
	67.0	6	-19	137.9		66.8	5	-32	144.2
	83.7	2	-21	133.3		80.2	2	-16	120.3
	93.4	0	-1	101.5		125.8	4	-7	101.5
	128.5	3	-11	114.2		145.8	2	-3	129.3
	164.8	3	15	46.1		157.9	1	8	51.2
	183.0	7	1	90.0		170.1	8	15	65.1
	202.8	1	-8	137.2		203.7	0	-7	135.4
	226.4	5	6	59.1		262.5	2	1	87.0
	290.8	4	10	78.7		293.0	8	10	80.0
	313.1	13	-21	155.9		323.7	13	-20	128.6
	370.1	18	56	15.7		382.6	19	60	13.1
	393.4	0	-8	121.1		404.4	0	-2	100.9
	443.5	25	-81	126.6		449.3	50	-100	112.4
	474.1	51	46	83.7		486.9	23	38	75.4
	542.6	9	2	85.5		524.7	9	23	40.0
	584.6	8	22	74.2		568.6	2	2	87.9
	601.8	1	-12	132.3		599.6	2	-19	125.2
	619.5	5	40	39.7		608.7	12	3	88.1
	627.9	9	-13	101.0		623.9	9	51	43.0
	700.9	0	-2	118.8		692.9	1	-6	136.1
	811.6	4	-11	124.6		789.0	3	-6	107.9
	825.9	6	6	32.4		829.4	3	14	56.8
	849.6	4	-14	124.6		875.3	3	-7	95.5
	874.0	3	-19	121.8		878.6	7	19	42.2
	895.6	10	7	73.6		901.3	10	36	19.1
	909.1	0	4	29.0		916.3	1	-8	114.3
	940.0	5	-14	107.5		949.4	2	-10	27.8
	957.5	4	-9	114.0		953.5	3	8	107.8

991.2	16	1	87.2	992.5	14	-9	101.2
1029.0	3	15	78.8	1018.6	3	16	64.6
1030.8	4	-19	129.1	1034.3	5	-6	89.5
1035.8	9	17	68.7	1044.6	16	-39	126.4
1066.6	3	7	55.2	1082.5	5	19	24.9
1106.7	1	0	134.4	1099.0	1	0	172.5
1128.1	2	-12	170.3	1128.5	2	-10	173.1
1144.6	12	-18	135.1	1149.4	5	6	75.1
1151.5	55	29	80.4	1153.2	108	-77	124.2
1179.5	42	-14	110.6	1169.1	17	27	63.4
1184.0	11	-15	110.5	1192.5	30	28	85.5
1196.2	62	-14	95.1	1200.2	24	45	58.0
1225.1	15	27	60.0	1235.3	32	-19	100.4
1241.8	4	13	30.3	1254.9	16	3	86.2
1289.2	53	-27	104.5	1293.9	5	7	77.7
1302.0	12	-28	146.6	1295.8	22	-30	114.8
1309.8	3	-11	107.1	1323.4	4	-27	162.4
1328.3	1	10	37.6	1337.1	16	38	65.6
1346.6	13	26	52.4	1344.0	1	-9	126.2
1358.3	22	-15	88.2	1356.6	60	18	30.0
1369.3	38	54	63.2	1363.8	52	102	46.9
1398.0	326	54	85.7	1393.9	274	-19	90.6
1411.0	20	-13	127.4	1410.2	19	-12	124.0
1435.4	9	18	87.7	1434.9	13	14	52.3
1439.1	12	-29	103.0	1452.0	4	-13	110.3
1454.1	18	18	61.2	1458.5	54	1	92.8
1458.4	49	-6	96.9	1459.9	20	-23	86.3
1463.5	4	-5	95.2	1462.9	8	-9	113.8
1467.9	10	-9	100.7	1467.4	9	-2	92.7
1477.6	6	-8	153.7	1475.0	4	-2	106.3
1495.6	2	2	72.8	1495.7	5	-5	149.9
1529.9	199	5	88.2	1530.5	204	0	89.5
1662.3	424	32	85.9	1658.4	430	-6	90.9
1690.0	239	-65	95.1	1689.5	230	-70	95.6
2913.0	68	-8	95.2	2889.7	44	17	85.0
2919.3	9	25	47.9	2910.8	17	5	84.1
2922.7	27	-28	133.4	2913.3	72	-5	93.3
2923.9	9	-9	99.7	2919.7	15	-18	148.1
2926.3	23	-5	94.9	2926.7	9	9	79.7
2931.7	21	-10	101.5	2927.7	33	-2	91.8
2960.6	12	-5	98.1	2950.3	6	-3	113.8
2964.8	27	68	56.2	2968.3	26	3	88.8
2968.6	26	3	89.1	2969.5	17	5	82.1
2976.6	21	-57	129.6	2978.0	33	15	84.2
2983.5	26	29	76.0	2991.6	19	-12	99.9
2987.3	34	17	71.5	2993.9	14	-4	94.9
2990.4	9	-8	108.2	3007.2	8	-2	93.2
3031.4	1	0	78.4	3026.8	10	-2	94.0
3033.6	9	2	85.0	3032.1	1	0	80.9
3470.3	24	-2	91.0	3470.0	25	-1	90.6

Dt-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Dt+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	35.2	2	-8	117.1		27.3	4	3	104.7
	50.5	5	5	76.7		37.6	3	29	90.1
	84.1	1	6	69.0		40.3	1	-3	53.2
	100.0	2	-16	150.9		67.0	6	-19	86.4
	111.0	3	5	78.3		83.7	2	-21	96.2
	130.2	3	17	55.3		93.4	0	-1	70.1
	147.6	8	-14	102.7		128.5	3	-11	101.7
	176.7	2	-10	126.4		164.8	3	15	95.7
	186.3	4	5	74.1		183.0	7	1	85.7
	194.2	5	-5	99.1		202.8	1	-8	77.1
	235.5	6	1	88.0		226.4	5	6	118.6
	279.1	8	-8	101.1		290.8	4	10	97.8
	309.7	1	0	92.0		313.1	13	-21	85.4
	352.5	5	10	70.4		370.1	18	56	68.2
	425.7	11	15	76.9		393.4	0	-8	66.7
	498.0	5	-30	153.1		443.5	25	-81	149.5
	524.4	11	-10	120.9		474.1	51	46	165.9
	580.4	13	-40	107.3		542.6	9	2	108.8
	600.0	7	14	26.4		584.6	8	22	61.6
	606.9	10	13	78.4		601.8	1	-12	110.2
	624.7	9	23	60.3		619.5	5	40	48.6
	681.7	3	-39	144.2		627.9	9	-13	107.8
	722.7	72	-19	96.4		700.9	0	-2	109.6
	765.0	4	-19	134.3		811.6	4	-11	54.6
	845.0	4	13	52.4		825.9	6	6	35.9
	861.2	2	-3	88.8		849.6	4	-14	54.6
	879.5	3	-10	153.9		874.0	3	-19	66.9
	898.8	0	-5	140.2		895.6	10	7	60.2
	912.9	9	0	59.0		909.1	0	4	103.6
	949.1	1	3	83.1		940.0	5	-14	41.1
	981.6	5	21	32.7		957.5	4	-9	76.6
	986.4	9	19	44.1		991.2	16	1	14.8
	1014.8	5	9	81.9		1029.0	3	15	46.7
	1037.4	4	0	87.1		1030.8	4	-19	169.0
	1058.0	5	6	73.6		1035.8	9	17	135.1
	1060.6	0	0	75.9		1066.6	3	7	60.9
	1119.3	1	3	82.1		1106.7	1	0	55.0
	1127.4	2	13	43.8		1128.1	2	-12	43.1
	1144.6	23	-15	142.5		1144.6	12	-18	132.1
	1167.1	2	-4	116.6		1151.5	55	29	71.2
	1182.4	6	13	49.0		1179.5	42	-14	111.7
	1184.5	12	-5	100.9		1184.0	11	-15	114.5
	1242.0	4	33	10.3		1196.2	62	-14	46.9
	1243.3	1	14	57.4		1225.1	15	27	90.9
	1274.5	18	-19	103.9		1241.8	4	13	35.4
	1293.2	68	-67	100.9		1289.2	53	-27	95.2
	1309.8	13	-20	103.1		1302.0	12	-28	96.8
	1321.2	1	-4	79.5		1309.8	3	-11	56.3

1328.9	1	-1	104.3	1328.3	1	10	122.9
1347.6	10	10	51.5	1346.6	13	26	50.6
1358.6	21	2	102.5	1358.3	22	-15	94.2
1377.1	0	0	78.4	1369.3	38	54	99.0
1405.6	279	41	84.4	1398.0	326	54	85.4
1420.6	20	6	87.4	1411.0	20	-13	59.8
1424.4	1	6	30.0	1435.4	9	18	89.5
1436.8	17	4	86.1	1439.1	12	-29	108.0
1445.8	11	-13	110.8	1454.1	18	18	109.3
1453.0	15	1	88.8	1458.4	49	-6	78.1
1467.4	5	1	82.9	1463.5	4	-5	63.3
1473.6	1	4	64.0	1467.9	10	-9	57.7
1479.2	7	1	87.5	1477.6	6	-8	58.4
1497.8	0	-4	131.9	1495.6	2	2	121.9
1570.9	121	-17	93.0	1529.9	199	5	92.0
1642.0	395	203	81.3	1662.3	424	32	80.0
1671.6	368	-111	102.0	1690.0	239	-65	101.4
2912.6	56	20	83.1	2913.0	68	-8	86.7
2917.7	29	-3	92.7	2919.3	9	25	83.2
2922.3	21	-4	94.7	2922.7	27	-28	66.2
2922.6	8	8	30.5	2923.9	9	-9	76.2
2927.9	24	-2	92.3	2926.3	23	-5	100.8
2941.9	15	-16	113.1	2931.7	21	-10	114.1
2954.1	21	46	64.6	2960.6	12	-5	93.7
2964.6	5	-18	144.3	2964.8	27	68	57.5
2976.0	26	-6	92.4	2968.6	26	3	93.1
2979.7	13	7	80.8	2976.6	21	-57	41.8
2984.2	10	-4	94.5	2983.5	26	29	102.6
2984.5	19	-33	130.2	2987.3	34	17	108.1
2992.7	39	25	81.7	2990.4	9	-8	89.9
3015.0	16	-1	90.4	3031.4	1	0	91.4
3037.9	5	0	89.7	3033.6	9	2	89.8
3279.4	472	137	85.9	3470.3	24	-2	85.3

