

Supplementary Information

Cyclometalated ruthenium complexes from naturally occurring quinones: Studies on their photophysical features, computational details and trypanocidal activity

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Contents

Computational details

S2

OPTIMIZED B3LYP/LANL2DZ/D95V GEOMETRIES.**COMPOUND 5**

52

scf done: -1334.999588

N	-5.113641	-1.978014	0.012961
C	-4.893601	-3.307103	-0.012873
C	-3.598639	-3.878525	-0.048003
C	-2.495399	-3.024349	-0.055762
H	-3.480884	-4.956772	-0.067869
H	-5.775494	-3.942744	-0.005393
H	-1.481266	-3.406072	-0.081636
C	-2.698006	-1.621272	-0.028984
C	-4.037388	-1.131055	0.004936
C	-4.282144	0.326235	0.032339
N	-5.575228	0.775141	0.062119
C	-5.801261	2.103183	0.087678
H	-6.842070	2.416122	0.110785
C	-4.762941	3.065851	0.085472
C	-3.441566	2.619210	0.054754
H	-5.002836	4.123684	0.107198
H	-2.608253	3.312464	0.051436
C	-3.175284	1.226373	0.027047
C	-1.568208	-0.693585	-0.035505
C	-1.807978	0.716174	-0.007015
N	-0.771423	1.591757	-0.011248
C	0.494311	1.111812	-0.043658
N	-0.306526	-1.186639	-0.068405
C	0.741781	-0.313323	-0.074493
C	2.086038	-0.833560	-0.112734
C	3.142489	0.061085	-0.096200
O	4.471627	-0.331278	-0.116392
C	1.620878	2.034595	-0.048574
C	2.946546	1.506642	-0.071355

C	4.051976	2.398897	-0.067985
H	5.055996	1.991136	-0.081425
C	3.845383	3.780691	-0.046798
H	4.696222	4.456628	-0.045078
C	2.526916	4.306100	-0.026078
H	2.373287	5.381547	-0.009242
C	1.430227	3.441227	-0.025788
H	0.416484	3.826366	-0.007904
C	4.810696	-1.789694	0.102550
C	2.325046	-2.328593	-0.193291
H	2.114325	-2.794940	0.779432
H	1.609963	-2.772573	-0.894080
C	6.210687	-1.937388	-0.500116
H	6.197119	-1.717406	-1.573737
H	6.571160	-2.963562	-0.360392
H	6.915548	-1.254747	-0.011615
C	3.765085	-2.640468	-0.646877
H	3.865265	-2.441924	-1.722381
H	3.989401	-3.701736	-0.486704
C	4.815702	-2.035390	1.622637
H	3.841098	-1.821426	2.074026
H	5.565408	-1.399039	2.106209
H	5.066162	-3.083112	1.829576

COMPOUND 6

52

scf done: -1345.775287

N	-5.506297	-2.548842	0.244279
N	-6.458074	0.003543	-0.366147
N	-0.963635	-0.807156	0.511866
C	-5.115956	-0.163600	-0.154069
N	-1.926570	1.772742	-0.084884
C	-4.201989	0.928725	-0.234834

C	-2.775706	0.717789	-0.005254
C	-2.284408	-0.590886	0.299980
C	-0.604255	1.569540	0.126675
C	-3.215742	-1.713899	0.386473
C	-4.611344	-1.515299	0.166526
C	-0.104331	0.248000	0.430461
C	1.302523	0.022698	0.651067
O	3.535342	0.986560	0.789733
C	2.164889	1.100974	0.588996
C	1.808359	-1.378880	0.920418
H	1.280485	-2.094041	0.286056
H	1.572959	-1.676740	1.953568
C	1.713971	2.451449	0.281523
C	-3.682049	-4.068362	0.767377
H	-3.370218	-5.081455	0.998156
C	-0.115228	4.001855	-0.257049
H	-1.172545	4.166410	-0.433792
C	0.326094	2.687197	0.045680
C	4.078425	-0.290730	1.357698
C	-5.049193	-3.782418	0.535829
H	-5.793213	-4.573278	0.587957
C	3.328437	-1.485041	0.720629
C	0.796212	5.058023	-0.324936
H	0.450910	6.061406	-0.558081
C	-2.762040	-3.022220	0.691021
H	-1.703692	-3.184008	0.859764
C	2.628671	3.535862	0.212475
H	3.680371	3.349699	0.396311
C	2.175780	4.823030	-0.087982
H	2.880867	5.648068	-0.140100
C	5.581636	-0.235024	1.074575
H	6.064809	-1.152816	1.429616
H	5.782765	-0.123846	0.005989
H	6.024501	0.615544	1.603689

C	-6.921063	1.234817	-0.657769
H	-7.992545	1.322642	-0.818698
C	-6.085260	2.373415	-0.757088
H	-6.512420	3.341859	-0.994917
C	-4.715791	2.214011	-0.543355
H	-4.030513	3.051325	-0.607718
C	3.823939	-0.276576	2.887831
H	4.189869	-1.204798	3.342068
H	2.764400	-0.164126	3.134284
H	4.369591	0.562828	3.331035
I	3.746918	-1.696969	-1.484478
H	3.718770	-2.426483	1.111067

COMPOUND 7

52

scf done: -1347.557635

N	-5.370834	-2.388117	0.167311
N	-6.201504	0.245838	-0.223466
N	-0.729828	-0.917440	0.340509
C	-4.862722	-0.006479	-0.088495
N	-1.567371	1.744489	-0.049136
C	-3.892524	1.038062	-0.141700
C	-2.471795	0.734776	0.004327
C	-2.043526	-0.616229	0.201909
C	-0.251029	1.455990	0.087961
C	-3.032461	-1.690665	0.257216
C	-4.422323	-1.402012	0.116971
C	0.184143	0.092371	0.287977
C	1.582742	-0.223112	0.436090
O	3.870478	0.604942	0.541033
C	2.502499	0.807378	0.401608
C	2.015767	-1.664558	0.604034
H	1.440688	-2.310764	-0.063065

H	1.785951	-2.016582	1.620911
C	2.118781	2.196752	0.192881
C	-3.615515	-4.037245	0.499353
H	-3.352665	-5.079537	0.645560
C	0.362505	3.877201	-0.168749
H	-0.689734	4.111429	-0.287297
C	0.738460	2.523464	0.033414
C	4.358110	-0.726644	1.025416
C	-4.972861	-3.662062	0.352768
H	-5.758015	-4.413156	0.386449
C	3.518818	-1.841386	0.361753
C	1.330556	4.883084	-0.213340
H	1.035188	5.916932	-0.369126
C	-2.641235	-3.039638	0.450858
H	-1.587388	-3.269435	0.558057
C	3.091755	3.230434	0.147941
H	4.137499	2.974571	0.272552
C	2.702731	4.557094	-0.053794
H	3.452029	5.343184	-0.087896
C	5.848571	-0.747210	0.679802
H	6.291774	-1.701372	0.987852
H	6.008607	-0.614959	-0.392945
H	6.360175	0.060088	1.214499
C	-6.606409	1.517420	-0.410044
H	-7.677331	1.673441	-0.512358
C	-5.712686	2.613730	-0.474383
H	-6.094571	3.617736	-0.626264
C	-4.346138	2.367229	-0.338823
H	-3.618591	3.169643	-0.380426
C	4.157599	-0.778006	2.561679
H	4.480228	-1.748481	2.956496
H	3.115360	-0.615294	2.851185
H	4.768382	0.003160	3.025726
Br	3.837255	-1.904771	-1.695350

H 3.870540 -2.824998 0.674775

COMPOUND 10

49

scf done: -1295.688223

N	1.200393	-1.258277	0.525118
N	1.340186	1.344378	-0.471122
N	-3.664985	-1.064622	0.414073
C	0.107155	0.785189	-0.266191
N	-3.527093	1.571873	-0.595166
C	-1.097239	1.496540	-0.547894
C	-2.396878	0.871951	-0.318400
C	-2.470262	-0.463542	0.192794
C	-4.730239	0.990067	-0.381335
C	-1.239855	-1.197054	0.483184
C	0.033137	-0.592982	0.261353
C	-4.802805	-0.365168	0.137429
C	-6.084303	-0.950423	0.351993
O	-8.396004	-0.929112	0.326348
C	-7.226215	-0.237505	0.070172
C	-6.445237	-2.323206	0.875349
H	-6.057406	-2.489448	1.887246
H	-6.044730	-3.121157	0.239073
C	-7.228543	1.109014	-0.445819
C	-0.082824	-3.189690	1.255498
H	-0.074181	-4.202654	1.643718
C	-5.925465	3.054090	-1.181292
H	-4.961859	3.521272	-1.353020
C	-5.957481	1.728899	-0.673735
C	-8.015291	-2.322808	0.863116
C	1.136836	-2.515245	1.006290
H	2.087006	-3.006034	1.201545
H	-8.385563	-4.353429	0.208673

