

Modeling Organic Electrochromic Materials through TDDFT

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DFT Gaussian Setup:

```
opt cc-pvdz scrf=(cpcm,solvent=dichloromethane) geom=connectivity
mpwlpbe
```

TDDFT Gaussian Setup:

```
td=(nstates=13)/cc-pvdz scrf=(cpcm,solvent=dichloromethane)
geom=connectivity mpwlpbe
```

neutral: charge 0 multiplicity 1

cation: charge 1 multiplicity 2

dication: charge 2 multiplicity 1

Cyan Cartesian Coordinates – N = 1

```
C      5.31543  2.25434  0.82958
C      5.13799  0.9282   0.54655
S      3.83964  3.13549  0.76221
C      3.76908  0.60948  0.26812
O      6.16917  0.04547  0.51121
C      2.91405  1.70148  0.3641
O      3.32487 -0.63234 -0.03538
C      5.89254 -1.24038  1.06272
C      1.47025  1.72217  0.18644
C      4.20794 -1.46771 -0.78544
H      6.86259 -1.6359   1.39428
H      5.24237 -1.13235  1.94387
C      5.241   -2.21141  0.06721
C      0.71966  2.94491  0.09099
C      0.70089  0.57041  0.09525
H      3.55661 -2.18765 -1.29932
H      4.72838 -0.86648 -1.54477
C      4.62322 -3.36964  0.85533
C      6.26973 -2.83499 -0.88126
C      -0.71957  2.94497 -0.09107
N      1.2389   4.17032  0.15815
H      1.1961  -0.39408  0.17216
C      -0.7012  0.57046 -0.09364
H      4.23147 -4.12905  0.14903
H      5.41203 -3.86717  1.45651
O      3.5971  -2.90354  1.69143
H      6.97288 -3.46304 -0.29798
H      5.75581 -3.50877 -1.59758
O      6.96638 -1.8305  -1.56997
N      -1.23857  4.17044 -0.15895
C      -1.47037  1.72228 -0.18572
```

S	0.00027	5.22973	-0.00078
H	-1.19659	-0.39399	-0.16982
C	3.03423	-3.93407	2.46504
C	7.91642	-2.35874	-2.46184
C	-2.91415	1.70165	-0.36348
H	2.24961	-3.48664	3.08821
H	2.58356	-4.72037	1.83141
H	3.78662	-4.4094	3.12174
H	8.41103	-1.51239	-2.95502
H	8.67906	-2.96178	-1.93499
H	7.44404	-2.99639	-3.23219
C	-3.76916	0.60962	-0.26769
S	-3.8398	3.13571	-0.76147
C	-5.13809	0.9283	-0.54608
O	-3.32484	-0.63219	0.03568
C	-5.31556	2.25452	-0.82884
O	-6.16924	0.04555	-0.51105
C	-4.20792	-1.46782	0.78546
H	-6.25149	2.74917	-1.07355
C	-5.89253	-1.24019	-1.06271
H	-3.55656	-2.18786	1.29915
H	-4.72839	-0.86681	1.54493
C	-5.24091	-2.21136	-0.06741
H	-6.86255	-1.63577	-1.39431
H	-5.24239	-1.132	-1.94387
C	-4.62304	-3.36934	-0.85582
C	-6.26957	-2.83525	0.88094
H	-4.2314	-4.12899	-0.14972
H	-5.41179	-3.86666	-1.45726
O	-3.59681	-2.90296	-1.69163
H	-6.97261	-3.46333	0.29756
H	-5.75555	-3.50905	1.59717
O	-6.9664	-1.83096	1.56975
C	-3.03396	-3.9332	-2.46564
C	-7.91712	-2.35943	2.46076
H	-2.24936	-3.48554	-3.08867
H	-2.58326	-4.71973	-1.83232
H	-3.78637	-4.40829	-3.12249
H	-8.4119	-1.5132	2.954
H	-8.67952	-2.96208	1.93311
H	-7.44538	-2.9975	3.23114
H	6.25139	2.74899	1.07432

Cyan Energy Levels – N = 1

Alpha occ. eigenvalues -- -89.15641 -89.09455 -89.09454 -19.26667 -19.26666
 Alpha occ. eigenvalues -- -19.25852 -19.25851 -19.23706 -19.23706 -19.23686
 Alpha occ. eigenvalues -- -19.23686 -14.44431 -14.44427 -10.31005 -10.31004
 Alpha occ. eigenvalues -- -10.30447 -10.30446 -10.30238 -10.30203 -10.29875