Et-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	15.4	4	-1	93.2
	28.7	1	-8	110.5
	40.2	2	-8	146.4
	74.5	9	13	74.7
	104.7	3	6	69.1
	126.7	0	0	84.2
	143.3	0	0	94.4
	169.2	3	3	78.3
	174.7	8	1	90.7
	201.1	0	3	51.3
	223.2	9	1	87.5
	276.4	7	8	73.2
	318.6	5	6	79.9
	366.6	16	-50	133.1
	413.2	3	4	76.9

459.5	68	16	87.2
507.7	11	3	95.1
518.2	8	25	22.9
582.5	4	-36	139.0
599.3	7	-4	93.5
617.2	11	4	81.2
640.1	3	36	29.9
726.6	2	-11	129.7
782.4	4	-13	159.7
823.3	4	-5	99.0
855.3	2	-3	104.2
868.6	1	-1	92.1
894.5	1	2	70.5
917.7	10	-38	125.6
940.5	3	3	79.1
967.5	15	20	63.3
999.4	1	-10	126.3
1034.9	4	-24	91.2
1035.8	5	22	92.4
1055.3	7	2	68.8
1073.5	3	-18	161.9
1102.2	2	-2	97.7
1127.7	4	17	20.9
1148.2	27	-9	111.7
1165.0	7	-20	143.8
1171.2	15	30	60.6
1197.0	95	8	42.2
1203.3	78	-4	86.3
1234.1	4	-39	154.6
1255.8	13	17	70.7
1302.8	2	-2	87.2
1311.8	29	-59	123.8
1328.7	23	21	60.1
1340.3	1	7	54.3
1348.5	17	-2	72.8
1354.4	20	6	96.6
1388.3	5	-3	91.3
1405.7	361	13	88.8
1409.2	13	3	96.5
1437.3	20	7	74.4
1441.2	12	5	112.5
1452.9	13	3	82.5
1457.7	46	7	86.3
1463.2	10	-8	98.3
1467.9	9	7	81.8
1472.2	7	-4	92.2
1489.9	2	2	83.4
1526.1	192	-8	91.7
1653.3	312	100	85.2
1686.2	245	-3	90.1

2888.1	60	-10	102.5
2909.4	78	48	46.1
2910.8	19	-38	170.2
2919.0	9	3	85.7
2921.2	12	3	79.8
2937.6	46	30	43.0
2951.4	48	-6	108.6
2959.8	18	23	72.8
2960.7	8	-9	111.6
2964.7	28	-4	91.3
2968.4	21	-21	102.4
2978.0	11	2	88.2
3010.2	19	5	86.0
3030.1	1	0	98.9
3033.9	8	-1	90.8
3470.2	25	2	88.4

Fc-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Fc+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	22.7	8	1	87.6		17.8	7	-2	93.9
	33.1	2	14	19.0		33.1	4	-6	103.1
	35.7	1	-30	157.2		46.9	0	7	25.0
	87.3	3	-6	99.0		74.7	4	-32	129.1
	90.9	1	17	14.7		83.8	1	9	47.4
	119.9	4	12	68.2		115.1	2	12	45.4
	142.4	1	-8	120.8		123.1	9	29	53.0
	165.8	13	8	65.3		152.0	1	-6	112.2
	186.5	1	12	43.1		178.3	8	1	89.1
	211.1	1	-6	117.7		220.7	2	14	17.0
	238.2	3	1	87.0		263.9	2	-7	108.9
	285.0	9	-17	106.1		288.4	8	-21	111.8
	314.3	4	9	57.5		312.1	4	11	60.8
	393.6	9	-34	129.5		398.1	13	-39	122.9
	415.2	34	-8	95.9		427.5	20	-1	85.3
	436.3	31	70	61.4		443.4	53	75	70.7
	493.3	38	36	74.4		493.6	28	17	80.9
	516.0	3	1	88.2		523.2	4	15	29.5
	592.9	8	10	84.0		580.6	2	-17	130.4
	605.3	2	-9	129.0		597.0	9	7	85.4
	625.7	7	-45	139.6		629.5	5	-15	164.8
	653.4	5	-23	125.3		641.1	6	-46	146.2
	721.5	0	3	61.6		710.2	0	2	67.7
	765.3	1	-7	142.9		770.2	2	-21	152.9
	833.8	0	-1	109.8		830.1	2	8	54.7
	859.3	8	-33	165.5		858.2	7	41	29.9
	877.2	1	10	65.2		873.7	3	-1	107.1
	894.0	5	-11	125.3		904.0	6	-9	109.6
	927.5	9	-12	109.6		930.3	1	6	38.4
	938.3	0	5	59.3		933.6	10	-15	117.3
	959.2	7	-7	96.0		951.9	2	-6	127.3
	987.2	14	-29	111.4		984.7	6	-18	111.7

1011.0	8	-7	106.5	1012.6	18	-7	96.4
1039.4	2	1	83.0	1037.5	1	5	72.1
1054.3	5	24	37.1	1050.7	6	-39	136.2
1067.3	5	11	66.5	1056.9	15	32	14.9
1112.2	5	4	91.7	1105.3	9	15	60.8
1125.9	14	-13	106.2	1124.3	22	-21	107.6
1135.2	12	11	80.7	1131.1	7	-3	95.9
1154.4	28	0	88.1	1154.1	27	-20	99.1
1178.7	29	-11	96.6	1184.8	14	18	69.1
1190.6	34	102	54.9	1192.8	56	155	30.6
1195.4	22	0	88.9	1204.6	46	23	76.7
1227.5	4	-3	93.8	1244.0	18	-95	132.4
1249.5	14	-10	98.1	1251.9	11	1	95.2
1277.4	36	-3	90.7	1280.3	30	66	62.6
1302.4	2	6	68.2	1298.0	12	-10	100.6
1313.9	16	-83	155.0	1304.4	2	8	54.8
1323.1	3	7	62.9	1321.2	27	-69	127.5
1347.2	19	6	97.0	1340.9	11	-39	134.3
1360.3	32	-12	88.9	1356.4	23	-8	93.2
1366.1	45	43	65.6	1367.8	21	22	51.3
1394.7	259	31	87.6	1401.1	248	49	85.1
1410.9	19	-19	113.5	1411.6	20	-23	116.9
1444.3	3	3	77.7	1440.9	2	3	70.6
1447.1	12	25	61.0	1446.9	11	27	53.9
1456.6	31	36	58.3	1456.6	29	36	56.9
1464.8	3	-17	93.8	1461.7	3	-3	112.5
1465.9	5	4	113.9	1465.2	7	-15	115.8
1469.7	28	-30	117.2	1470.1	23	-25	100.9
1480.5	4	-1	96.7	1475.3	7	-7	145.7
1498.9	3	0	91.0	1488.7	6	-2	109.0
1533.5	175	33	85.2	1533.7	176	30	85.8
1658.3	374	-3	90.2	1662.8	382	-27	92.9
1685.7	247	95	82.2	1684.7	247	96	82.3
2915.0	53	-12	94.1	2888.5	44	8	87.8
2919.3	9	-3	95.0	2914.3	25	0	91.2
2920.6	7	23	53.5	2915.0	44	13	85.2
2926.8	24	-4	93.3	2920.1	8	-2	93.0
2929.2	18	-10	103.3	2929.7	33	5	86.0
2934.2	47	1	89.5	2933.3	33	-43	158.4
2961.2	12	47	44.1	2961.9	11	5	84.0
2966.8	11	-36	137.6	2969.1	16	30	44.9
2973.1	26	5	88.3	2973.1	26	2	89.1
2977.0	24	-50	125.6	2982.5	27	9	86.7
2985.4	43	53	72.7	2992.3	28	-24	110.9
2991.0	22	-12	106.0	2998.2	6	-7	106.3
2997.1	5	-6	106.7	3022.6	5	-2	97.6
3032.5	1	1	66.7	3032.2	1	1	67.4
3037.8	4	4	74.0	3039.1	4	4	72.9
3472.9	23	-1	90.8	3472.9	23	-1	90.3