H	-8.190791	-3.194366	-1.125121
H	-9.701002	-3.221144	-0.180565
C	-7.112555	3.739954	-1.453089
H	-7.076459	4.754000	-1.841388
C	-1.278068	-2.520611	0.990066
H	-2.241121	-2.987424	1.161652
C	-8.426814	1.815429	-0.725576
H	-9.381433	1.331208	-0.547251
C	-8.369310	3.118893	-1.224614
H	-9.286109	3.660831	-1.439215
C	-8.630570	-2.418604	2.262865
H	-8.404728	-3.398574	2.701554
H	-8.222032	-1.644070	2.922251
H	-9.719491	-2.302844	2.217074
C	1.410650	2.601091	-0.952145
H	2.408274	3.006800	-1.100049
C	0.267474	3.378340	-1.258640
H	0.383150	4.385955	-1.643870
C	-0.993534	2.817791	-1.053397
H	-1.901233	3.368796	-1.271412
C	-8.612182	-3.332312	-0.122625

COMPOUND 13

46

scf done: -1256.375443

N	1.074045	1.264678	-0.581162
N	1.130263	-1.266178	0.592874
N	-3.796706	1.160386	-0.620039
C	-0.084090	-0.700813	0.310015
N	-3.740845	-1.399892	0.574948
C	-1.310149	-1.370110	0.600396
C	-2.589520	-0.740801	0.286120
C	-2.620840	0.556930	-0.318487

C	-4.925630	-0.814345	0.282928
C	-1.367701	1.247783	-0.617726
C	-0.114059	0.639055	-0.312466
C	-4.955589	0.501072	-0.332938
C	-6.218850	1.090520	-0.629688
O	-8.531426	1.115491	-0.666822
C	-7.381312	0.419913	-0.330084
C	-6.540745	2.436808	-1.245423
H	-6.093348	2.557174	-2.237979
H	-6.179736	3.263989	-0.621621
C	-7.426670	-0.884230	0.282226
C	-0.147449	3.162330	-1.484970
H	-0.106922	4.145848	-1.940911
C	-6.183840	-2.794140	1.192608
H	-5.235487	-3.265796	1.425957
C	-6.174827	-1.508674	0.590650
C	-8.101682	2.425792	-1.322714
C	1.050270	2.486444	-1.148933
H	2.015395	2.946809	-1.344771
H	-8.554079	4.520858	-1.087608
H	-8.474601	3.626159	0.448246
H	-9.888867	3.444094	-0.622465
C	-7.391598	-3.436851	1.478429
H	-7.386397	-4.420788	1.939044
C	-1.363477	2.533624	-1.215131
H	-2.310511	3.004823	-1.451397
C	-8.646356	-1.546557	0.577361
H	-9.585868	-1.059612	0.336893
C	-8.628832	-2.811346	1.170041
H	-9.561798	-3.319791	1.396421
H	0.078050	-4.202013	1.940124
C	-1.248221	-2.654669	1.198709
H	-2.172629	-3.173539	1.424697
C	-8.800659	3.570564	-0.597152

C	1.161511	-2.487467	1.161021
H	2.146010	-2.899010	1.368535
C	-0.005561	-3.221681	1.483054
H	-8.452128	2.342417	-2.356101

COMPOUND 15

93

scf done: -2430.176967

Ru	3.885144	-0.088708	0.012773
N	2.082111	-1.156035	-0.163428
N	2.491799	1.486762	0.016142
N	-2.730217	-0.463384	-0.491801
N	5.571291	1.101013	0.352722
C	1.182511	1.071916	-0.097829
N	4.091396	-0.219367	-2.068014
N	-2.301751	2.318607	-0.281861
N	3.913354	0.002035	2.105282
N	5.140499	-1.752157	-0.175503
C	0.097434	1.977730	-0.115195
C	-1.259300	1.452412	-0.254145
C	-1.480346	0.039447	-0.363949
C	-3.556866	1.828708	-0.412910
C	-0.342989	-0.881734	-0.336867
C	0.961722	-0.354403	-0.203845
C	-3.784068	0.401915	-0.517388
C	-5.116725	-0.125993	-0.649617
O	-7.496560	0.350165	-0.831572
C	-6.178453	0.759293	-0.700144
C	-5.335236	-1.623621	-0.706468
H	-4.663254	-2.125772	-0.007328
H	-5.063953	-2.010316	-1.700606
C	-6.005739	2.202385	-0.595936
C	4.873840	-1.258899	-2.520568

C	0.653226	-3.091703	-0.398630
H	0.581481	-4.170857	-0.471318
C	4.938349	0.742982	2.651622
C	-4.520549	4.144754	-0.345586
H	-3.516441	4.539172	-0.235029
C	-4.691936	2.739719	-0.448193
C	5.474787	-2.099746	-1.466283
C	-7.784017	-1.078910	-1.188536
C	1.924523	-2.496947	-0.262527
H	2.821841	-3.101067	-0.226012
C	3.496882	0.607641	-2.970799
H	2.895938	1.412957	-2.569689
C	5.062893	-1.474226	-3.897922
H	5.676760	-2.295689	-4.246266
C	6.332696	-3.184691	-1.723113
H	6.593512	-3.449669	-2.740414
C	5.872900	1.338766	1.676031
C	-6.799820	-1.996189	-0.424811
C	3.652726	0.441290	-4.352710
H	3.160219	1.126664	-5.033227
C	4.448602	-0.618883	-4.825427
H	4.587771	-0.776256	-5.889829
C	-5.625722	4.997817	-0.387515
H	-5.487570	6.072382	-0.308207
C	-0.488727	-2.286041	-0.435904
H	-1.480236	-2.711065	-0.537726
C	-7.119396	3.081906	-0.639896
H	-8.113961	2.667470	-0.755620
C	6.379516	1.611847	-0.615906
H	6.102327	1.402243	-1.640542
C	5.651979	-2.471957	0.860358
H	5.362208	-2.164848	1.856350
C	6.855543	-3.925778	-0.652341
H	7.517667	-4.764610	-0.839557

C	3.001367	-0.581225	2.930226
H	2.215271	-1.155220	2.457694
C	7.513754	2.376979	-0.316282
H	8.126565	2.763557	-1.122786
C	7.000903	2.099326	2.034044
H	7.232584	2.280839	3.076342
C	-6.931717	4.462714	-0.535942
H	-7.788091	5.130401	-0.569843
C	6.507945	-3.562684	0.662223
H	6.888534	-4.106585	1.519400
C	3.068447	-0.459358	4.323889
H	2.319406	-0.943889	4.940004
C	5.053369	0.899649	4.044965
H	5.861552	1.483828	4.467540
C	4.112385	0.294481	4.892116
H	4.192170	0.408637	5.968053
C	7.831409	2.624683	1.032280
H	8.703849	3.212425	1.297822
C	-9.263360	-1.274872	-0.849473
H	-9.562470	-2.308592	-1.058592
H	-9.464830	-1.058013	0.202493
H	-9.873464	-0.607046	-1.466851
C	2.744288	2.811940	0.128369
H	3.780886	3.110543	0.215861
C	1.710963	3.771989	0.123449
H	1.967017	4.821446	0.213947
C	0.381120	3.360209	-0.000553
H	-0.434627	4.073276	-0.011446
C	-7.561875	-1.236931	-2.715488
H	-7.746170	-2.273770	-3.019935
H	-6.549016	-0.960231	-3.020939
H	-8.268322	-0.590788	-3.246654
I	-7.131992	-1.968988	1.804118
H	-6.998279	-3.041923	-0.664820

COMPOUND 16

93

scf done: -2431.959057

Ru	3.614655	-0.079353	0.014693
N	1.831515	-1.187583	0.140516
N	2.185348	1.437984	-0.263387
N	-3.003165	-0.656864	-0.157724
N	5.277369	1.190012	0.027312
C	0.882896	0.989173	-0.231532
N	3.754118	-0.645403	-1.997782
N	-2.634801	2.118892	-0.513511
N	3.712669	0.457792	2.037613
N	4.901021	-1.725193	0.133468
C	-0.222787	1.855512	-0.390435
C	-1.571264	1.292475	-0.358944
C	-1.762412	-0.116901	-0.172087
C	-3.881748	1.591893	-0.496405
C	-0.604000	-0.994010	0.005440
C	0.691943	-0.430481	-0.025622
C	-4.077144	0.167497	-0.320969
C	-5.398676	-0.402516	-0.320934
O	-7.791142	-0.021541	-0.541150
C	-6.482414	0.435601	-0.508386
C	-5.576815	-1.890938	-0.105950
H	-4.908610	-2.240188	0.684526
H	-5.275783	-2.444003	-1.008168
C	-6.343566	1.877274	-0.666695
C	4.539475	-1.748492	-2.250005
C	0.440208	-3.150500	0.377540
H	0.390996	-4.221270	0.538871
C	4.730189	1.324574	2.371274
C	-4.902619	3.862988	-0.812968