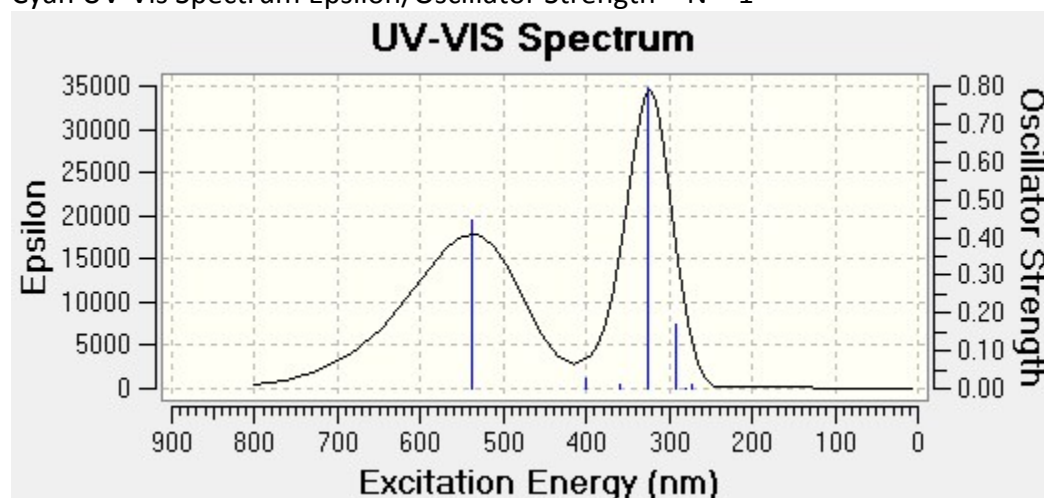
Alpha occ. eigenvalues -- -10.29874 -10.29587 -10.29586 -10.29369 -10.29369
 Alpha occ. eigenvalues -- -10.29363 -10.29363 -10.28255 -10.28254 -10.28239
 Alpha occ. eigenvalues -- -10.28238 -10.28131 -10.28130 -10.27754 -10.27752
 Alpha occ. eigenvalues -- -10.26560 -10.26560 -10.26485 -10.26485 -10.25446
 Alpha occ. eigenvalues -- -10.25401 -8.09644 -8.03775 -8.03775 -6.03628
 Alpha occ. eigenvalues -- -6.03045 -6.02798 -5.97653 -5.97652 -5.97283
 Alpha occ. eigenvalues -- -5.97283 -5.96898 -5.96898 -1.11854 -1.11853
 Alpha occ. eigenvalues -- -1.09368 -1.09366 -1.07862 -1.07862 -1.07687
 Alpha occ. eigenvalues -- -1.07687 -1.05584 -0.93136 -0.91793 -0.90937
 Alpha occ. eigenvalues -- -0.88596 -0.85909 -0.85872 -0.81792 -0.78913
 Alpha occ. eigenvalues -- -0.77726 -0.76512 -0.76307 -0.75429 -0.74609
 Alpha occ. eigenvalues -- -0.74598 -0.72085 -0.71541 -0.71534 -0.69878
 Alpha occ. eigenvalues -- -0.68300 -0.68241 -0.66826 -0.64616 -0.64607
 Alpha occ. eigenvalues -- -0.64069 -0.63905 -0.60533 -0.60496 -0.59620
 Alpha occ. eigenvalues -- -0.59533 -0.58509 -0.57078 -0.54504 -0.53620
 Alpha occ. eigenvalues -- -0.53259 -0.53214 -0.52747 -0.52137 -0.51978
 Alpha occ. eigenvalues -- -0.51380 -0.50376 -0.50322 -0.49605 -0.49529
 Alpha occ. eigenvalues -- -0.48768 -0.48766 -0.48257 -0.48189 -0.47808
 Alpha occ. eigenvalues -- -0.47739 -0.47173 -0.46902 -0.46541 -0.46494
 Alpha occ. eigenvalues -- -0.46149 -0.45820 -0.44274 -0.44042 -0.43698
 Alpha occ. eigenvalues -- -0.42732 -0.42662 -0.42325 -0.41964 -0.41300
 Alpha occ. eigenvalues -- -0.41232 -0.40796 -0.40146 -0.40135 -0.39817
 Alpha occ. eigenvalues -- -0.39647 -0.39419 -0.38640 -0.38463 -0.38219
 Alpha occ. eigenvalues -- -0.37535 -0.37170 -0.36564 -0.36463 -0.36142
 Alpha occ. eigenvalues -- -0.35415 -0.34566 -0.34510 -0.34456 -0.33701
 Alpha occ. eigenvalues -- -0.33346 -0.33170 -0.33168 -0.32251 -0.32107
 Alpha occ. eigenvalues -- -0.31379 -0.30546 -0.30254 -0.28538 -0.27913
 Alpha occ. eigenvalues -- -0.27896 -0.27673 -0.27110 -0.27108 -0.24356
 Alpha occ. eigenvalues -- -0.23115 -0.23112 -0.19920
 Alpha virt. eigenvalues -- -0.09154 -0.03315 -0.00655 0.01454 0.02009
 Alpha virt. eigenvalues -- 0.04017 0.04065 0.05255 0.05969 0.06367
 Alpha virt. eigenvalues -- 0.06965 0.07823 0.07947 0.08032 0.08369
 Alpha virt. eigenvalues -- 0.09691 0.09739 0.09824 0.10039 0.10366
 Alpha virt. eigenvalues -- 0.10386 0.10949 0.11153 0.11726 0.11802
 Alpha virt. eigenvalues -- 0.12004 0.12927 0.13172 0.13370 0.13886
 Alpha virt. eigenvalues -- 0.13932 0.13955 0.14041 0.14069 0.14207
 Alpha virt. eigenvalues -- 0.14231 0.14883 0.14887 0.14969 0.15574
 Alpha virt. eigenvalues -- 0.15813 0.15837 0.16789 0.16900 0.17521
 Alpha virt. eigenvalues -- 0.17858 0.18339 0.18488 0.19155 0.20070
 Alpha virt. eigenvalues -- 0.20245 0.20743 0.20917 0.21593 0.21660
 Alpha virt. eigenvalues -- 0.22706 0.22949 0.23189 0.23513 0.23598
 Alpha virt. eigenvalues -- 0.23973 0.24143 0.26060 0.26242 0.26715
 Alpha virt. eigenvalues -- 0.27093 0.27811 0.28177 0.28279 0.28729
 Alpha virt. eigenvalues -- 0.29161 0.29497 0.29863 0.30368 0.30687
 Alpha virt. eigenvalues -- 0.32868 0.33251 0.36141 0.36166 0.36809
 Alpha virt. eigenvalues -- 0.37982 0.40454 0.40645 0.42469 0.42626
 Alpha virt. eigenvalues -- 0.43035 0.43181 0.43258 0.44211 0.44690
 Alpha virt. eigenvalues -- 0.44882 0.45074 0.45344 0.45508 0.45780