Gt-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Gt+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	32.1	5	-1	112.5		28.0	14	-11	103.4
	42.1	14	0	88.7		36.2	3	5	52.3
	70.1	1	-5	121.2		67.4	2	-2	109.8
	83.7	4	-14	110.8		89.1	1	-6	134.2
	102.2	2	-1	98.2		102.7	1	12	54.3
	108.2	1	9	47.5		113.0	2	8	74.0
	132.4	1	3	84.1		118.3	6	-20	115.0
	160.7	2	-5	106.5		158.3	0	-10	170.5
	177.9	3	13	53.1		191.2	1	9	35.0
	226.7	1	-6	131.7		221.1	7	13	67.0
	238.8	7	-7	100.0		264.2	10	-10	102.6
	275.8	11	13	76.2		278.5	4	12	73.3
	301.5	0	1	67.5		306.2	1	-1	101.3
	393.5	22	32	68.1		392.7	19	7	83.4
	430.0	10	-1	108.5		426.7	10	29	41.6
	446.6	5	-30	130.5		469.6	7	-27	123.2
	499.2	113	-48	99.7		498.8	117	-53	100.5
	515.7	3	11	29.3		519.4	5	0	90.8
	592.9	7	-11	103.0		585.3	3	5	39.6
	604.8	8	19	69.2		597.3	5	-10	103.3
	617.2	6	14	56.7		611.2	11	19	61.5
	655.2	10	50	42.3		644.0	11	51	33.3
	728.4	3	9	74.9		705.9	3	0	97.8
	763.3	5	-18	132.2		759.4	5	-32	126.9
	846.3	0	-2	142.1		838.0	3	8	60.2
	860.0	4	-15	131.6		859.5	2	21	4.4
	870.4	3	-18	133.3		878.2	3	-4	128.1
	893.6	1	-2	100.9		891.5	9	29	8.4
	911.4	9	1	95.2		903.9	1	10	56.6
	947.0	4	10	63.2		934.4	7	15	42.9
	970.8	18	32	47.8		981.8	10	1	88.8
	988.1	0	3	21.6		990.0	4	8	53.0
	1013.6	4	-7	125.0		1022.4	6	7	82.2
	1035.5	5	-12	97.7		1036.1	3	-14	102.9
	1043.8	2	6	81.0		1040.5	7	-13	123.1
	1063.8	6	11	42.1		1065.2	10	-1	49.6
	1109.1	7	11	76.7		1102.3	11	22	65.7
	1122.2	14	42	50.8		1122.1	14	45	49.4
	1144.0	6	-32	151.1		1150.8	14	-51	144.3
	1165.9	5	-7	105.2		1165.7	7	-22	173.6
	1180.2	5	-4	109.0		1172.6	29	-1	64.8
	1185.2	17	-20	109.9		1192.3	2	3	83.8
	1200.7	37	52	67.8		1209.7	28	106	45.0
	1240.8	3	10	71.6		1241.4	25	4	82.0
	1261.1	21	61	44.3		1263.9	9	10	71.8
	1287.6	46	-67	123.2		1280.5	55	-35	99.4
	1303.9	7	-6	98.6		1304.0	4	13	72.4
	1317.3	9	2	81.4		1314.1	7	11	65.9
	1328.8	4	2	84.8		1329.4	13	3	84.3

1344.8	19	-2	69.7	1343.9	6	-4	113.5
1352.6	29	16	99.3	1357.6	11	14	78.5
1374.6	2	-19	118.0	1373.8	3	-13	103.1
1401.0	304	39	86.0	1409.5	271	19	86.6
1413.0	17	9	82.6	1414.1	32	-10	113.5
1435.9	14	-1	92.3	1440.6	13	-10	116.7
1447.8	15	-10	75.2	1445.6	6	9	28.7
1449.7	2	-4	133.7	1448.2	12	-13	123.5
1452.5	14	4	80.2	1454.4	14	5	79.7
1466.0	4	1	78.4	1461.6	3	0	81.0
1471.6	17	6	82.3	1471.4	17	3	76.8
1475.7	8	-1	147.1	1475.4	2	2	87.8
1495.0	0	2	53.8	1493.0	1	-3	137.7
1524.1	153	-36	94.6	1522.3	149	-21	92.7
1659.5	314	113	83.0	1659.9	352	45	87.0
1690.8	265	-209	106.2	1694.0	251	-125	99.5
2900.7	48	-13	98.3	2892.2	41	6	87.6
2915.0	42	18	83.0	2911.9	12	-5	99.2
2918.9	19	-7	102.4	2915.1	46	18	83.8
2920.8	10	6	80.6	2920.1	9	9	77.9
2926.7	30	1	89.2	2928.4	29	-3	90.7
2937.5	10	-14	113.3	2929.4	33	-16	112.6
2949.9	30	44	71.0	2943.4	4	6	64.3
2964.5	9	-4	109.3	2973.7	25	43	39.2
2976.5	22	-49	129.8	2981.8	4	16	70.0
2980.8	9	3	86.0	2984.8	7	-16	111.6
2985.0	28	36	73.2	2985.3	25	7	87.1
2985.7	29	-5	92.6	2986.3	55	-47	106.9
2989.9	34	-1	90.2	3009.3	18	-1	90.4
3025.5	7	-4	96.2	3025.4	7	-4	95.9
3035.7	7	0	90.5	3035.4	6	-1	91.3
3453.5	20	6	85.3	3450.6	16	5	86.1

He-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	He+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	36.2	15	-28	136.9		23.0	8	5	83.1
	40.9	4	16	38.7		47.6	3	7	143.7
	55.4	2	6	76.0		48.7	2	7	40.8
	67.3	1	7	52.0		67.3	6	-29	147.5
	95.3	1	-25	146.0		92.3	2	-11	108.9
	100.5	2	1	87.9		106.4	0	-4	120.2
	113.6	1	0	84.8		135.8	1	4	71.7
	165.8	11	9	74.5		152.5	7	5	84.0
	188.2	5	7	67.9		190.2	7	14	62.4
	215.4	2	-2	100.2		217.9	1	-3	113.7
	221.1	5	12	58.6		252.9	3	-11	123.5
	262.8	6	-13	107.5		279.0	11	1	87.7
	314.7	5	10	68.0		322.0	8	-1	92.5
	386.1	24	33	68.4		392.0	11	-9	102.8
	417.1	9	-64	119.9		400.6	9	58	33.6
	423.9	60	22	92.9		459.7	60	-21	94.7

485.4	14	-5	101.7	513.5	6	7	64.6
522.2	7	18	41.8	546.0	2	-10	174.9
588.2	10	38	67.9	557.1	6	23	59.3
590.1	9	42	21.9	574.7	5	3	85.8
603.9	1	-11	126.9	608.2	9	62	45.7
636.7	7	-14	108.1	618.9	12	-28	164.5
742.1	2	-9	110.7	707.8	0	0	67.9
793.1	3	-19	147.0	776.8	5	-11	103.3
817.1	2	-6	128.7	836.4	5	16	49.8
849.9	0	1	87.9	850.5	6	-6	103.3
880.0	1	-20	146.1	878.0	2	16	32.9
889.8	4	-10	115.8	892.1	2	4	49.6
907.9	4	-1	116.0	914.5	5	4	78.3
936.0	10	-20	109.2	947.0	3	-20	129.7
948.5	4	18	68.8	956.3	4	3	91.0
986.4	4	4	84.3	983.0	2	-4	99.6
1017.0	19	-26	115.0	1009.6	16	1	91.4
1033.3	3	2	88.6	1035.4	4	-9	95.6
1058.0	2	0	76.7	1044.3	4	-6	100.6
1075.4	2	2	40.4	1072.2	5	1	28.7
1101.0	0	-2	112.4	1097.8	2	15	23.8
1126.0	6	24	54.1	1128.1	3	15	47.4
1145.7	14	44	36.2	1153.2	7	24	24.9
1158.6	3	-10	104.4	1167.3	2	14	25.2
1171.8	12	19	69.7	1176.4	25	-36	142.3
1187.7	9	1	91.8	1192.5	19	-60	165.4
1207.0	42	-80	150.4	1209.9	27	-67	128.4
1236.5	9	31	56.4	1245.2	25	128	39.9
1261.4	58	-54	99.5	1261.1	44	-75	110.7
1273.8	9	-8	101.9	1284.8	10	11	36.7
1298.1	9	7	81.2	1298.3	4	-8	111.9
1313.1	6	16	52.6	1326.4	8	-5	96.5
1328.8	1	2	87.5	1335.7	24	2	96.5
1345.5	17	20	66.2	1345.5	4	5	85.9
1357.6	43	-20	95.6	1353.6	82	4	60.6
1374.3	6	-2	116.9	1368.0	51	89	43.5
1390.3	332	-57	98.9	1386.0	224	-100	110.5
1416.6	13	29	39.3	1418.9	10	17	42.5
1437.6	5	6	84.6	1438.0	15	-4	106.0
1444.4	7	3	65.1	1444.6	19	-7	40.8
1447.0	20	-17	145.7	1446.2	8	4	118.0
1455.7	16	-8	95.5	1460.0	9	-19	125.2
1464.1	11	-8	134.7	1463.7	4	-5	159.5
1472.3	7	3	82.3	1474.0	6	3	79.5
1477.9	9	2	86.6	1475.1	6	-3	94.0
1495.2	7	11	54.6	1493.2	10	-2	107.8
1521.2	143	25	85.8	1523.3	137	44	81.4
1662.8	460	-56	93.4	1661.1	482	-35	92.4
1686.7	190	-15	91.7	1686.9	217	-20	92.4
2909.5	43	13	86.2	2898.4	45	6	74.1

2921.6	3	-21	139.0	2901.2	20	23	76.9
2923.4	29	-10	114.1	2915.0	44	11	85.9
2924.9	5	12	53.9	2925.5	31	-11	102.0
2930.0	23	-21	113.9	2926.8	4	-7	98.4
2944.1	51	33	63.6	2936.1	15	-5	99.2
2951.3	18	-14	117.4	2943.1	17	2	85.5
2967.4	19	57	53.2	2978.5	23	56	47.5
2983.3	23	-5	92.6	2982.5	21	-6	93.1
2985.5	9	-5	95.7	2987.3	31	-41	109.3
2987.9	6	5	83.8	2990.7	4	10	60.2
2990.5	25	-47	151.3	2992.2	17	-22	110.5
2999.0	29	27	73.6	3009.1	8	-1	92.2
3022.5	7	-2	92.2	3018.9	10	-1	90.6
3034.8	7	2	86.5	3030.5	7	-1	91.4
3465.5	26	3	88.6	3455.8	58	11	87.0

Ic-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	~0	8	-6	-
	25.9	0	-6	103.0
	44.7	3	-5	161.3
	74.2	6	12	76.1
	91.2	0	6	43.9
	100.9	0	1	64.7
	135.2	3	20	53.4
	164.5	1	-5	128.6
	183.4	10	-11	140.6
	211.8	3	-16	155.1
	234.8	7	39	47.9
	281.1	5	1	88.0
	315.3	6	-14	133.8
	351.1	18	-10	98.6
	393.8	2	7	78.9
	450.9	41	88	55.3
	472.9	39	-64	101.3
	537.4	6	30	22.7
	584.9	6	16	77.2
	600.3	1	1	96.5
	613.0	8	-32	117.4
	643.9	7	-26	131.8
	721.0	1	-12	165.8
	807.9	6	-5	85.0
	812.2	1	-4	131.2
	850.3	2	-5	116.1
	888.0	2	-15	108.2
	896.6	12	10	63.2
	906.0	2	10	63.1
	938.2	5	-7	99.8
	968.5	6	9	48.2
	986.3	11	-6	93.3
	1011.1	10	15	66.1