H	-3.906775	4.292045	-0.804709
C	-5.040166	2.458991	-0.658160
C	5.195152	-2.337179	-1.065563
C	-8.040729	-1.495453	-0.669954
C	1.701069	-2.520731	0.336964
H	2.612100	-3.089723	0.469364
C	3.116319	-0.032345	-3.032059
H	2.516623	0.834151	-2.787266
C	4.684157	-2.248501	-3.557043
H	5.299348	-3.119214	-3.747662
C	6.067954	-3.439187	-1.118911
H	6.297285	-3.913614	-2.065112
C	5.614055	1.715914	1.255470
C	-7.030308	-2.252602	0.220371
C	3.228509	-0.484230	-4.352897
H	2.702934	0.038719	-5.143936
C	4.024319	-1.613837	-4.620581
H	4.129453	-1.991060	-5.632381
C	-6.030286	4.671881	-0.971487
H	-5.917872	5.746085	-1.087739
C	-0.720546	-2.389416	0.211240
H	-1.704328	-2.842531	0.238292
C	-7.480245	2.711378	-0.833122
H	-8.466347	2.262121	-0.843437
C	6.037166	1.498143	-1.059202
H	5.732828	1.066278	-2.003228
C	5.466272	-2.198296	1.277759
H	5.204531	-1.688665	2.195414
C	6.646871	-3.925017	0.063490
H	7.320902	-4.774650	0.033233
C	2.847800	0.043704	3.003586
H	2.067135	-0.639259	2.696063
C	7.155822	2.336697	-0.975590
H	7.729465	2.554125	-1.869517

C	6.729014	2.561940	1.397555
H	6.989765	2.969953	2.366350
C	-7.325576	4.092137	-0.982097
H	-8.199441	4.725297	-1.107552
C	6.339654	-3.293117	1.282941
H	6.764187	-3.634474	2.220348
C	2.955016	0.466866	4.334350
H	2.242692	0.108557	5.068933
C	4.883663	1.783501	3.692232
H	5.684486	2.466449	3.947394
C	3.990605	1.353007	4.685466
H	4.100380	1.700834	5.707265
C	7.509469	2.877460	0.274757
H	8.371388	3.528910	0.373767
C	-9.510103	-1.678007	-0.283680
H	-9.780803	-2.739264	-0.329494
H	-9.705056	-1.309421	0.726213
H	-10.144823	-1.128947	-0.987197
C	2.411662	2.760225	-0.445034
H	3.444228	3.083694	-0.469235
C	1.357095	3.682887	-0.605488
H	1.591956	4.731473	-0.748335
C	0.033174	3.235290	-0.579765
H	-0.798643	3.918629	-0.703147
C	-7.817881	-1.888405	-2.152409
H	-7.971005	-2.965342	-2.286957
H	-6.814274	-1.634276	-2.505226
H	-8.544985	-1.356292	-2.774218
Br	-7.357021	-1.855196	2.237343
H	-7.203870	-3.327960	0.169909

COMPOUND 17

scf done: -2380.089881

Ru	2.866291	-0.034683	0.009142
N	1.184905	-1.195560	0.510124
N	1.310553	1.274107	-0.524694
N	-3.686108	-1.055117	0.450744
N	4.421457	1.306258	-0.388547
C	0.050884	0.765185	-0.295051
N	2.954367	-1.063009	-1.815155
N	-3.553888	1.575895	-0.586470
N	3.016412	0.981718	1.834439
N	4.285807	-1.512109	0.433127
C	-1.126684	1.495787	-0.575745
C	-2.423451	0.874942	-0.316201
C	-2.494783	-0.457445	0.213294
C	-4.754647	0.998929	-0.353808
C	-1.262456	-1.192510	0.505894
C	-0.017486	-0.572387	0.252824
C	-4.825594	-0.355884	0.175493
C	-6.103865	-0.937951	0.400965
O	-8.413707	-0.910330	0.393178
C	-7.248061	-0.222715	0.126409
C	-6.464249	-2.303562	0.943363
H	-6.117004	-2.432541	1.975610
H	-6.026064	-3.113332	0.349244
C	-7.252331	1.123356	-0.392449
C	3.817071	-2.136675	-1.848030
C	-0.035656	-3.131134	1.290911
H	0.006979	-4.135150	1.697314
C	3.976727	1.968249	1.886312
C	-5.952252	3.063056	-1.147895
H	-4.990352	3.528806	-1.332173
C	-5.982663	1.739934	-0.635656
C	4.573668	-2.374123	-0.602528
C	-8.031330	-2.330240	0.864109

C	1.168688	-2.451201	1.016521
H	2.126493	-2.915674	1.211584
C	2.217616	-0.767433	-2.920816
H	1.558504	0.087891	-2.852161
C	3.941480	-2.927793	-3.004780
H	4.618573	-3.772898	-3.022951
C	5.529774	-3.394460	-0.447842
H	5.754537	-4.066174	-1.267076
C	4.773568	2.134676	0.654695
H	-8.338807	-4.320793	0.067462
H	-8.086463	-3.080771	-1.181106
H	-9.645227	-3.179083	-0.324395
C	2.304006	-1.518912	-4.099571
H	1.697820	-1.243695	-4.955264
C	3.179879	-2.619714	-4.142524
H	3.268364	-3.223591	-5.039505
C	-7.141045	3.750561	-1.408570
H	-7.106783	4.763321	-1.800015
C	-1.259187	-2.503979	1.037818
H	-2.202301	-2.997610	1.240047
C	-8.451732	1.831047	-0.661004
H	-9.405666	1.349828	-0.471650
C	5.101781	1.390789	-1.564440
H	4.787688	0.723341	-2.355840
C	4.939334	-1.654588	1.618729
H	4.680228	-0.956623	2.403685
C	6.199186	-3.539713	0.776853
H	6.937824	-4.323761	0.906480
C	2.232698	0.758442	2.924537
H	1.494637	-0.027986	2.839689
C	6.153100	2.296099	-1.755955
H	6.664676	2.327973	-2.711304
C	5.824154	3.060310	0.518377
H	6.098761	3.705835	1.343503

C	-8.396229	3.133163	-1.164468
H	-9.313917	3.676549	-1.370873
C	5.897453	-2.654423	1.828402
H	6.390330	-2.729734	2.791118
C	2.368030	1.497163	4.106654
H	1.721083	1.281282	4.949427
C	4.154188	2.742996	3.047227
H	4.908483	3.519495	3.080392
C	3.345045	2.508249	4.169588
H	3.473975	3.099989	5.069759
C	6.522319	3.145041	-0.695938
H	7.334039	3.855603	-0.811273
C	-8.711126	-2.524474	2.221436
H	-8.479734	-3.523519	2.611184
H	-8.356983	-1.781993	2.945577
H	-9.799357	-2.434029	2.128071
C	1.423426	2.524477	-1.030675
H	2.424682	2.896286	-1.205036
C	0.292720	3.312750	-1.329857
H	0.436804	4.308266	-1.733994
C	-0.988732	2.802322	-1.104910
H	-1.876575	3.381968	-1.327857
C	-8.560058	-3.283555	-0.213414

COMPOUND 18

87

scf done: -2340.777163

Ru	-2.701693	0.019103	-0.000722
N	-1.057542	1.200778	0.568991
N	-1.105571	-1.220929	-0.580873
N	3.815289	1.174381	0.598592
N	-4.212835	-1.346810	-0.473209
C	0.137231	-0.692159	-0.308088

N	-2.808554	1.127881	-1.775122
N	3.765085	-1.401284	-0.575744
N	-2.833400	-1.085002	1.774892
N	-4.162926	1.435060	0.482113
C	1.336867	-1.379159	-0.604705
C	2.613662	-0.741242	-0.292408
C	2.643244	0.565040	0.302559
C	4.947374	-0.810648	-0.288034
C	1.388638	1.258043	0.602903
C	0.163655	0.619853	0.302137
C	4.975661	0.513212	0.317723
C	6.235367	1.106062	0.610839
O	8.545867	1.130226	0.654151
C	7.400032	0.433024	0.319190
C	6.554982	2.457181	1.216514
H	6.100154	2.587705	2.204274
H	6.201281	3.279141	0.581900
C	7.447871	-0.876124	-0.283463
C	-3.699147	2.179074	-1.763656
C	0.101757	3.130016	1.451480
H	0.027979	4.114020	1.900147
C	-3.761179	-2.103498	1.770738
C	6.208666	-2.795019	-1.180714
H	5.261886	-3.270544	-1.412236
C	6.197694	-1.505279	-0.588654
C	-4.469779	2.336227	-0.514019
C	8.114976	2.443438	1.306942
C	-1.080806	2.432706	1.130119
H	-2.053241	2.863031	1.331194
C	-2.058355	0.903136	-2.888126
H	-1.377892	0.062539	-2.853635
C	-3.835630	3.021832	-2.882049
H	-4.532777	3.850502	-2.864493
C	-5.455776	3.320351	-0.318056