Alpha virt. eigenvalues --	0.46554	0.46568	0.46994	0.47042	0.47155
Alpha virt. eigenvalues --	0.47236	0.47278	0.47429	0.47647	0.48058
Alpha virt. eigenvalues --	0.48138	0.48442	0.48627	0.48799	0.48815
Alpha virt. eigenvalues --	0.49372	0.49488	0.49985	0.50048	0.50391
Alpha virt. eigenvalues --	0.50602	0.50760	0.51286	0.51361	0.51513
Alpha virt. eigenvalues --	0.51803	0.52089	0.52468	0.52597	0.52904
Alpha virt. eigenvalues --	0.53352	0.53696	0.54683	0.55014	0.55195
Alpha virt. eigenvalues --	0.55333	0.55819	0.56003	0.56449	0.56661
Alpha virt. eigenvalues --	0.56725	0.56975	0.57584	0.58339	0.58879
Alpha virt. eigenvalues --	0.59477	0.60068	0.60304	0.60476	0.61029
Alpha virt. eigenvalues --	0.61135	0.61191	0.61614	0.62005	0.62102
Alpha virt. eigenvalues --	0.62232	0.62615	0.63327	0.63378	0.63670
Alpha virt. eigenvalues --	0.63698	0.63880	0.63938	0.64358	0.64574
Alpha virt. eigenvalues --	0.64840	0.64874	0.65217	0.65444	0.65965
Alpha virt. eigenvalues --	0.66360	0.66624	0.66796	0.66837	0.66963
Alpha virt. eigenvalues --	0.67100	0.67605	0.67881	0.68076	0.68336
Alpha virt. eigenvalues --	0.68457	0.68710	0.68714	0.69102	0.69640
Alpha virt. eigenvalues --	0.70056	0.70240	0.70763	0.71155	0.72028
Alpha virt. eigenvalues --	0.72491	0.72616	0.73177	0.73362	0.74401
Alpha virt. eigenvalues --	0.74463	0.74569	0.74935	0.75097	0.75391
Alpha virt. eigenvalues --	0.75789	0.75929	0.76223	0.76230	0.76864
Alpha virt. eigenvalues --	0.76886	0.77052	0.77462	0.78375	0.78515
Alpha virt. eigenvalues --	0.78961	0.81387	0.81500	0.83017	0.83305
Alpha virt. eigenvalues --	0.84143	0.84781	0.85599	0.85645	0.87394
Alpha virt. eigenvalues --	0.87705	0.87859	0.88097	0.88471	0.88478
Alpha virt. eigenvalues --	0.89378	0.90969	0.91594	0.91653	0.91855
Alpha virt. eigenvalues --	0.92359	0.92986	0.94128	0.94384	0.94584
Alpha virt. eigenvalues --	0.95852	0.96117	0.96195	0.97415	0.97859
Alpha virt. eigenvalues --	0.98902	0.99369	0.99885	0.99932	1.00622
Alpha virt. eigenvalues --	1.00889	1.00979	1.01006	1.02422	1.02868
Alpha virt. eigenvalues --	1.03027	1.03598	1.04102	1.04290	1.05020
Alpha virt. eigenvalues --	1.06744	1.07801	1.08033	1.08044	1.09155
Alpha virt. eigenvalues --	1.09829	1.10492	1.11079	1.11988	1.13692
Alpha virt. eigenvalues --	1.13796	1.14632	1.15415	1.15802	1.16257
Alpha virt. eigenvalues --	1.16762	1.17306	1.18261	1.19456	1.19679
Alpha virt. eigenvalues --	1.20008	1.20748	1.21075	1.22022	1.22073
Alpha virt. eigenvalues --	1.22962	1.23911	1.24160	1.24202	1.24961
Alpha virt. eigenvalues --	1.25755	1.26707	1.27040	1.27450	1.28040
Alpha virt. eigenvalues --	1.28107	1.29185	1.29710	1.30504	1.30672
Alpha virt. eigenvalues --	1.31665	1.31800	1.32730	1.33101	1.34614
Alpha virt. eigenvalues --	1.34628	1.34979	1.35673	1.36228	1.37051
Alpha virt. eigenvalues --	1.37309	1.38739	1.38797	1.39586	1.40367
Alpha virt. eigenvalues --	1.40548	1.41017	1.41179	1.41425	1.41448
Alpha virt. eigenvalues --	1.41502	1.41957	1.42315	1.43055	1.43826
Alpha virt. eigenvalues --	1.44294	1.44597	1.44751	1.45297	1.45604
Alpha virt. eigenvalues --	1.45974	1.46158	1.47130	1.47269	1.47759
Alpha virt. eigenvalues --	1.48314	1.48893	1.49489	1.49762	1.50362
Alpha virt. eigenvalues --	1.50625	1.51994	1.52619	1.52642	1.53017