1031.4	3	6	86.7
1050.8	7	-19	113.4
1065.4	2	4	21.8
1103.6	11	-24	117.7
1126.6	17	33	35.1
1148.4	5	-3	87.1
1152.2	11	-47	114.0
1170.1	91	20	72.5
1184.4	9	-4	109.7
1206.3	5	-12	113.8
1229.3	43	1	89.4
1240.2	16	48	44.0
1278.7	29	15	71.1
1303.3	8	-25	116.1
1322.0	6	-13	113.0
1336.0	5	-8	141.0
1346.3	4	17	32.9
1356.7	15	-30	111.1
1364.1	58	46	53.6
1397.5	322	26	88.2
1409.8	22	24	65.3
1438.5	7	11	48.5
1442.5	6	-15	154.6
1455.2	31	15	31.8
1456.5	36	-23	97.0
1467.2	9	-4	151.5
1469.0	12	10	84.0
1476.7	7	-6	123.8
1495.9	3	0	88.6
1527.6	205	10	87.3
1663.3	456	-8	91.3
1688.2	213	54	85.4
2912.2	67	12	88.8
2920.9	7	-19	127.7
2922.8	28	26	76.5
2923.7	19	-4	81.9
2927.7	2	-4	95.2
2931.5	29	-18	99.8
2950.6	25	-7	103.2
2966.1	23	58	60.1
2968.7	25	-4	91.1
2972.2	25	-2	89.2
2983.1	41	-17	95.0
2984.7	15	0	93.6
3016.0	4	3	79.5
3031.8	1	-1	100.4
3033.1	9	2	84.3
3472.5	23	-2	91.0

Jc-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Jc+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	28.4	5	-1	94.5		27.2	0	-4	102.1
	32.9	0	-5	167.2		34.9	1	4	71.0
	39.2	1	1	81.4		41.4	4	-5	98.9
	49.4	0	-4	108.0		72.4	2	-12	124.9
	84.7	2	-8	123.8		99.3	0	0	90.3
	104.6	1	5	8.6		108.7	3	-7	100.2
	122.0	3	-14	102.5		134.1	4	-1	91.6
	169.7	13	20	68.6		151.2	2	-3	94.7
	176.8	0	-2	113.0		179.1	12	13	77.2
	214.0	2	1	83.8		231.6	4	15	64.2
	233.8	4	22	58.4		265.1	2	-5	115.8
	285.7	7	-20	116.1		286.3	6	-1	91.8
	315.7	4	-14	147.1		317.1	5	-13	114.2
	384.9	29	25	57.0		391.9	27	-5	92.7
	401.8	12	42	57.7		417.9	23	79	50.7
	439.4	26	-59	118.1		441.7	22	-53	120.7
	474.4	31	12	87.6		474.1	30	-1	90.0
	521.3	4	0	84.3		530.5	5	2	85.6
	586.3	3	-9	99.7		567.6	2	-20	131.7
	601.6	3	-2	91.2		600.8	4	-1	89.2
	617.6	9	10	81.5		618.6	12	25	71.6
	662.6	7	35	48.6		643.1	4	18	58.6
	722.0	1	1	80.3		700.5	0	-5	139.4
	766.3	3	-5	120.3		770.6	1	-4	114.3
	837.1	0	-3	103.2		836.8	6	-5	99.6
	855.8	1	9	33.6		865.6	8	40	32.7
	872.6	9	-46	126.5		873.8	3	-5	108.8
	893.6	4	3	81.0		905.9	2	4	68.3
	911.4	8	-31	136.5		918.8	6	3	74.0
	934.1	2	11	60.7		932.4	4	-2	99.3
	968.6	10	35	42.8		955.6	1	-2	120.1
	991.3	9	-1	82.2		996.5	7	4	78.8
	1011.2	9	-2	102.5		1016.3	20	1	102.9
	1037.2	7	-21	107.2		1038.9	6	-4	87.6
	1047.6	9	24	36.9		1044.4	3	-23	120.6
	1063.8	2	7	48.7		1058.4	13	18	50.4
	1109.8	14	26	62.0		1102.7	21	23	52.7
	1129.1	0	-3	106.7		1128.6	1	-7	145.2
	1139.5	6	0	77.3		1137.5	10	-6	64.7
	1152.0	29	12	84.6		1152.3	28	-35	113.3
	1180.4	7	-15	163.6		1183.6	26	50	49.0
	1183.0	14	23	76.6		1190.7	44	113	37.7
	1199.2	92	50	66.8		1199.6	30	-50	114.2
	1230.0	3	11	72.9		1237.7	66	-1	91.7
	1251.9	24	43	35.1		1261.5	5	24	47.7
	1268.9	40	-61	141.8		1272.3	46	-32	140.3
	1303.6	2	6	66.0		1303.0	9	22	62.6
	1316.4	16	9	79.4		1315.5	12	16	76.1
	1324.9	5	-1	95.0		1324.9	12	-1	84.5

1343.4	16	19	81.2	1338.2	8	-26	125.6
1354.0	19	-45	146.5	1358.9	14	-31	79.4
1363.5	20	5	41.6	1361.3	21	28	111.6
1391.8	316	-1	90.2	1388.5	281	28	87.4
1410.2	20	7	81.2	1409.0	20	1	89.6
1442.1	10	22	44.4	1445.1	10	9	59.9
1446.7	11	11	67.7	1449.9	14	28	63.9
1457.1	14	-66	133.3	1458.2	15	-60	73.1
1459.7	47	5	78.9	1459.8	54	-15	118.3
1464.0	4	3	74.4	1460.5	5	-8	119.0
1468.2	10	11	77.8	1467.7	9	1	92.1
1481.1	5	-1	98.5	1474.5	4	-2	85.5
1498.6	3	1	82.1	1493.6	8	-9	137.6
1528.2	186	-3	90.3	1527.3	180	-8	90.9
1661.0	356	6	89.2	1661.9	357	-23	94.9
1695.8	248	-122	99.8	1697.6	250	-114	98.8
2912.0	63	8	86.6	2893.4	42	8	87.3
2913.6	20	-5	96.3	2907.1	16	-5	95.7
2925.9	29	-17	122.1	2912.1	64	10	85.8
2928.4	4	13	72.7	2924.5	39	-14	100.6
2932.1	12	11	77.9	2929.0	29	-13	100.5
2935.0	38	-30	112.8	2930.9	3	-6	110.7
2953.1	22	16	60.7	2938.7	18	8	80.7
2965.6	14	48	46.9	2965.7	28	0	89.8
2966.1	29	7	88.0	2969.8	23	62	41.6
2974.4	27	-72	126.9	2982.0	39	-25	97.6
2986.1	48	23	83.3	2987.0	19	-10	101.4
2992.9	13	4	84.4	3006.3	15	-14	104.4
2997.6	13	-12	107.8	3023.4	5	-5	102.9
3030.0	1	-1	115.6	3026.0	9	1	87.2
3030.9	6	1	86.0	3030.6	0	0	106.0
3469.7	22	-1	91.0	3467.4	21	-1	90.9

Kc-	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$	Kc+	$\nu_{\text{calc}} / \text{cm}^{-1}$	$I_{\text{IR,calc}}$	R_{calc}	$\tau / ^\circ$
	25.4	1	-16	143.8		17.9	5	-5	102.1
	26.8	1	-3	98.4		45.2	1	-3	112.6
	32.4	3	10	67.3		50.4	1	9	37.9
	57.1	0	-3	151.9		63.0	2	17	48.7
	92.6	0	11	11.4		97.5	1	-2	107.0
	110.6	3	5	64.7		112.9	8	20	75.3
	125.2	5	18	73.1		152.2	2	-3	95.3
	162.2	6	2	88.0		194.3	0	-1	85.2
	180.4	2	-8	108.2		200.2	1	1	63.1
	207.0	8	7	72.5		208.5	14	-7	108.8
	220.0	0	2	82.5		253.2	1	9	56.2
	276.1	1	-10	155.6		282.0	1	4	75.5
	322.0	15	-7	98.4		311.7	15	-30	147.6
	385.0	13	28	29.1		389.5	25	51	41.5
	409.4	11	-78	145.6		402.8	56	-50	96.1
	452.2	52	28	86.2		434.0	6	-18	137.9