H	-5.696350	4.022482	-1.106794
C	-4.545564	-2.234281	0.526764
H	8.577591	4.536049	1.077113
H	8.507098	3.643325	-0.460278
H	9.911729	3.454621	0.622126
C	-2.156966	1.707004	-4.030695
H	-1.539049	1.487701	-4.894129
C	-3.059559	2.786943	-4.027542
H	-3.157190	3.430783	-4.895318
C	7.418219	-3.437510	-1.459841
H	7.415405	-4.424830	-1.912876
C	1.344335	2.544522	1.191218
H	2.271433	3.051664	1.430505
C	8.668811	-1.537970	-0.571592
H	9.607414	-1.048059	-0.334002
C	-4.881876	-1.396614	-1.657454
H	-4.582803	-0.683532	-2.414015
C	-4.824720	1.504304	1.669491
H	-4.548579	0.778054	2.422174
C	-6.134231	3.389790	0.908369
H	-6.895751	4.145572	1.069566
C	-2.066293	-0.888239	2.881721
H	-1.355932	-0.073093	2.841965
C	-5.903477	-2.323467	-1.899886
H	-6.407052	-2.326002	-2.860026
C	-5.566928	-3.183289	0.338980
H	-5.827380	-3.874734	1.130848
C	8.653644	-2.807444	-1.154843
H	9.587699	-3.315777	-1.376440
C	-5.811518	2.466112	1.919894
H	-6.310184	2.483265	2.882436
C	-2.184733	-1.688259	4.025112
H	-1.552035	-1.491839	4.883339
C	-3.919216	-2.940935	2.890232

H	-4.645932	-3.743890	2.878144
C	-3.125999	-2.734639	4.029450
H	-3.239896	-3.374701	4.898040
C	-6.254101	-3.231732	-0.883613
H	-7.043130	-3.960123	-1.038498
H	-0.137053	-4.168572	-1.924781
C	1.240246	-2.660883	-1.199599
H	2.145866	-3.206621	-1.436385
C	8.824347	3.585349	0.587588
C	-1.178956	-2.447173	-1.149198
H	-2.167972	-2.835025	-1.355477
C	-0.024348	-3.191128	-1.469759
H	8.456647	2.356848	2.342859

VIBRATIONAL ANALYSIS
HARMONIC FREQUENCIES in CM⁻¹.

COMPOUND 5

Frequencies --	24.4901	41.3897	65.7676
Frequencies --	73.8953	87.7523	93.9075
Frequencies --	111.1154	130.2425	152.6318
Frequencies --	165.5669	178.2526	199.4334
Frequencies --	207.2268	207.7643	232.8029
Frequencies --	249.6404	262.2346	269.3582
Frequencies --	292.3738	308.1763	337.7469
Frequencies --	357.9594	391.8637	407.3061
Frequencies --	411.2435	418.9972	436.9975
Frequencies --	444.8186	453.0049	457.8423
Frequencies --	464.2324	484.3427	503.4622
Frequencies --	511.2879	547.4858	550.1637
Frequencies --	583.8808	586.1326	597.9003
Frequencies --	610.2566	629.5480	637.6873

Frequencies --	668.7976	679.5192	690.5867
Frequencies --	693.7628	697.0849	722.1047
Frequencies --	746.8543	761.3168	789.9068
Frequencies --	811.7670	824.6462	827.8065
Frequencies --	837.1345	861.0101	866.0129
Frequencies --	870.3410	891.5745	899.6821
Frequencies --	935.4502	958.5429	961.2149
Frequencies --	974.6524	991.4150	994.5653
Frequencies --	997.0122	1012.2691	1016.7313
Frequencies --	1022.2863	1028.2975	1043.7798
Frequencies --	1051.7861	1053.2225	1054.6534
Frequencies --	1055.9605	1065.4443	1067.6862
Frequencies --	1072.2190	1101.1174	1103.2160
Frequencies --	1126.4048	1138.3502	1144.6596
Frequencies --	1150.1021	1170.1691	1190.8532
Frequencies --	1200.8490	1212.8647	1220.3609
Frequencies --	1262.2339	1271.1523	1274.6820
Frequencies --	1278.2668	1300.3148	1307.0295
Frequencies --	1325.5037	1327.7373	1338.4513
Frequencies --	1345.2061	1361.5468	1371.8832
Frequencies --	1391.6569	1393.6213	1403.0315
Frequencies --	1423.3251	1424.5814	1438.2535
Frequencies --	1441.0283	1454.2937	1465.1467
Frequencies --	1471.2717	1483.4637	1492.1270
Frequencies --	1498.0696	1504.6401	1505.7887
Frequencies --	1506.8381	1508.0346	1513.9155
Frequencies --	1525.0679	1538.8939	1547.5558
Frequencies --	1581.2388	1593.4697	1604.3207
Frequencies --	1624.0179	1629.7431	1638.4712
Frequencies --	1658.5579	3049.4865	3050.7671
Frequencies --	3054.3428	3063.7142	3114.2844
Frequencies --	3124.9499	3141.5172	3146.4415
Frequencies --	3147.6606	3150.0880	3205.9526
Frequencies --	3206.4918	3206.6938	3223.9859

Frequencies --	3235.2677	3237.1505	3241.8682
Frequencies --	3251.9134	3252.9216	3255.3765

COMPOUND 6

Frequencies --	17.3238	24.3931	34.1455
Frequencies --	61.0512	76.7191	90.1099
Frequencies --	94.0964	109.8379	127.2854
Frequencies --	136.6203	159.6155	166.2432
Frequencies --	185.3504	199.0753	204.7841
Frequencies --	209.2399	228.1504	241.4793
Frequencies --	258.1501	278.7517	297.6842
Frequencies --	330.1750	347.7417	358.4690
Frequencies --	376.8959	409.6959	411.7218
Frequencies --	419.5013	439.6213	447.0610
Frequencies --	452.0114	458.4506	466.6687
Frequencies --	485.4693	504.9678	511.1498
Frequencies --	545.8737	549.9482	585.2718
Frequencies --	587.0030	597.0694	610.4765
Frequencies --	626.4085	628.5136	638.4635
Frequencies --	677.1925	685.9093	692.5312
Frequencies --	693.6096	698.6912	724.1006
Frequencies --	753.3279	788.6243	798.0779
Frequencies --	811.6336	825.0526	831.0505
Frequencies --	859.8110	864.5245	865.3875
Frequencies --	886.1921	895.4027	932.7173
Frequencies --	951.9328	964.5351	970.8889
Frequencies --	974.1408	992.9104	993.7504
Frequencies --	1007.0922	1011.7901	1017.4161
Frequencies --	1026.9914	1036.7655	1046.1816
Frequencies --	1051.4141	1051.5298	1053.4615
Frequencies --	1054.2384	1066.4123	1072.9975
Frequencies --	1101.1121	1102.4346	1124.8029
Frequencies --	1138.4725	1144.3685	1150.9536

Frequencies --	1170.2947	1188.1011	1200.0784
Frequencies --	1204.1265	1212.0281	1220.4993
Frequencies --	1248.2924	1260.6828	1267.4165
Frequencies --	1274.9742	1305.6881	1317.2355
Frequencies --	1327.4392	1330.5123	1339.2028
Frequencies --	1346.3174	1360.3737	1375.8904
Frequencies --	1393.6702	1402.1594	1423.7093
Frequencies --	1427.8889	1442.3030	1444.2092
Frequencies --	1456.7717	1465.3680	1472.0569
Frequencies --	1484.5349	1491.3879	1495.1295
Frequencies --	1504.9290	1505.8971	1508.9168
Frequencies --	1513.9764	1530.1229	1540.4532
Frequencies --	1549.8587	1582.1421	1593.8223
Frequencies --	1606.2827	1623.6258	1632.8371
Frequencies --	1639.4402	1659.8792	3039.8327
Frequencies --	3061.3656	3065.9438	3147.6303
Frequencies --	3150.2691	3156.3552	3165.8792
Frequencies --	3166.5793	3172.7682	3206.9366
Frequencies --	3207.4178	3208.2015	3225.1125
Frequencies --	3236.5025	3236.9964	3241.8831
Frequencies --	3251.3607	3254.1252	3254.7782