Alpha virt. eigenvalues --	1.53483	1.53571	1.55956	1.56200	1.56364
Alpha virt. eigenvalues --	1.57039	1.57254	1.57538	1.58077	1.58110
Alpha virt. eigenvalues --	1.58702	1.58840	1.59033	1.59626	1.59845
Alpha virt. eigenvalues --	1.60014	1.61244	1.61250	1.61657	1.61996
Alpha virt. eigenvalues --	1.62611	1.62627	1.62748	1.62819	1.63317
Alpha virt. eigenvalues --	1.63541	1.64010	1.64221	1.64554	1.65405
Alpha virt. eigenvalues --	1.65490	1.65717	1.65825	1.66969	1.67165
Alpha virt. eigenvalues --	1.67523	1.68002	1.68828	1.68927	1.69346
Alpha virt. eigenvalues --	1.69370	1.69770	1.70426	1.71076	1.71505
Alpha virt. eigenvalues --	1.71712	1.72097	1.72221	1.72705	1.72854
Alpha virt. eigenvalues --	1.73074	1.73840	1.74386	1.74716	1.75098
Alpha virt. eigenvalues --	1.75128	1.75733	1.76627	1.76881	1.77236
Alpha virt. eigenvalues --	1.77913	1.78099	1.78581	1.79107	1.79363
Alpha virt. eigenvalues --	1.79683	1.80060	1.81523	1.81928	1.81960
Alpha virt. eigenvalues --	1.82688	1.82717	1.83179	1.83218	1.84050
Alpha virt. eigenvalues --	1.84812	1.85784	1.86025	1.86806	1.86816
Alpha virt. eigenvalues --	1.87006	1.87354	1.87770	1.87869	1.88734
Alpha virt. eigenvalues --	1.89395	1.89814	1.90496	1.90780	1.91877
Alpha virt. eigenvalues --	1.93072	1.93706	1.94458	1.94543	1.95313
Alpha virt. eigenvalues --	1.96477	1.97173	1.98049	1.98408	1.98641
Alpha virt. eigenvalues --	1.98920	1.99409	1.99728	1.99998	2.00452
Alpha virt. eigenvalues --	2.00516	2.02009	2.02103	2.02814	2.03408
Alpha virt. eigenvalues --	2.03544	2.04121	2.04593	2.06794	2.07062
Alpha virt. eigenvalues --	2.07765	2.07919	2.08342	2.09268	2.09906
Alpha virt. eigenvalues --	2.10047	2.10790	2.11229	2.12527	2.12610
Alpha virt. eigenvalues --	2.13245	2.13322	2.14299	2.14734	2.14895
Alpha virt. eigenvalues --	2.15394	2.18172	2.18186	2.18512	2.19724
Alpha virt. eigenvalues --	2.19933	2.20926	2.21916	2.22220	2.23148
Alpha virt. eigenvalues --	2.23288	2.24452	2.26575	2.26731	2.27537
Alpha virt. eigenvalues --	2.28004	2.28760	2.29784	2.30608	2.30754
Alpha virt. eigenvalues --	2.32404	2.33080	2.34712	2.34713	2.36028
Alpha virt. eigenvalues --	2.37848	2.39265	2.39635	2.39890	2.40383
Alpha virt. eigenvalues --	2.42552	2.42611	2.42869	2.43401	2.43678
Alpha virt. eigenvalues --	2.43882	2.43967	2.44060	2.44996	2.45385
Alpha virt. eigenvalues --	2.45649	2.45767	2.46946	2.47780	2.47987
Alpha virt. eigenvalues --	2.48064	2.48858	2.49182	2.49873	2.49881
Alpha virt. eigenvalues --	2.50131	2.50764	2.51285	2.51528	2.53319
Alpha virt. eigenvalues --	2.53401	2.55370	2.55829	2.56181	2.56511
Alpha virt. eigenvalues --	2.56883	2.58338	2.58375	2.59747	2.61157
Alpha virt. eigenvalues --	2.61626	2.65522	2.67699	2.69556	2.71357
Alpha virt. eigenvalues --	2.73493	2.75605	2.80030	2.82992	2.84669
Alpha virt. eigenvalues --	2.86024	2.91929	2.92794	2.95134	2.95337
Alpha virt. eigenvalues --	2.96782	2.98500	2.99201	2.99249	2.99557
Alpha virt. eigenvalues --	3.00059	3.00941	3.02821	3.02947	3.05010
Alpha virt. eigenvalues --	3.05395	3.08324	3.08349	3.09001	3.09003
Alpha virt. eigenvalues --	3.11098	3.11102	3.13370	3.13729	3.14345
Alpha virt. eigenvalues --	3.14693	3.24563	3.24567	3.26655	3.26692
Alpha virt. eigenvalues --	3.32131	3.32332	3.35792	3.37539	3.37642