496.3	20	40	72.5	492.7	9	26	60.7
531.0	8	16	49.8	540.9	6	18	53.4
585.0	7	-23	158.0	552.5	1	12	36.3
591.5	4	14	78.0	576.1	5	-1	90.8
602.1	7	-8	108.7	604.8	2	19	60.8
642.6	4	-22	123.0	620.6	12	-47	140.1
740.1	1	-14	152.2	709.6	0	-2	90.1
792.4	5	-17	156.9	798.9	1	1	73.9
817.1	1	-2	123.8	824.8	4	8	65.6
847.5	2	-4	114.1	863.8	2	9	48.9
862.8	2	5	83.1	888.1	2	12	55.3
891.9	4	-18	137.6	902.6	5	14	70.2
922.2	4	-12	121.1	918.6	2	-7	97.8
929.4	12	21	65.9	937.5	1	0	84.5
949.2	4	-12	124.7	953.4	3	-20	130.5
995.6	6	0	84.4	994.5	6	11	57.8
1029.3	15	-12	81.5	1020.5	11	-23	128.3
1032.6	8	-37	151.6	1034.6	16	-16	104.5
1043.8	4	6	74.1	1038.4	6	-1	79.2
1068.7	2	8	26.2	1058.4	8	7	88.8
1102.0	2	3	74.5	1101.4	6	7	89.8
1128.0	1	9	34.0	1126.6	9	24	7.9
1146.6	11	-16	120.9	1149.9	14	16	40.5
1159.1	41	28	79.7	1167.8	13	15	84.3
1164.2	63	46	66.4	1178.8	28	-56	121.2
1189.7	8	5	58.2	1191.2	38	13	92.2
1205.7	73	-61	114.2	1197.6	10	4	43.0
1230.9	6	13	67.3	1242.9	22	32	74.9
1254.5	10	36	50.2	1269.5	48	-67	125.2
1286.8	58	-78	129.0	1278.3	47	-37	114.1
1299.4	8	-17	117.9	1294.1	6	-19	140.9
1313.4	8	24	52.5	1324.6	5	1	82.3
1324.0	3	8	56.7	1333.9	13	2	97.7
1345.8	9	10	81.1	1343.7	1	0	89.9
1359.0	25	-20	104.3	1352.3	21	-1	76.0
1381.5	12	10	60.5	1371.3	68	69	58.1
1399.5	369	-51	95.9	1395.2	273	-42	96.1
1409.8	19	12	71.2	1417.4	12	24	50.1
1437.3	6	15	60.8	1441.7	17	17	75.3
1445.4	11	12	65.2	1445.3	20	-20	101.7
1457.7	23	-21	94.6	1455.0	13	-12	111.0
1458.0	29	20	65.8	1459.8	4	-5	143.5
1463.1	7	-1	133.9	1469.1	3	3	75.9
1468.1	9	3	128.6	1471.6	16	18	135.3
1472.7	7	-6	86.8	1472.0	3	-6	77.1
1491.6	6	2	82.0	1497.0	5	2	70.5
1526.7	174	-14	92.7	1513.0	188	-31	94.5
1664.6	373	-4	90.3	1665.2	349	19	88.5
1694.9	243	157	76.5	1694.1	256	58	85.6
2911.5	52	31	62.1	2875.4	39	9	66.3

2912.4	31	-17	113.1	2897.3	33	18	82.9
2918.9	4	-18	120.6	2915.4	50	45	47.1
2923.0	13	17	66.2	2916.9	21	-32	127.4
2928.6	34	-19	121.9	2922.4	12	0	90.2
2936.4	65	20	49.3	2923.5	30	-50	146.3
2950.2	27	15	69.1	2925.7	37	35	54.2
2966.3	27	-2	90.6	2970.4	30	67	20.6
2968.9	20	-46	120.9	2980.7	39	-54	108.4
2976.5	13	-3	92.8	2985.5	21	-9	93.9
2979.8	8	32	57.8	2989.6	9	-7	100.1
2982.9	18	1	89.7	2999.8	10	-7	102.0
2996.5	41	4	88.2	3004.8	10	-1	92.8
3030.4	0	0	86.4	3021.6	9	-4	93.9
3034.1	8	1	87.4	3029.0	8	2	86.7
3473.4	23	1	88.8	3476.8	23	-1	91.1

Table S3. Assignments of MI spectra of Ac-β³-HPro-NHMe^d

Ar	Kr	Calculated	Assignment
amide A			
3494, ^a 3485	3481	3470	Cc- ν_1
3428	3425, 3414 ^a	3420	At+ ν_1
3344, 3331 ^{a,b}	3338	3343	Bt- ν_1
3287	3282	3279	Dt- ν_1
3246	3240		overtone (or dimer)
amide I (C-terminal)			
1700 ^b	1699 ^b	1690	Cc- ν_{17}
1696 ^b	1695 ^b	1689	Bt- ν_{17}
1691	1690	1681	At+ ν_{17}
1681 ^b	1680 ^b	1672	Dt- ν_{17}
amide I (N-terminal)			
1669	1665	1662	Cc- ν_{18}
1654	1652	1643	At+ ν_{18}
1649 ^b	1647 ^b	1642	Dt- ν_{18}
1640	1638	1640	Bt- ν_{18}
amide II			
1553 ^c	1549 ^c	1570, 1571	Bt- ν_{19} and Dt- ν_{19}
1534 ^c	1530 ^c	1536, 1530	At+ ν_{19} and Cc- ν_{19}
1471 ^b	1467 ^b	1476, 1473	At+ ν_{21} and At+ ν_{22}
1462 ^b	1460 ^b	1465	Bt- ν_{23}
1454 ^b	1451 ^b	1458	Cc- ν_{24}
1447	1446	1455	At+ ν_{24}
1441	1439	1448	At+ ν_{26}
1435 ^b	1433 ^b	1438	At+ ν_{27}
1423	1421	1415 and 1413	At+ ν_{28} and At+ ν_{29}
1420 ^b	1418 ^b	1414	Bt- ν_{28}
1417	1415	1406	Dt- ν_{29}
1410	1408	1398	Cc- ν_{29}
1366	1365	1371 and 1369	At+ ν_{30} and Cc- ν_{30}
1354	1352	1355	At+ ν_{31}
1341	1340	1346 and 1345	At+ ν_{32} and At+ ν_{33}
1328	1326	1331	At+ ν_{34}
1309	1308	1310	Dt- ν_{35}
1300	1299	1303	At+ ν_{35}
1292	1290	1289, 1293	Cc- ν_{36} and Dt- ν_{36}
1280	1279	1282	At+ ν_{36}
1265 ^b	1264 ^b	1265	Bt- ν_{37}
1259	1258	1259	At+ ν_{37}
1251	1250	1249	At+ ν_{38}
1245 ^b	1245 ^b	1247	Bt- ν_{38}
1236	1238	1225	Cc- ν_{38}
1215 ^c	1214 ^c	1209 and 1206	At+ ν_{39} and Bt- ν_{39}
1202	1201	1195	At+ ν_{40}
1191	1191	1180	Cc- ν_{41}
1172 ^c	1169 ^c	1164	At+ ν_{42}
1164 ^c	1164 ^c	1157	Bt- ν_{42}
1159 ^d	1158 ^c	1152	Cc- ν_{42}
1155 ^c	1153 ^c	1147	At+ ν_{43}
1151 ^c	1150 ^c	1145	Dt- ν_{43}
1131	1129	1125	At+ ν_{44}
1119	1118	1116	Bt- ν_{45}

1112	1111	1109	<i>At</i> − ν_{45} ?
1105	1105	1100	<i>At</i> + ν_{45}
1081	1080	1074	<i>At</i> + ν_{46}
1074 ^b	1073 ^b	1067 and 1067	<i>Bt</i> − ν_{46} and <i>Cc</i> − ν_{46}
1058	1055	1058	<i>Dt</i> − ν_{47}
1035	1034	1035 and 1036	<i>At</i> + ν_{48} and <i>Cc</i> − ν_{47}
1029 ^b	1028 ^b	1031	<i>Cc</i> − ν_{48}
1020	1018	1013 and 1016	<i>At</i> + ν_{49} and <i>Bt</i> − ν_{49}
1001	1000	991	<i>Cc</i> − ν_{50}
994	993	990	<i>At</i> + ν_{50}
980	980	982	<i>At</i> + ν_{51}
971	970	961	<i>Bt</i> − ν_{51}
959	958	957	<i>Cc</i> − ν_{51}
946 ^c	946 ^c	937, 935 and 940	<i>At</i> + ν_{52} , <i>Bt</i> − ν_{52} and <i>Cc</i> − ν_{52}
925	925	911 and 913	<i>At</i> + ν_{53} and <i>Dt</i> − ν_{53}
917	916	906	<i>At</i> + ν_{54}
888	887	896	<i>Cc</i> − ν_{54}
877 ^c	876 ^c	880	<i>Dt</i> − ν_{55}
875 ^c	874 ^c	877	<i>At</i> + ν_{55}
870 ^c	869 ^c	874	<i>Cc</i> − ν_{55}
854	853	864	<i>Bt</i> − ν_{56}
845	844	862	<i>At</i> + ν_{56}
837 ^c	835 ^c	850 and 845	<i>Cc</i> − ν_{56} and <i>Dt</i> − ν_{57}
824	823	833 and 840	<i>At</i> + ν_{57} + <i>Bt</i> − ν_{57}
813	813	826	<i>Cc</i> − ν_{57}
797	797	812	<i>Cc</i> − ν_{58}
780	778	795 and 798	<i>At</i> + ν_{58} + <i>Bt</i> − ν_{58}
754	753	765	<i>Dt</i> − ν_{58}
713 ^c	711 ^c	734 and 723	<i>Bt</i> − ν_{59} and <i>Dt</i> − ν_{59}
675	675	686	<i>Bt</i> − ν_{60}
635	633	641	<i>Bt</i> − ν_{61}
620	619	630	<i>At</i> + ν_{60}
602	602	615	<i>At</i> + ν_{61}
593	593	599	<i>At</i> + ν_{62}
572	570	570	<i>At</i> + ν_{63}
539 ^b	535 ^b	543	<i>Cc</i> − ν_{64}
528	528	537	<i>At</i> + ν_{64}
518 ^b	516 ^b	529	<i>At</i> + ν_{65}
511 ^b	509 ^b	526	<i>Bt</i> − ν_{65}
489 ^c	487 ^c	483	<i>At</i> + ν_{66}
480 ^c	480 ^c	474	<i>Cc</i> − ν_{65}
438 ^c	438 ^c	443	<i>Cc</i> − ν_{66}
427 ^c	427 ^c	423	<i>At</i> + ν_{67}
416 ^c	416 ^c	420	<i>Bt</i> − ν_{67}

^a Site splitting.

^b Shoulder.

^c Broad, unresolved.

^d Tentative in the fingerprint region.