COMPOUND 7

Frequencies --	18.8130	30.5755	41.1534
Frequencies --	61.6809	78.4211	90.5563
Frequencies --	98.6876	109.2044	129.1048
Frequencies --	140.4665	163.5227	172.5664
Frequencies --	191.1133	203.5855	205.0604
Frequencies --	216.3645	235.1806	252.8721
Frequencies --	259.8226	282.1742	297.0172
Frequencies --	332.9432	347.8941	362.1302
Frequencies --	372.7277	410.2112	412.3848
Frequencies --	418.7960	439.4673	448.5764

Frequencies --	451.9868	458.4856	468.3000
Frequencies --	486.0028	505.2579	511.0836
Frequencies --	548.4138	556.9626	585.1962
Frequencies --	587.7734	597.2945	609.9071
Frequencies --	629.5351	633.8716	638.8174
Frequencies --	678.3322	687.0647	692.3070
Frequencies --	693.6162	699.4458	724.5960
Frequencies --	753.1397	789.0703	802.2128
Frequencies --	811.5760	824.8625	831.6712
Frequencies --	860.1412	865.2737	867.2075
Frequencies --	886.8781	897.0901	934.1198
Frequencies --	954.3639	965.9904	972.8312
Frequencies --	975.0302	994.4593	995.2514
Frequencies --	1005.9941	1012.1652	1017.2311
Frequencies --	1027.0752	1038.2365	1047.6247
Frequencies --	1051.4727	1052.4960	1054.0152
Frequencies --	1054.5874	1067.1723	1075.5747
Frequencies --	1101.0844	1102.6381	1126.0195
Frequencies --	1138.9010	1144.5620	1156.4396
Frequencies --	1173.0652	1197.9841	1205.0292
Frequencies --	1211.1482	1212.4687	1220.4074
Frequencies --	1257.0911	1264.1843	1270.0979
Frequencies --	1275.4089	1306.1200	1321.8831
Frequencies --	1327.9789	1333.3782	1340.0736
Frequencies --	1346.3041	1360.4848	1378.0089
Frequencies --	1393.5976	1402.4213	1423.7353
Frequencies --	1430.5193	1442.3345	1445.3828
Frequencies --	1456.8779	1465.3771	1471.9996
Frequencies --	1483.5172	1493.5505	1494.3295
Frequencies --	1504.8811	1506.6540	1509.1094
Frequencies --	1513.8187	1528.7119	1540.4001
Frequencies --	1550.0633	1582.1575	1593.7905
Frequencies --	1606.2502	1623.3686	1632.9663
Frequencies --	1639.4580	1659.7708	3044.8983

Frequencies --	3062.6204	3067.1665	3145.1321
Frequencies --	3151.8135	3157.5384	3164.7301
Frequencies --	3176.7032	3178.7714	3206.5552
Frequencies --	3207.2325	3208.3802	3225.4492
Frequencies --	3236.1399	3237.2484	3242.6004
Frequencies --	3252.0472	3253.8868	3255.0476

COMPOUND 10

Frequencies --	19.7120	33.3655	49.3324
Frequencies --	85.4374	86.3733	95.1199
Frequencies --	113.4851	134.7545	148.4376
Frequencies --	153.0503	200.5984	204.7041
Frequencies --	214.5029	223.2984	257.0848
Frequencies --	266.7917	277.5407	285.1481
Frequencies --	326.4238	335.9882	345.7462
Frequencies --	390.9793	410.5964	410.7468
Frequencies --	432.5882	444.8067	446.9546
Frequencies --	452.3399	459.5716	464.5146
Frequencies --	487.8799	508.9499	530.6562
Frequencies --	564.1130	579.9033	598.1518
Frequencies --	610.0227	625.5573	629.9793
Frequencies --	640.0377	677.3724	684.0711
Frequencies --	685.3117	692.2997	703.5136
Frequencies --	728.1093	752.4230	755.7532
Frequencies --	789.7727	811.7231	823.3376
Frequencies --	829.2743	851.7783	860.9528
Frequencies --	866.2985	886.6006	892.4664
Frequencies --	941.6593	959.3064	966.6389
Frequencies --	974.7823	979.3187	986.2563
Frequencies --	994.6634	1013.3827	1014.9659
Frequencies --	1025.9872	1027.2607	1040.0372
Frequencies --	1051.0146	1053.6375	1054.6424
Frequencies --	1055.9865	1055.9928	1067.1725

Frequencies --	1095.3339	1100.9923	1115.3801
Frequencies --	1137.7539	1142.0404	1147.1295
Frequencies --	1150.0978	1187.4033	1202.6352
Frequencies --	1213.2112	1220.1773	1263.9396
Frequencies --	1268.6858	1276.3086	1305.8037
Frequencies --	1309.8402	1312.2235	1327.2798
Frequencies --	1333.3510	1342.5879	1360.4738
Frequencies --	1369.5049	1389.1361	1404.1437
Frequencies --	1421.2041	1425.7474	1437.9745
Frequencies --	1441.5578	1458.7064	1465.6382
Frequencies --	1478.0072	1491.2636	1493.5544
Frequencies --	1499.6452	1505.9153	1507.5010
Frequencies --	1509.0145	1513.4114	1517.3048
Frequencies --	1542.6514	1560.5335	1581.0180
Frequencies --	1593.4706	1601.9467	1623.2802
Frequencies --	1634.3226	1643.2459	1668.7122
Frequencies --	3046.6700	3051.7962	3066.5005
Frequencies --	3113.0471	3137.9640	3143.4584
Frequencies --	3145.6226	3150.2387	3206.3749
Frequencies --	3206.8544	3208.0848	3223.1245
Frequencies --	3235.2044	3236.2625	3236.6741
Frequencies --	3244.6418	3252.7593	3253.8039

COMPOUND 13

Frequencies --	21.5698	34.6248	51.7838
Frequencies --	86.5695	90.1111	104.1637
Frequencies --	112.6813	136.1566	151.2907
Frequencies --	167.8082	205.2486	212.0803
Frequencies --	222.5338	247.7302	263.4364
Frequencies --	285.6974	296.5088	344.6080
Frequencies --	351.4867	386.0901	410.5179
Frequencies --	412.7955	444.0826	447.2761
Frequencies --	451.5090	457.0689	470.8915

Frequencies --	487.3874	507.9796	535.7347
Frequencies --	559.6446	579.6676	597.2827
Frequencies --	610.0966	630.6998	635.6616
Frequencies --	661.0419	676.7310	686.7681
Frequencies --	688.9238	693.4206	724.4902
Frequencies --	732.7041	751.2059	787.8164
Frequencies --	789.0185	810.8447	823.5503
Frequencies --	830.3199	860.4533	866.0860
Frequencies --	881.9899	885.4004	904.0558
Frequencies --	943.9588	963.8823	966.8960
Frequencies --	974.5069	993.7509	1012.9367
Frequencies --	1014.7874	1024.6045	1025.7969
Frequencies --	1049.2648	1051.8721	1052.3948
Frequencies --	1053.5447	1054.8328	1057.1100
Frequencies --	1067.9368	1095.4744	1100.7809
Frequencies --	1113.4457	1116.0491	1138.4482
Frequencies --	1143.1740	1151.8342	1158.6702
Frequencies --	1197.7600	1211.0929	1218.2244
Frequencies --	1229.2734	1264.3216	1272.5651
Frequencies --	1299.4747	1304.9747	1323.3084
Frequencies --	1329.6556	1335.7290	1342.4312
Frequencies --	1360.3080	1367.4395	1382.7897
Frequencies --	1389.4917	1408.9663	1421.2223
Frequencies --	1433.1336	1441.6867	1458.1491
Frequencies --	1465.3507	1477.3627	1490.8032
Frequencies --	1496.9834	1505.8992	1507.0553
Frequencies --	1509.5140	1513.9077	1542.9234
Frequencies --	1560.6624	1581.0921	1593.5937
Frequencies --	1602.0328	1623.0042	1634.2011
Frequencies --	1643.3823	1668.9259	3050.2739
Frequencies --	3066.1391	3109.1509	3125.0901
Frequencies --	3142.1686	3152.4574	3206.5916
Frequencies --	3207.1544	3208.4656	3223.3623
Frequencies --	3236.0246	3236.6267	3236.7932

Frequencies --	3244.7008	3253.6872	3254.4496
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COMPOUND 14