Alpha virt. eigenvalues -- 3.37660 3.37896 3.41771 3.42681 3.43891
 Alpha virt. eigenvalues -- 3.45610 3.52313 3.53351

Cyan UV-Vis Spectrum Epsilon/Oscillator Strength – N = 1



Cyan Table of 10 Lowest Excited States – N = 1

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	2.30	537.99	0.4425
2	3.10	400.11	0.0283
3	3.10	399.71	0.0020
4	3.45	359.36	0.0126
5	3.81	325.70	0.7962
6	4.26	290.89	0.1682
7	4.41	280.89	0.0002
8	4.41	280.84	0.0000
9	4.54	272.83	0.0009
10	4.56	271.84	0.0091

Cyan Cartesian Coordinates – N = 2

C 0.04312 3.20976 -0.13059
 C -1.28498 2.73137 -0.15421
 C -1.37078 1.33322 -0.12674
 C -0.11505 0.69296 -0.13434
 S 1.17898 1.87527 -0.13701
 O -2.49603 0.60688 -0.10867
 O -2.34634 3.55705 -0.20564
 C -3.46363 3.10954 -0.98639
 H -3.98486 4.02624 -1.29014
 H -3.09134 2.60181 -1.88772
 C -3.6202 1.16312 0.5921
 H -4.24622 0.29949 0.8482
 H -3.2635 1.63013 1.52091
 C -4.41789 2.1812 -0.22777

C	-5.32454	2.95417	0.73414
H	-5.9958	3.61562	0.15105
H	-5.97254	2.24405	1.28727
C	-5.32882	1.50109	-1.2536
H	-6.10627	0.9165	-0.72268
H	-5.85698	2.2716	-1.8518
O	-4.54589	3.70565	1.62671
O	-4.56766	0.66771	-2.08575
C	-5.33359	4.41997	2.54902
H	-4.65008	4.97726	3.20168
H	-6.00695	5.13406	2.04045
H	-5.9502	3.74305	3.16852
C	-5.35559	0.01026	-3.04895
H	-4.68384	-0.61439	-3.65089
H	-6.11901	-0.63494	-2.57678
H	-5.87096	0.72796	-3.71347
C	0.4788	4.57489	-0.12073
C	1.86828	4.9456	-0.21293
C	-0.40394	5.65885	-0.0185
C	2.28459	6.33052	-0.21016
N	2.88368	4.09304	-0.30967
H	-1.46737	5.45486	0.06669
C	0.00027	7.00056	-0.01733
N	3.60256	6.48061	-0.30868
C	1.33468	7.41093	-0.10691
S	4.25811	4.98346	-0.39433
H	-0.77388	7.7594	0.04946
C	1.73319	8.79476	-0.10483
C	0.93259	9.91493	0.14831
S	3.37728	9.31097	-0.43962
C	1.63543	11.15316	0.02609
O	-0.36978	9.80694	0.46195
C	2.956	10.96835	-0.28688
O	1.09403	12.38174	0.20846
C	-0.93259	10.82207	1.30226
H	3.6977	11.74737	-0.44284
C	-0.20515	12.56184	-0.35676
H	-1.81175	10.35055	1.76024
H	-0.21675	11.07354	2.09716
C	-1.34382	12.09804	0.56348
H	-0.29422	13.63816	-0.55623
H	-0.26607	12.02366	-1.31451
C	-2.604	11.90262	-0.2835
C	-1.68527	13.15341	1.62032
H	-3.46108	11.66567	0.37817
H	-2.84998	12.85316	-0.79994
O	-2.40807	10.87623	-1.22018
H	-2.08712	14.05623	1.11819