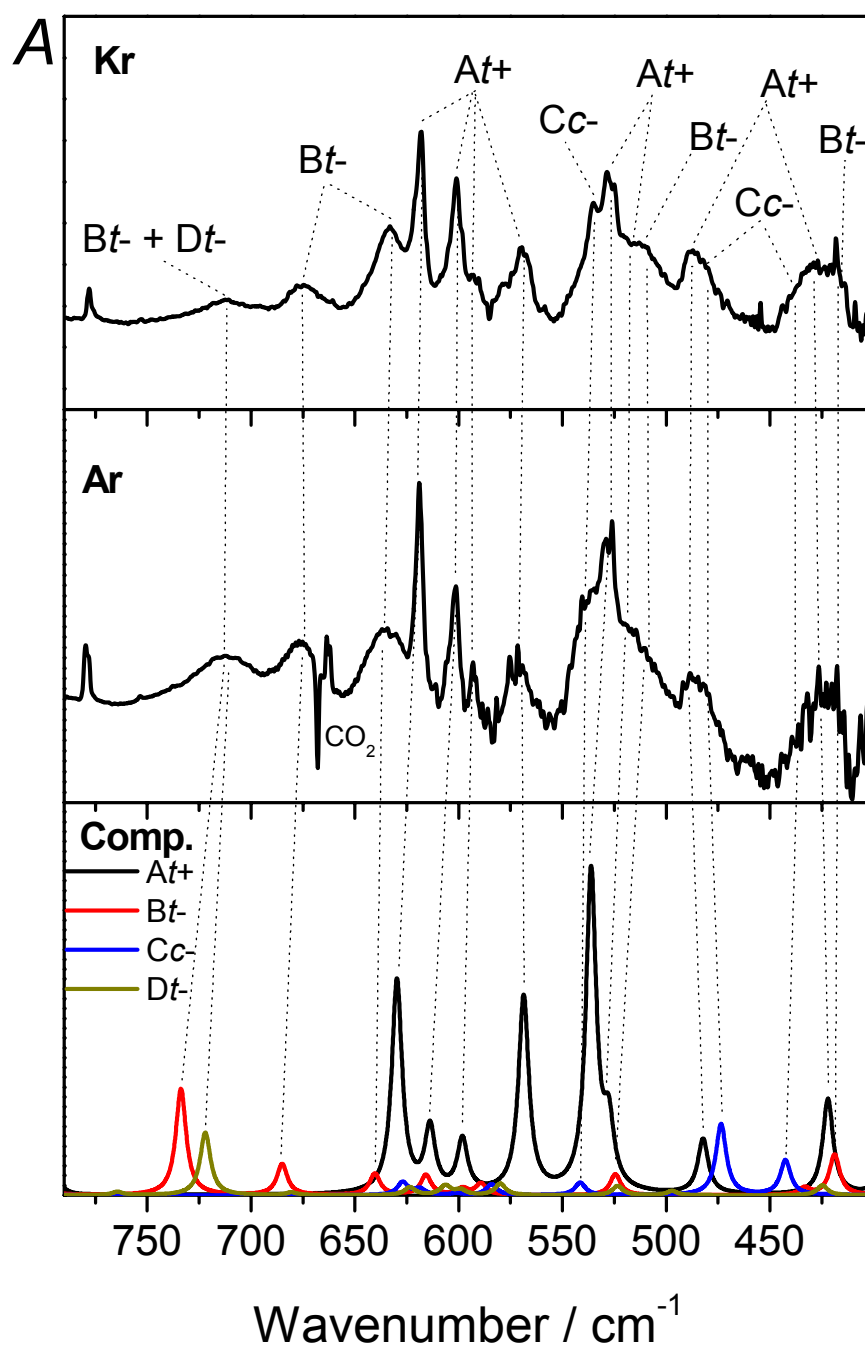


Figure S1. Computed and MI-IR spectra of Ac- β^3 -HPro-NHMe in the 750–400 cm^{-1} region.

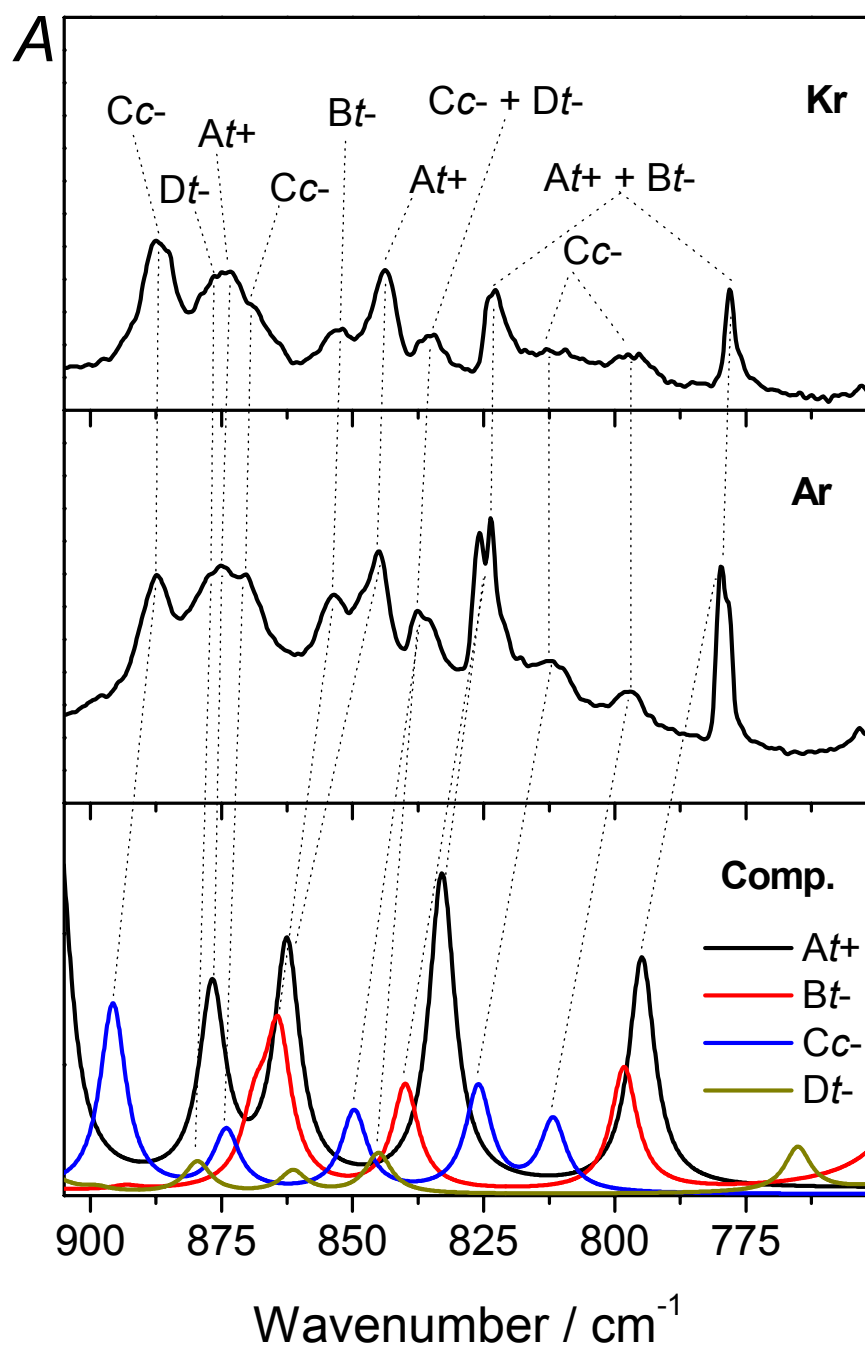


Figure S2. Computed and MI-IR spectra of Ac- β^3 -HPro-NHMe in the 900–750 cm⁻¹ region.

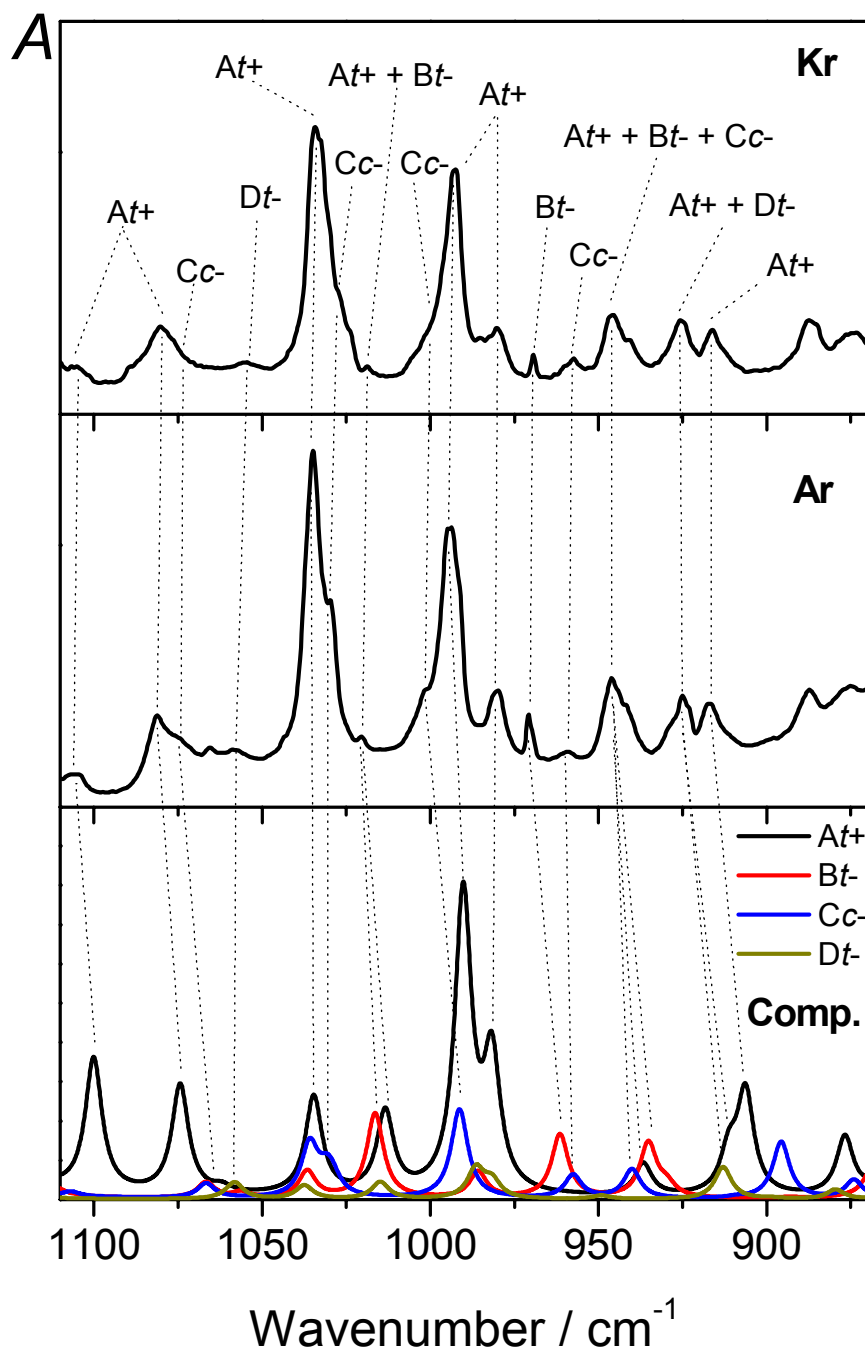


Figure S3. Computed and MI-IR spectra of Ac- β^3 -HPro-NHMe in the 1100–900 cm⁻¹ region.