Frequencies --	12.4280	17.4180	32.4564
Frequencies --	35.5578	36.0044	38.7648
Frequencies --	44.2610	52.6227	65.8960
Frequencies --	71.8295	73.8332	81.8931
Frequencies --	86.1232	93.4367	118.5710
Frequencies --	122.8463	124.6053	129.4501
Frequencies --	151.3686	164.7222	168.9665
Frequencies --	172.9760	176.7190	180.2234
Frequencies --	183.8654	194.7337	197.5691
Frequencies --	211.2001	220.5936	227.5637
Frequencies --	231.0410	236.3486	247.3807
Frequencies --	261.9084	263.1328	279.0791
Frequencies --	281.2173	287.9035	303.0845
Frequencies --	320.1485	325.7213	330.3500
Frequencies --	342.2600	366.8155	367.9607
Frequencies --	369.8130	373.1052	395.6306
Frequencies --	409.2831	423.6250	436.1598
Frequencies --	438.4455	440.4033	442.7346
Frequencies --	449.2616	458.7455	465.3024
Frequencies --	467.5909	470.0905	477.0176
Frequencies --	483.6985	484.5918	498.8334
Frequencies --	501.1113	502.6932	509.0537
Frequencies --	545.5138	554.6193	563.2514
Frequencies --	573.4445	575.8568	583.6993
Frequencies --	586.3525	588.4140	631.6206
Frequencies --	642.0226	655.2454	658.6182
Frequencies --	663.8226	666.5090	666.9156
Frequencies --	669.9173	675.9466	679.4526
Frequencies --	680.2066	693.9521	696.6405
Frequencies --	727.7173	735.9421	743.2446

Frequencies --	760.6427	766.0359	767.9390
Frequencies --	771.3405	777.7795	778.5606
Frequencies --	779.4134	781.8266	794.7489
Frequencies --	796.4248	806.9080	823.3730
Frequencies --	833.1108	835.2390	836.7332
Frequencies --	838.7264	841.0014	862.5935
Frequencies --	873.6757	885.1503	905.0467
Frequencies --	925.8186	927.3410	931.6010
Frequencies --	933.0203	935.8667	938.3406
Frequencies --	960.3109	962.8132	992.3630
Frequencies --	995.7827	998.2570	1004.1504
Frequencies --	1008.4223	1012.3005	1012.6725
Frequencies --	1016.0998	1016.4217	1019.3967
Frequencies --	1022.9268	1026.3379	1027.7316
Frequencies --	1033.5733	1042.3344	1050.6015
Frequencies --	1050.8366	1051.1629	1052.1439
Frequencies --	1052.6398	1053.5638	1054.6324
Frequencies --	1054.7580	1059.8499	1065.9483
Frequencies --	1066.5813	1066.6979	1070.3650
Frequencies --	1081.2347	1082.3086	1083.5191
Frequencies --	1093.1531	1093.9016	1117.4983
Frequencies --	1118.3765	1127.7199	1132.0937
Frequencies --	1133.2038	1142.0840	1152.0264
Frequencies --	1152.9391	1153.7350	1154.3724
Frequencies --	1175.0528	1188.9683	1200.8313
Frequencies --	1204.5915	1204.8129	1213.1199
Frequencies --	1215.6759	1220.9765	1222.9443
Frequencies --	1261.8005	1271.7651	1273.7858
Frequencies --	1285.9356	1299.8038	1304.0038
Frequencies --	1304.8579	1306.1868	1309.0081
Frequencies --	1320.9495	1324.3306	1325.1214
Frequencies --	1325.3805	1328.4723	1345.0112
Frequencies --	1347.4016	1353.2971	1354.4286
Frequencies --	1355.4038	1355.9372	1360.5023

Frequencies --	1372.7933	1392.5693	1394.1621
Frequencies --	1403.3280	1428.1761	1429.2484
Frequencies --	1441.6083	1448.8750	1457.1842
Frequencies --	1459.8289	1460.8538	1474.9555
Frequencies --	1475.9410	1476.3303	1481.1713
Frequencies --	1483.2706	1491.9392	1496.1335
Frequencies --	1498.8489	1499.1412	1506.0549
Frequencies --	1507.9839	1508.8922	1510.5174
Frequencies --	1525.1963	1525.6416	1527.0369
Frequencies --	1527.6017	1540.0955	1544.4697
Frequencies --	1594.2434	1595.7235	1596.2738
Frequencies --	1605.6037	1606.0803	1607.6336
Frequencies --	1615.1019	1625.5339	1628.8801
Frequencies --	1639.2089	1642.0708	1642.8835
Frequencies --	1643.8315	1644.7722	1657.6310
Frequencies --	3051.0536	3051.9933	3055.3354
Frequencies --	3064.5479	3113.8028	3126.4113
Frequencies --	3142.0250	3147.7046	3148.1122
Frequencies --	3151.0260	3208.7259	3225.5423
Frequencies --	3235.9747	3236.5133	3237.0872
Frequencies --	3237.7796	3242.2595	3244.1620
Frequencies --	3245.0949	3250.2716	3250.7696
Frequencies --	3252.8088	3252.9302	3253.3887
Frequencies --	3259.1610	3259.8003	3260.7248
Frequencies --	3261.1007	3267.3189	3267.6029
Frequencies --	3274.0542	3275.4092	3277.1025
Frequencies --	3277.3412	3278.8185	3279.8250

COMPOUND 15

Frequencies --	12.5838	13.7940	25.3094
Frequencies --	31.8090	34.5469	37.4651
Frequencies --	38.3237	45.2604	51.6429
Frequencies --	56.8521	71.1330	85.4801

Frequencies --	86.3070	90.7493	96.8465
Frequencies --	113.1715	124.0372	127.0182
Frequencies --	129.8478	145.1071	160.9949
Frequencies --	168.6192	173.2732	175.5087
Frequencies --	178.8178	183.7820	190.4026
Frequencies --	197.9696	199.5214	213.3770
Frequencies --	223.3509	229.0404	232.7787
Frequencies --	233.7084	245.9443	252.3201
Frequencies --	266.5302	279.2789	281.6138
Frequencies --	305.2377	309.8382	325.8943
Frequencies --	331.0597	341.9155	343.1376
Frequencies --	360.5340	368.3488	372.3862
Frequencies --	378.4925	379.2580	411.6989
Frequencies --	425.6585	435.7729	440.8639
Frequencies --	442.2508	443.4566	454.0680
Frequencies --	460.1764	463.9534	468.3899
Frequencies --	470.3770	477.9802	484.1220
Frequencies --	484.8191	499.3111	501.2342
Frequencies --	503.6359	510.8464	543.2561
Frequencies --	553.0575	563.7584	575.1197
Frequencies --	575.4433	584.3452	587.5794
Frequencies --	589.6635	627.0681	631.6317
Frequencies --	642.4513	655.1935	658.8845
Frequencies --	663.5980	666.3737	666.7883
Frequencies --	676.3725	678.7173	680.5345
Frequencies --	686.8913	694.1856	698.6822
Frequencies --	730.7630	737.1658	746.7510
Frequencies --	766.4708	769.1315	770.8938
Frequencies --	777.8863	777.9546	779.0791
Frequencies --	782.0282	795.6056	796.4139
Frequencies --	800.2435	807.5956	824.1753
Frequencies --	836.4393	837.1557	840.1853
Frequencies --	841.1243	862.7623	866.9561
Frequencies --	880.5064	900.7740	925.6275

Frequencies --	930.3112	931.5355	932.1374
Frequencies --	933.6416	936.3373	951.5258
Frequencies --	964.7815	971.5259	994.5419
Frequencies --	1000.8631	1002.7486	1008.4875
Frequencies --	1012.0986	1012.5760	1012.9697
Frequencies --	1014.1054	1016.3559	1019.5070
Frequencies --	1026.7970	1027.8768	1033.9413
Frequencies --	1040.4199	1043.4118	1050.3100
Frequencies --	1051.3955	1051.7341	1052.0212
Frequencies --	1054.3932	1054.6889	1054.8311
Frequencies --	1055.4717	1059.5197	1065.6656
Frequencies --	1066.6645	1071.6793	1082.2747
Frequencies --	1083.0926	1083.8791	1093.0423
Frequencies --	1093.3440	1116.6666	1117.4984
Frequencies --	1127.7384	1132.1918	1133.2355
Frequencies --	1144.0202	1152.0577	1152.9790
Frequencies --	1153.4056	1156.6079	1175.6679
Frequencies --	1187.6174	1202.5503	1203.5536
Frequencies --	1203.7326	1205.6254	1213.7843
Frequencies --	1214.8031	1220.9971	1222.5080
Frequencies --	1249.0783	1262.8696	1268.5381
Frequencies --	1283.4560	1305.5289	1306.4595
Frequencies --	1306.8220	1309.1544	1316.9087
Frequencies --	1321.8854	1325.2853	1325.8862
Frequencies --	1326.6692	1333.5323	1345.8382
Frequencies --	1347.0065	1353.8657	1354.5052
Frequencies --	1354.8413	1357.9885	1359.9882
Frequencies --	1378.3413	1395.2881	1402.7108
Frequencies --	1429.3705	1430.9906	1447.7546
Frequencies --	1451.3437	1459.5920	1460.1981
Frequencies --	1461.4201	1475.4273	1476.1422
Frequencies --	1477.4311	1481.6814	1484.5638
Frequencies --	1492.8402	1495.7499	1496.2652
Frequencies --	1499.6021	1506.5751	1509.4821