H	-2.48666	12.77176	2.2858
O	-0.54095	13.47441	2.36575
C	-3.52432	10.70258	-2.05869
C	-0.80548	14.43412	3.35982
H	-3.2871	9.89063	-2.75761
H	-4.42762	10.42796	-1.48327
H	-3.74742	11.61926	-2.63547
H	0.1355	14.62485	3.89096
H	-1.16956	15.38248	2.92343
H	-1.55991	14.07428	4.08374
C	0.11505	-0.69296	-0.13434
C	1.37078	-1.33322	-0.12674
S	-1.17898	-1.87527	-0.13701
C	1.28498	-2.73137	-0.15421
O	2.49603	-0.60688	-0.10867
C	-0.04312	-3.20976	-0.13059
O	2.34634	-3.55705	-0.20564
C	3.6202	-1.16312	0.5921
C	-0.4788	-4.57489	-0.12073
C	3.46363	-3.10954	-0.98639
H	4.24622	-0.29949	0.8482
H	3.2635	-1.63013	1.52091
C	4.41789	-2.1812	-0.22777
C	-1.86828	-4.9456	-0.21293
C	0.40394	-5.65885	-0.0185
H	3.98486	-4.02624	-1.29014
H	3.09134	-2.60181	-1.88772
C	5.32454	-2.95417	0.73414
C	5.32882	-1.50109	-1.2536
C	-2.28459	-6.33052	-0.21016
N	-2.88368	-4.09304	-0.30967
H	1.46737	-5.45486	0.06669
C	-0.00027	-7.00056	-0.01733
H	5.9958	-3.61562	0.15105
H	5.97254	-2.24405	1.28727
O	4.54589	-3.70565	1.62671
H	6.10627	-0.9165	-0.72268
H	5.85698	-2.2716	-1.8518
O	4.56766	-0.66771	-2.08575
N	-3.60256	-6.48061	-0.30868
C	-1.33468	-7.41093	-0.10691
S	-4.25811	-4.98346	-0.39433
H	0.77388	-7.7594	0.04946
C	5.33359	-4.41997	2.54902
C	5.35559	-0.01026	-3.04895
C	-1.73319	-8.79476	-0.10483
H	4.65008	-4.97726	3.20168
H	6.00695	-5.13406	2.04045

H	5.9502	-3.74305	3.16852
H	4.68384	0.61439	-3.65089
H	6.11901	0.63494	-2.57678
H	5.87096	-0.72796	-3.71347
C	-0.93259	-9.91493	0.14831
S	-3.37728	-9.31097	-0.43962
C	-1.63543	-11.15316	0.02609
O	0.36978	-9.80694	0.46195
C	-2.956	-10.96835	-0.28688
O	-1.09403	-12.38174	0.20846
C	0.93259	-10.82207	1.30226
H	-3.6977	-11.74737	-0.44284
C	0.20515	-12.56184	-0.35676
H	1.81175	-10.35055	1.76024
H	0.21675	-11.07354	2.09716
C	1.34382	-12.09804	0.56348
H	0.29422	-13.63816	-0.55623
H	0.26607	-12.02366	-1.31451
C	2.604	-11.90262	-0.2835
C	1.68527	-13.15341	1.62032
H	3.46108	-11.66567	0.37817
H	2.84998	-12.85316	-0.79994
O	2.40807	-10.87623	-1.22018
H	2.08712	-14.05623	1.11819
H	2.48666	-12.77176	2.2858
O	0.54095	-13.47441	2.36575
C	3.52432	-10.70258	-2.05869
C	0.80548	-14.43412	3.35982
H	3.2871	-9.89063	-2.75761
H	4.42762	-10.42796	-1.48327
H	3.74742	-11.61926	-2.63547
H	-0.1355	-14.62485	3.89096
H	1.16956	-15.38248	2.92343
H	1.55991	-14.07428	4.08374

Cyan Energy Levels – N = 2

Neutral

Alpha occ. eigenvalues -- -89.15573 -89.15573 -89.09439 -89.09439 -89.09417
Alpha occ. eigenvalues -- -89.09417 -19.26689 -19.26689 -19.26610 -19.26610
Alpha occ. eigenvalues -- -19.26591 -19.26591 -19.25840 -19.25840 -19.23693
Alpha occ. eigenvalues -- -19.23693 -19.23690 -19.23690 -19.23655 -19.23655
Alpha occ. eigenvalues -- -19.23606 -19.23606 -14.44401 -14.44401 -14.44354
Alpha occ. eigenvalues -- -14.44354 -10.31114 -10.31114 -10.30927 -10.30927
Alpha occ. eigenvalues -- -10.30731 -10.30730 -10.30426 -10.30426 -10.30208
Alpha occ. eigenvalues -- -10.30208 -10.30162 -10.30162 -10.29895 -10.29895
Alpha occ. eigenvalues -- -10.29834 -10.29834 -10.29819 -10.29819 -10.29571
Alpha occ. eigenvalues -- -10.29571 -10.29359 -10.29359 -10.29342 -10.29342
Alpha occ. eigenvalues -- -10.29341 -10.29341 -10.29327 -10.29327 -10.28560