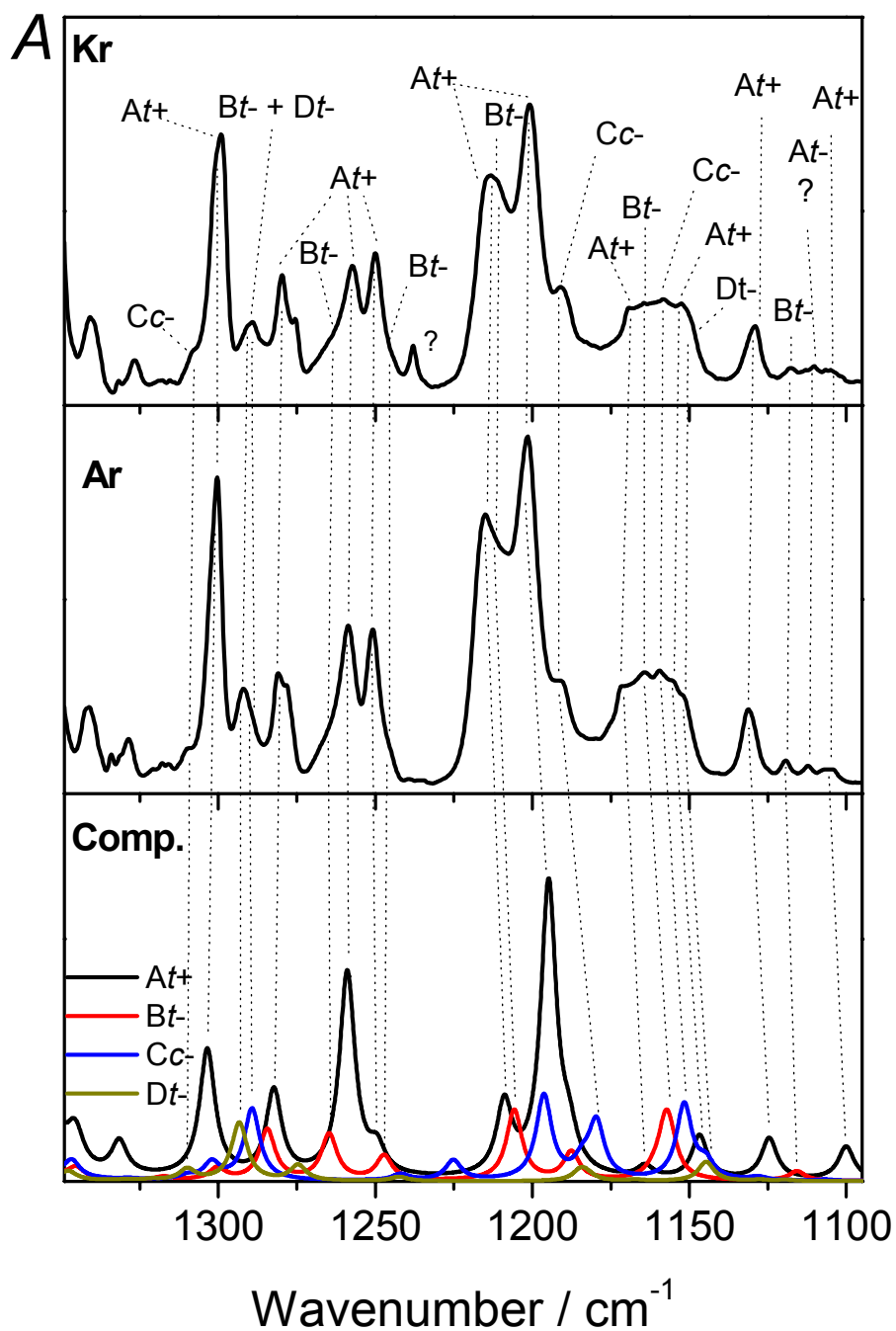


Figure S4. Computed and MI-IR spectra of Ac-β³-HPro-NHMe in the 1300–1100 cm⁻¹ region.

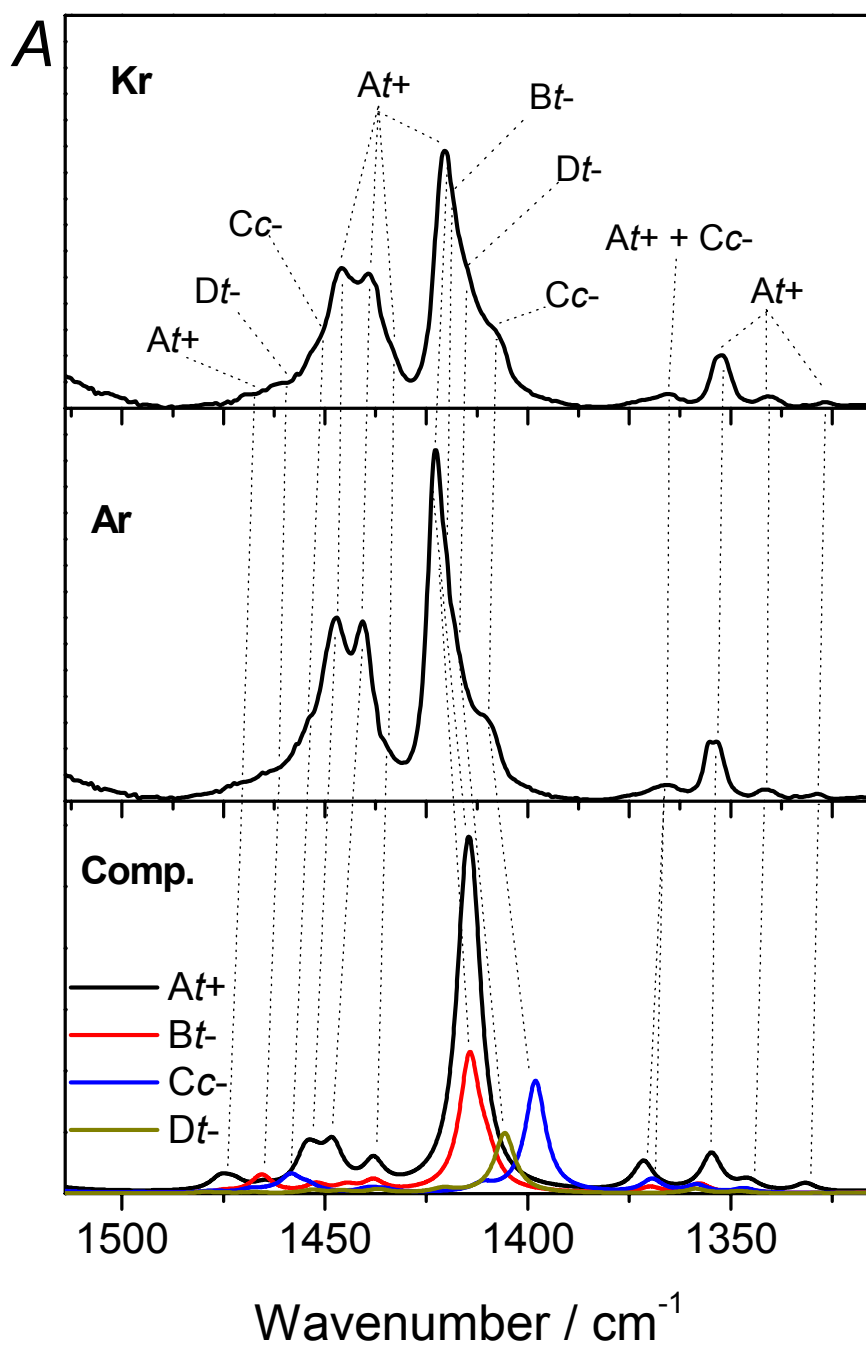


Figure S5. Computed and MI-IR spectra of Ac- β^3 -HPro-NHMe in the 1500–1300 cm^{-1} region.