Frequencies --	1510.2855	1526.3518	1527.2408
Frequencies --	1527.5279	1529.4498	1541.9147
Frequencies --	1547.5505	1595.7603	1596.2228
Frequencies --	1596.9801	1605.7329	1606.2348
Frequencies --	1608.1265	1615.4077	1627.8331
Frequencies --	1629.9548	1640.0968	1642.2066
Frequencies --	1643.2432	1644.2246	1644.6146
Frequencies --	1659.0184	3040.6064	3062.2584
Frequencies --	3066.8715	3147.9255	3151.2794
Frequencies --	3157.4304	3166.5069	3171.1201
Frequencies --	3175.0823	3209.6734	3226.5123
Frequencies --	3235.5833	3235.6637	3237.2427
Frequencies --	3237.3717	3243.3140	3244.2535
Frequencies --	3245.1353	3249.0785	3249.4884
Frequencies --	3252.7098	3252.9471	3253.1457
Frequencies --	3258.2847	3259.2764	3259.3546
Frequencies --	3259.9760	3266.7939	3267.5266
Frequencies --	3272.8049	3274.5941	3275.6941
Frequencies --	3277.0844	3278.8008	3279.2491

COMPOUND 16

Frequencies --	10.4339	13.4465	28.0614
Frequencies --	31.1657	34.7857	37.6273
Frequencies --	40.7460	43.4112	49.5188
Frequencies --	56.8437	68.3379	79.0839
Frequencies --	84.2114	88.2244	98.8649
Frequencies --	113.8284	119.2174	126.5580
Frequencies --	129.8477	148.1344	162.4424
Frequencies --	167.6777	171.9692	173.5844
Frequencies --	178.5974	182.7159	189.8571
Frequencies --	196.6779	198.2660	214.0961
Frequencies --	226.1114	229.7827	231.8615
Frequencies --	235.3202	246.8077	257.6797

Frequencies --	272.1789	278.0670	281.6415
Frequencies --	304.5243	310.5918	326.5260
Frequencies --	331.2422	342.2564	344.9727
Frequencies --	361.2627	367.6241	371.9636
Frequencies --	375.1022	378.3909	413.9288
Frequencies --	426.6379	435.6424	439.2461
Frequencies --	441.4591	442.8369	454.9017
Frequencies --	459.8784	464.0940	467.8334
Frequencies --	470.5345	478.7353	483.8416
Frequencies --	486.0034	498.8845	501.0997
Frequencies --	503.4553	511.2955	547.3972
Frequencies --	557.8849	564.0360	573.9160
Frequencies --	575.0435	583.3854	587.3176
Frequencies --	590.3105	630.5977	634.1051
Frequencies --	642.5353	655.1292	658.6388
Frequencies --	663.5518	666.2980	666.7248
Frequencies --	675.6792	679.1204	679.9957
Frequencies --	688.6721	694.4124	699.0405
Frequencies --	730.7756	736.7900	746.5988
Frequencies --	765.4799	768.0510	769.4876
Frequencies --	777.4948	777.8515	779.4259
Frequencies --	783.6745	796.0161	797.1938
Frequencies --	802.2879	807.5817	823.8365
Frequencies --	835.7344	836.5852	838.5430
Frequencies --	840.9198	860.3810	869.5015
Frequencies --	881.0142	901.9386	925.4622
Frequencies --	928.9572	931.7131	933.7393
Frequencies --	935.2801	937.5335	954.2548
Frequencies --	966.1864	973.5274	994.6563
Frequencies --	995.8570	1003.1192	1006.9876
Frequencies --	1009.8848	1011.9951	1013.0025
Frequencies --	1014.2510	1016.5783	1019.6412
Frequencies --	1026.7503	1028.1978	1033.7232
Frequencies --	1039.2594	1042.9706	1049.4549

Frequencies --	1050.2189	1051.5602	1053.0799
Frequencies --	1054.5144	1055.2319	1055.3034
Frequencies --	1055.5763	1059.5809	1065.4389
Frequencies --	1066.2955	1072.9282	1081.4020
Frequencies --	1081.9704	1083.5609	1093.3700
Frequencies --	1094.2494	1115.6435	1117.7079
Frequencies --	1128.3373	1131.5173	1132.8291
Frequencies --	1144.5129	1151.7565	1152.7186
Frequencies --	1153.3001	1159.9252	1176.1712
Frequencies --	1200.2571	1203.8358	1204.1405
Frequencies --	1204.8862	1211.0179	1213.2123
Frequencies --	1214.8262	1219.5123	1222.2667
Frequencies --	1255.9361	1262.7137	1268.9367
Frequencies --	1283.6620	1304.5964	1305.8259
Frequencies --	1306.8371	1309.1322	1319.1854
Frequencies --	1322.9383	1324.8583	1325.7227
Frequencies --	1326.0314	1335.9947	1344.9504
Frequencies --	1346.9465	1353.4090	1355.0891
Frequencies --	1355.3917	1358.4452	1360.7688
Frequencies --	1379.5204	1394.5318	1402.6391
Frequencies --	1429.3810	1432.3309	1448.5810
Frequencies --	1450.7220	1459.4513	1460.1145
Frequencies --	1460.8240	1475.0151	1475.8226
Frequencies --	1476.3950	1481.1529	1483.9110
Frequencies --	1492.6462	1494.0966	1496.2240
Frequencies --	1499.5592	1506.8226	1509.3348
Frequencies --	1510.0566	1526.2067	1526.7874
Frequencies --	1527.8106	1529.5678	1541.6647
Frequencies --	1547.4973	1595.5054	1595.9175
Frequencies --	1597.0303	1605.5399	1605.9090
Frequencies --	1608.0409	1615.1401	1627.9696
Frequencies --	1630.1790	1640.1498	1642.2094
Frequencies --	1643.2083	1644.4899	1645.0018
Frequencies --	1659.0714	3046.1420	3064.3443

Frequencies --	3068.0772	3144.9635	3153.0005
Frequencies --	3159.1065	3166.6503	3176.6744
Frequencies --	3178.9883	3209.9861	3226.9115
Frequencies --	3236.1183	3236.5996	3237.3610
Frequencies --	3237.7486	3243.6333	3244.5960
Frequencies --	3245.2350	3250.0870	3250.9260
Frequencies --	3252.8289	3253.0090	3254.0260
Frequencies --	3259.0129	3259.5407	3260.6008
Frequencies --	3261.7227	3267.2756	3267.5777
Frequencies --	3272.8206	3273.3046	3275.4338
Frequencies --	3277.1257	3277.5859	3277.9099

COMPOUND 17

Frequencies --	13.4940	16.7246	29.2953
Frequencies --	32.4810	35.6377	38.0866
Frequencies --	41.2279	52.4235	53.5560
Frequencies --	72.7748	80.7431	82.4648
Frequencies --	91.7651	94.7547	118.9058
Frequencies --	122.9383	126.7426	130.0547
Frequencies --	143.8049	161.1247	172.2540
Frequencies --	173.3293	179.2116	183.3548
Frequencies --	193.0615	198.4440	210.5513
Frequencies --	216.7972	229.3729	230.8208
Frequencies --	238.0740	248.4225	259.6787
Frequencies --	260.9260	279.1557	281.3949
Frequencies --	299.3806	303.1095	315.3221
Frequencies --	326.8145	337.6888	342.7979
Frequencies --	360.8951	367.7314	369.5970
Frequencies --	373.1763	393.3786	417.1655
Frequencies --	432.5227	435.7100	439.6585
Frequencies --	442.5102	446.5840	448.4951
Frequencies --	459.1932	465.9184	469.4065
Frequencies --	469.4626	478.7460	484.0416