Alpha occ. eigenvalues -- -10.28523 -10.28232 -10.28232 -10.28218 -10.28218
 Alpha occ. eigenvalues -- -10.28215 -10.28215 -10.28138 -10.28138 -10.28127
 Alpha occ. eigenvalues -- -10.28126 -10.28098 -10.28098 -10.27717 -10.27717
 Alpha occ. eigenvalues -- -10.27645 -10.27645 -10.26547 -10.26547 -10.26511
 Alpha occ. eigenvalues -- -10.26511 -10.26456 -10.26456 -10.25381 -10.25381
 Alpha occ. eigenvalues -- -10.25319 -10.25318 -8.09577 -8.09577 -8.03741
 Alpha occ. eigenvalues -- -8.03741 -8.03703 -8.03702 -6.03562 -6.03562
 Alpha occ. eigenvalues -- -6.02979 -6.02979 -6.02728 -6.02728 -5.97618
 Alpha occ. eigenvalues -- -5.97618 -5.97599 -5.97599 -5.97248 -5.97248
 Alpha occ. eigenvalues -- -5.97219 -5.97219 -5.96863 -5.96863 -5.96788
 Alpha occ. eigenvalues -- -5.96788 -1.12214 -1.12170 -1.11798 -1.11798
 Alpha occ. eigenvalues -- -1.09775 -1.09743 -1.09333 -1.09333 -1.07837
 Alpha occ. eigenvalues -- -1.07837 -1.07831 -1.07830 -1.07661 -1.07661
 Alpha occ. eigenvalues -- -1.07643 -1.07643 -1.05521 -1.05521 -0.93252
 Alpha occ. eigenvalues -- -0.93061 -0.92412 -0.91614 -0.91225 -0.90628
 Alpha occ. eigenvalues -- -0.88775 -0.88387 -0.85989 -0.85965 -0.85868
 Alpha occ. eigenvalues -- -0.85855 -0.82709 -0.81495 -0.79364 -0.78828
 Alpha occ. eigenvalues -- -0.78620 -0.77544 -0.76670 -0.76476 -0.76346
 Alpha occ. eigenvalues -- -0.76280 -0.75492 -0.75451 -0.74579 -0.74576
 Alpha occ. eigenvalues -- -0.74571 -0.74558 -0.72864 -0.72032 -0.71843
 Alpha occ. eigenvalues -- -0.71504 -0.71504 -0.71429 -0.70831 -0.69037
 Alpha occ. eigenvalues -- -0.68360 -0.68243 -0.68221 -0.68207 -0.67136
 Alpha occ. eigenvalues -- -0.66503 -0.64834 -0.64594 -0.64578 -0.64573
 Alpha occ. eigenvalues -- -0.64534 -0.64023 -0.63982 -0.63389 -0.61214
 Alpha occ. eigenvalues -- -0.60973 -0.60537 -0.60481 -0.60080 -0.59675
 Alpha occ. eigenvalues -- -0.59469 -0.59143 -0.58520 -0.57765 -0.57052
 Alpha occ. eigenvalues -- -0.56600 -0.54692 -0.54116 -0.53657 -0.53419
 Alpha occ. eigenvalues -- -0.53365 -0.53271 -0.53229 -0.53128 -0.52805
 Alpha occ. eigenvalues -- -0.52744 -0.52183 -0.52172 -0.51979 -0.51943
 Alpha occ. eigenvalues -- -0.51707 -0.51158 -0.50552 -0.50370 -0.50292
 Alpha occ. eigenvalues -- -0.50219 -0.49909 -0.49543 -0.49538 -0.48788
 Alpha occ. eigenvalues -- -0.48759 -0.48745 -0.48743 -0.48721 -0.48329
 Alpha occ. eigenvalues -- -0.48327 -0.48130 -0.48020 -0.47886 -0.47769
 Alpha occ. eigenvalues -- -0.47713 -0.47324 -0.47189 -0.47148 -0.47029
 Alpha occ. eigenvalues -- -0.46914 -0.46559 -0.46500 -0.46493 -0.46218
 Alpha occ. eigenvalues -- -0.46143 -0.46080 -0.45682 -0.45297 -0.44432
 Alpha occ. eigenvalues -- -0.44315 -0.44115 -0.43928 -0.43774 -0.43350
 Alpha occ. eigenvalues -- -0.43250 -0.42676 -0.42657 -0.42464 -0.42391
 Alpha occ. eigenvalues -- -0.42032 -0.42011 -0.41563 -0.41329 -0.41305
 Alpha occ. eigenvalues -- -0.41235 -0.41035 -0.40588 -0.40207 -0.40124
 Alpha occ. eigenvalues -- -0.40114 -0.40092 -0.39817 -0.39797 -0.39650
 Alpha occ. eigenvalues -- -0.39602 -0.39448 -0.39311 -0.38778 -0.38613
 Alpha occ. eigenvalues -- -0.38590 -0.38249 -0.38237 -0.38081 -0.37699
 Alpha occ. eigenvalues -- -0.37696 -0.37360 -0.36936 -0.36883 -0.36463
 Alpha occ. eigenvalues -- -0.36455 -0.36259 -0.36155 -0.36125 -0.35542
 Alpha occ. eigenvalues -- -0.35268 -0.34660 -0.34576 -0.34515 -0.34498
 Alpha occ. eigenvalues -- -0.34495 -0.34133 -0.33821 -0.33641 -0.33415
 Alpha occ. eigenvalues -- -0.33307 -0.33184 -0.33152 -0.33141 -0.33137