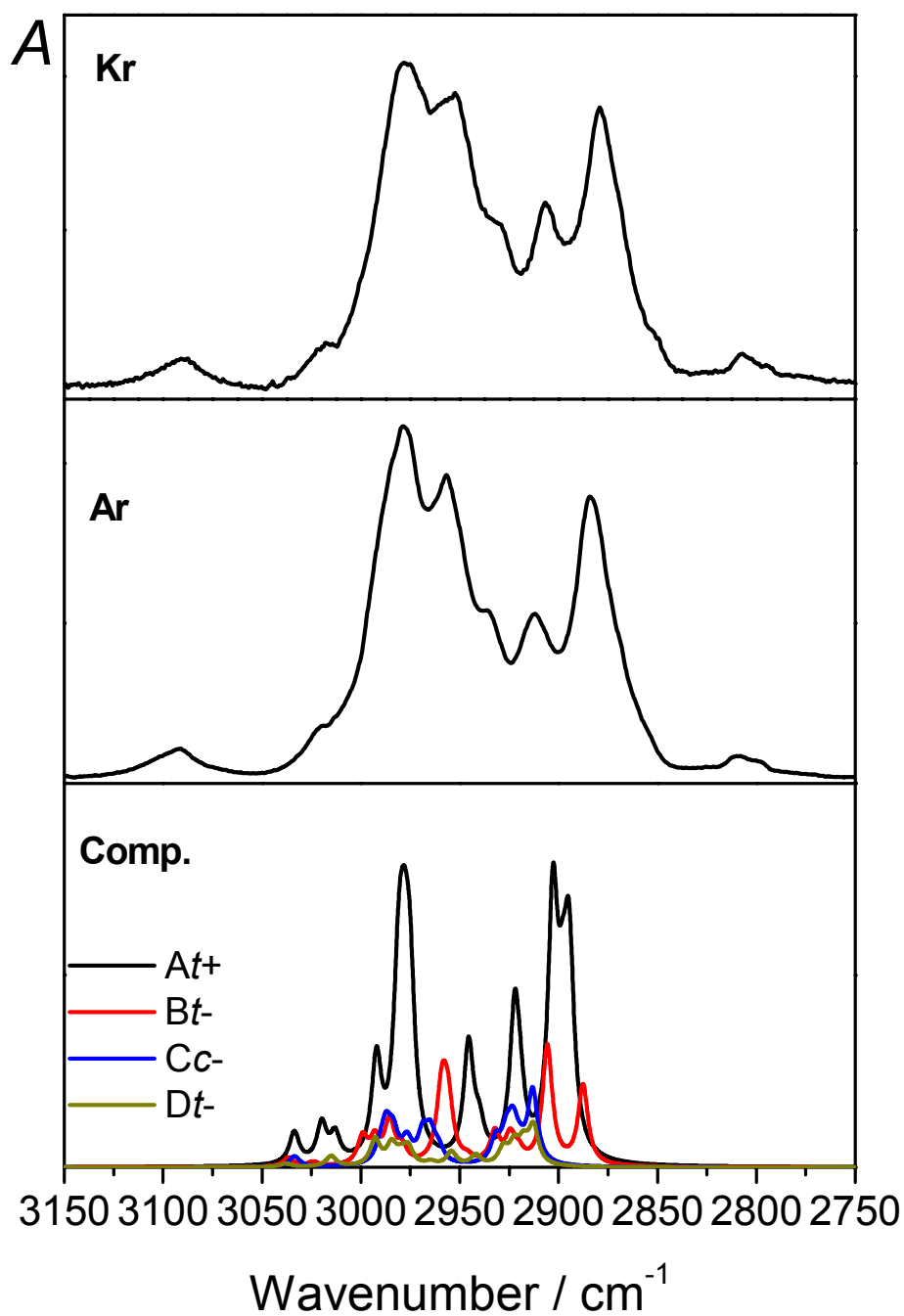
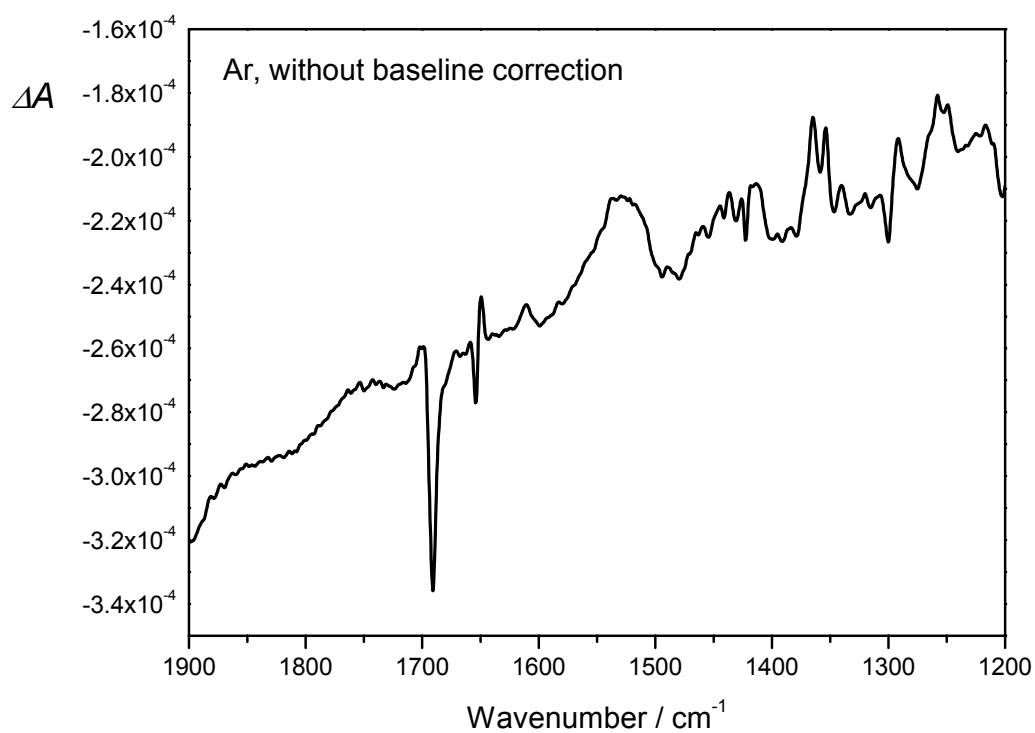


Figure S6. Computed and MI-IR spectra of Ac- β^3 -HPro-NHMe in the 3150–2750 cm^{-1} region.



**Figure S7. Raw MI-VCD spectrum
(as measured in Ar without baseline correction)
of Ac-β³-HPro-NHMe.**

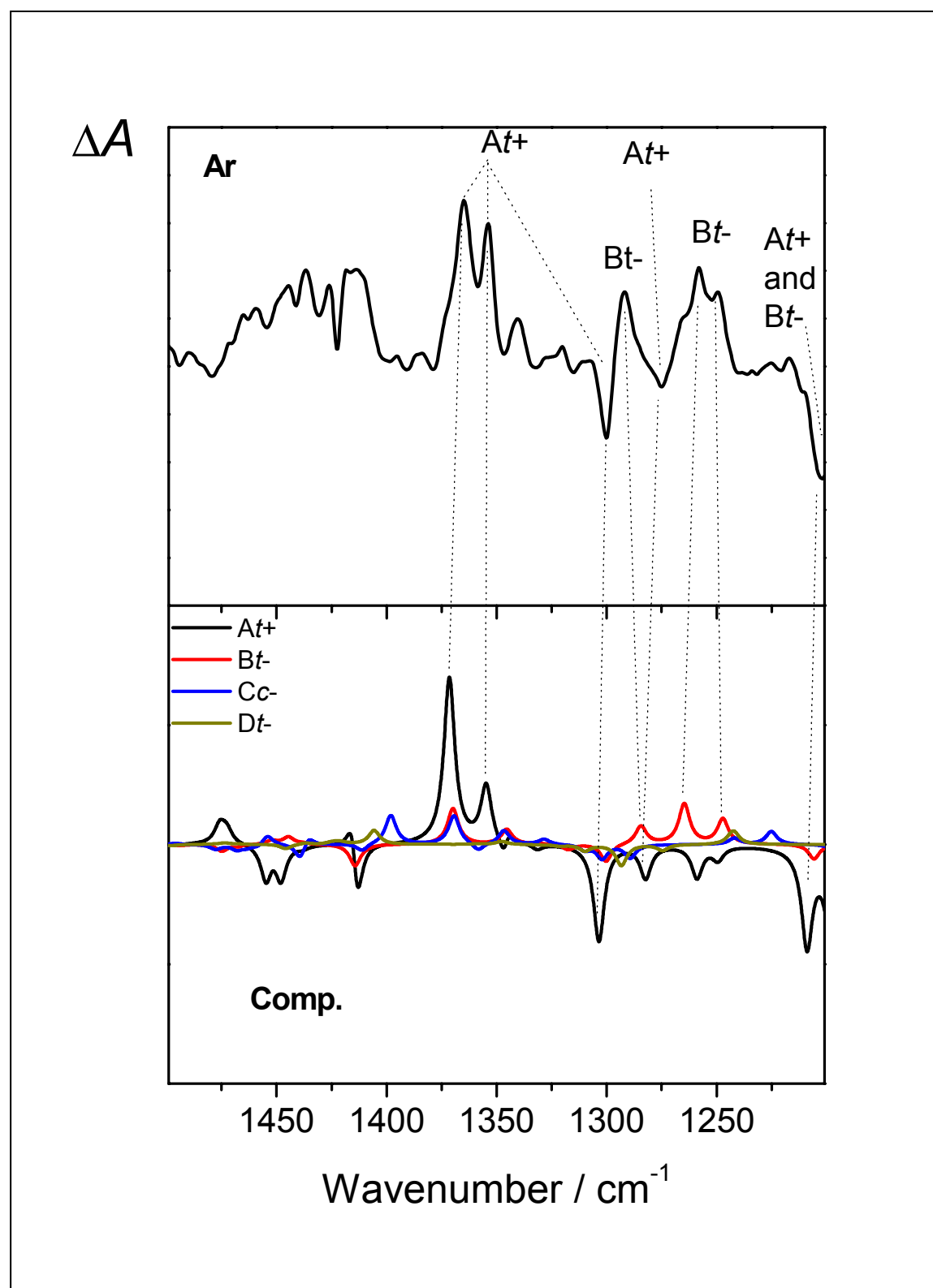


Figure S8. Computed and MI-VCD spectra of Ac- β^3 -HPro-NHMe in the 1500–1200 cm^{-1} region.