Frequencies --	486.5876	499.4283	501.5886
Frequencies --	504.7141	535.5681	548.1994
Frequencies --	573.3125	575.7023	578.6078
Frequencies --	579.6580	586.5039	628.8451
Frequencies --	631.6443	641.8150	655.4025
Frequencies --	658.7031	663.7810	666.5524
Frequencies --	666.9517	675.9832	677.7949
Frequencies --	680.2626	683.8543	687.5987
Frequencies --	702.0578	733.0119	736.1938
Frequencies --	744.6525	758.0004	766.1113
Frequencies --	767.8158	771.3667	777.7715
Frequencies --	778.6537	779.7161	781.8999
Frequencies --	794.6808	796.1785	806.6369
Frequencies --	821.0613	835.0438	836.4931
Frequencies --	836.7641	840.8433	853.0385
Frequencies --	862.3775	877.2393	901.8551
Frequencies --	926.9512	927.6716	932.2967
Frequencies --	932.7585	934.6630	942.0525
Frequencies --	958.0037	972.0187	977.5793
Frequencies --	989.2312	995.3178	998.1751
Frequencies --	1008.7340	1011.8622	1012.9790
Frequencies --	1014.8388	1016.3363	1019.4083
Frequencies --	1022.4475	1025.4843	1033.5853
Frequencies --	1039.2279	1040.7294	1046.2522
Frequencies --	1050.5266	1050.5769	1051.2198
Frequencies --	1052.2111	1053.5191	1054.3538
Frequencies --	1054.4210	1054.8230	1062.0305
Frequencies --	1066.2032	1066.7252	1078.6304
Frequencies --	1082.3468	1083.6833	1093.1482
Frequencies --	1094.0089	1103.0372	1118.2737
Frequencies --	1124.1660	1132.3068	1133.2711
Frequencies --	1139.1212	1148.3655	1152.0136
Frequencies --	1153.0688	1153.9254	1158.0859
Frequencies --	1189.2901	1202.5682	1204.7491

Frequencies --	1205.0242	1213.4940	1215.7710
Frequencies --	1220.5797	1222.6957	1264.7223
Frequencies --	1269.6623	1284.6983	1303.7563
Frequencies --	1304.7633	1306.2797	1306.4716
Frequencies --	1309.0191	1317.4246	1322.4828
Frequencies --	1324.3488	1325.2189	1325.3265
Frequencies --	1339.0954	1346.8162	1352.5786
Frequencies --	1354.2706	1355.4344	1356.3390
Frequencies --	1360.3132	1372.2689	1391.6362
Frequencies --	1404.7043	1426.8478	1427.5826
Frequencies --	1439.2668	1446.8316	1459.8531
Frequencies --	1460.7815	1465.3689	1475.5837
Frequencies --	1476.0664	1479.6005	1480.9727
Frequencies --	1493.1011	1494.0813	1496.2624
Frequencies --	1499.0962	1499.7859	1505.4918
Frequencies --	1510.4377	1510.8658	1519.3982
Frequencies --	1525.6614	1527.1058	1528.4761
Frequencies --	1541.8814	1560.5301	1593.4296
Frequencies --	1595.7748	1596.2743	1605.6645
Frequencies --	1606.0767	1607.2100	1615.0674
Frequencies --	1627.6343	1631.2306	1641.9686
Frequencies --	1642.8560	1643.2194	1643.8974
Frequencies --	1644.7193	1666.4168	3048.6814
Frequencies --	3052.9705	3068.0625	3116.6201
Frequencies --	3139.8686	3144.2018	3147.6043
Frequencies --	3151.3672	3210.4360	3224.9222
Frequencies --	3235.9808	3236.4108	3237.0897
Frequencies --	3237.7214	3237.7376	3243.9848
Frequencies --	3244.7680	3245.9095	3250.4428
Frequencies --	3250.7985	3252.7688	3253.3443
Frequencies --	3258.7333	3259.4837	3260.8872
Frequencies --	3261.1589	3267.3230	3267.6584
Frequencies --	3273.2850	3274.5820	3277.3321
Frequencies --	3277.4451	3278.3519	3279.0301

COMPOUND 18

Frequencies --	12.2151	17.0323	33.6827
Frequencies --	34.0001	35.0866	41.4463
Frequencies --	42.4955	52.8315	54.4199
Frequencies --	75.7396	82.3250	83.9639
Frequencies --	93.7457	105.9336	123.3256
Frequencies --	126.9254	129.6637	133.3548
Frequencies --	147.8360	166.2547	174.7317
Frequencies --	179.4703	183.7545	188.0398
Frequencies --	195.4043	201.5271	215.8361
Frequencies --	231.0150	231.9096	240.1229
Frequencies --	250.3257	254.1418	267.0576
Frequencies --	280.8151	283.1278	303.3245
Frequencies --	308.6206	327.0279	342.4334
Frequencies --	349.2550	360.9560	363.6218
Frequencies --	368.4155	373.2423	390.0836
Frequencies --	420.2215	435.3023	440.6289
Frequencies --	442.8302	445.9307	453.9953
Frequencies --	460.3172	464.2433	469.2893
Frequencies --	472.7805	478.5762	484.4780
Frequencies --	487.0561	499.2864	501.2583
Frequencies --	505.1617	541.8246	549.0513
Frequencies --	573.7706	574.6094	575.5053
Frequencies --	578.9626	586.5285	631.7586
Frequencies --	640.1434	655.3279	658.4943
Frequencies --	660.8600	664.4571	666.5955
Frequencies --	666.8543	675.8810	676.8162
Frequencies --	680.0056	687.6424	694.3367
Frequencies --	720.6380	734.5796	742.8515
Frequencies --	743.8566	766.8482	768.3351
Frequencies --	771.0310	777.5992	778.6514
Frequencies --	781.1227	783.1806	787.4215

Frequencies --	795.3751	796.2827	806.0336
Frequencies --	821.6586	835.5599	836.4373
Frequencies --	839.3575	840.0563	861.0054
Frequencies --	877.3880	886.7836	909.8553
Frequencies --	926.7229	931.4703	932.9542
Frequencies --	933.3143	934.5624	944.5439
Frequencies --	962.6650	972.0319	996.2584
Frequencies --	998.8468	1011.6832	1012.2793
Frequencies --	1012.7692	1015.4420	1016.6391
Frequencies --	1019.7675	1022.2281	1026.0186
Frequencies --	1033.6733	1038.8681	1045.9203
Frequencies --	1049.6705	1049.8311	1051.2060
Frequencies --	1051.5862	1051.8330	1053.9036
Frequencies --	1053.9476	1054.4614	1056.7869
Frequencies --	1062.0297	1066.1076	1066.7042
Frequencies --	1079.7606	1083.5186	1084.5575
Frequencies --	1093.5087	1094.3543	1103.5443
Frequencies --	1116.8644	1118.3215	1123.2454
Frequencies --	1132.0461	1132.7587	1144.4486
Frequencies --	1149.8216	1152.4760	1153.4040
Frequencies --	1153.9685	1165.1673	1199.9215
Frequencies --	1204.2581	1204.5082	1215.3327
Frequencies --	1215.8973	1219.1193	1222.3450
Frequencies --	1230.0062	1264.3232	1280.2137
Frequencies --	1300.5423	1305.2299	1305.7968
Frequencies --	1308.2077	1310.3568	1318.9361
Frequencies --	1322.1738	1325.6855	1325.9307
Frequencies --	1333.5489	1339.0441	1347.0369
Frequencies --	1353.2761	1355.6868	1356.5683
Frequencies --	1359.9014	1361.2042	1369.6933
Frequencies --	1385.2949	1392.2351	1409.6251
Frequencies --	1428.2432	1434.1481	1447.3348
Frequencies --	1460.0432	1460.8061	1465.7331
Frequencies --	1475.1070	1475.6171	1479.8332

Frequencies -- 1481.1717	1493.9897	1496.7618
Frequencies -- 1497.4004	1500.0288	1506.0550
Frequencies -- 1510.0769	1512.4664	1526.8457
Frequencies -- 1527.7077	1528.8272	1542.3639
Frequencies -- 1560.6878	1593.6101	1595.7613
Frequencies -- 1596.2732	1605.5493	1605.9667
Frequencies -- 1607.1616	1615.3763	1628.0573
Frequencies -- 1631.6819	1642.1930	1643.0561
Frequencies -- 1643.6462	1644.5693	1644.9140
Frequencies -- 1667.0298	3050.6226	3068.1745
Frequencies -- 3111.5211	3127.1127	3142.3983
Frequencies -- 3153.2969	3210.7226	3225.3244
Frequencies -- 3236.2252	3236.3918	3237.6543
Frequencies -- 3237.8514	3238.3561	3243.4885
Frequencies -- 3244.4549	3246.3781	3250.7897
Frequencies -- 3251.0756	3253.0870	3253.4068
Frequencies -- 3258.4503	3259.0092	3261.3012
Frequencies -- 3261.6062	3268.0153	3268.2660
Frequencies -- 3272.4064	3273.5606	3276.0873
Frequencies -- 3277.7018	3278.4093	3279.3181