Alpha occ. eigenvalues --	-0.32591	-0.32302	-0.32134	-0.32065	-0.31430
Alpha occ. eigenvalues --	-0.31183	-0.30890	-0.30617	-0.30362	-0.30107
Alpha occ. eigenvalues --	-0.28815	-0.28242	-0.27890	-0.27886	-0.27874
Alpha occ. eigenvalues --	-0.27864	-0.27637	-0.27635	-0.27085	-0.27085
Alpha occ. eigenvalues --	-0.27063	-0.27063	-0.26050	-0.23591	-0.23526
Alpha occ. eigenvalues --	-0.23064	-0.23063	-0.22708	-0.20815	-0.18137
Alpha virt. eigenvalues --	-0.09738	-0.08726	-0.04653	-0.02759	-0.01631
Alpha virt. eigenvalues --	0.00535	0.01416	0.01772	0.02027	0.02039
Alpha virt. eigenvalues --	0.03446	0.04057	0.04069	0.05211	0.05214
Alpha virt. eigenvalues --	0.05507	0.05954	0.06086	0.06329	0.06409
Alpha virt. eigenvalues --	0.06450	0.07150	0.07459	0.07845	0.07953
Alpha virt. eigenvalues --	0.08003	0.08043	0.08183	0.08637	0.09074
Alpha virt. eigenvalues --	0.09324	0.09714	0.09818	0.09877	0.09953
Alpha virt. eigenvalues --	0.10017	0.10213	0.10320	0.10333	0.10494
Alpha virt. eigenvalues --	0.10650	0.10798	0.10981	0.11086	0.11298
Alpha virt. eigenvalues --	0.11596	0.11776	0.11874	0.11949	0.12131
Alpha virt. eigenvalues --	0.12613	0.12949	0.13123	0.13173	0.13257
Alpha virt. eigenvalues --	0.13376	0.13541	0.13812	0.13926	0.13944
Alpha virt. eigenvalues --	0.13962	0.14013	0.14021	0.14059	0.14145
Alpha virt. eigenvalues --	0.14196	0.14214	0.14268	0.14279	0.14380
Alpha virt. eigenvalues --	0.14743	0.14907	0.14915	0.14954	0.14991
Alpha virt. eigenvalues --	0.15022	0.15131	0.15621	0.15632	0.15844
Alpha virt. eigenvalues --	0.15849	0.16582	0.16748	0.16855	0.16908
Alpha virt. eigenvalues --	0.17139	0.17301	0.17481	0.17693	0.17860
Alpha virt. eigenvalues --	0.17868	0.18383	0.18399	0.18541	0.18974
Alpha virt. eigenvalues --	0.19307	0.19363	0.20100	0.20183	0.20407
Alpha virt. eigenvalues --	0.20688	0.20757	0.20815	0.21099	0.21280
Alpha virt. eigenvalues --	0.21582	0.21611	0.21741	0.22586	0.22626
Alpha virt. eigenvalues --	0.22888	0.22971	0.23189	0.23196	0.23357
Alpha virt. eigenvalues --	0.23581	0.23619	0.23678	0.23915	0.24000
Alpha virt. eigenvalues --	0.24155	0.24264	0.25704	0.26064	0.26166
Alpha virt. eigenvalues --	0.26249	0.26548	0.26686	0.26866	0.27126
Alpha virt. eigenvalues --	0.27367	0.27743	0.28035	0.28265	0.28295
Alpha virt. eigenvalues --	0.28490	0.28581	0.29115	0.29134	0.29209
Alpha virt. eigenvalues --	0.29317	0.29817	0.29922	0.30267	0.30330
Alpha virt. eigenvalues --	0.30642	0.30934	0.32501	0.32843	0.32949
Alpha virt. eigenvalues --	0.33203	0.33753	0.35553	0.36045	0.36254
Alpha virt. eigenvalues --	0.36809	0.37013	0.37438	0.38398	0.39490
Alpha virt. eigenvalues --	0.40167	0.40468	0.40703	0.41030	0.42313
Alpha virt. eigenvalues --	0.42493	0.42591	0.42617	0.42891	0.42965
Alpha virt. eigenvalues --	0.43009	0.43120	0.43359	0.44027	0.44047
Alpha virt. eigenvalues --	0.44298	0.44374	0.44743	0.44775	0.44911
Alpha virt. eigenvalues --	0.45017	0.45183	0.45312	0.45401	0.45525
Alpha virt. eigenvalues --	0.45654	0.45880	0.46147	0.46220	0.46557
Alpha virt. eigenvalues --	0.46561	0.46701	0.46825	0.46944	0.46977
Alpha virt. eigenvalues --	0.47099	0.47164	0.47168	0.47182	0.47358
Alpha virt. eigenvalues --	0.47371	0.47495	0.47579	0.47601	0.47765
Alpha virt. eigenvalues --	0.47833	0.48066	0.48116	0.48202	0.48314

Alpha virt. eigenvalues --	0.48377	0.48445	0.48750	0.48753	0.48902
Alpha virt. eigenvalues --	0.48962	0.49062	0.49126	0.49276	0.49428
Alpha virt. eigenvalues --	0.49527	0.49613	0.49735	0.50058	0.50098
Alpha virt. eigenvalues --	0.50279	0.50357	0.50371	0.50548	0.50610
Alpha virt. eigenvalues --	0.50777	0.51030	0.51182	0.51303	0.51356
Alpha virt. eigenvalues --	0.51446	0.51697	0.51976	0.52048	0.52254
Alpha virt. eigenvalues --	0.52343	0.52445	0.52560	0.52711	0.52928
Alpha virt. eigenvalues --	0.53286	0.53365	0.53438	0.53576	0.53725
Alpha virt. eigenvalues --	0.54107	0.54643	0.54858	0.54905	0.55154
Alpha virt. eigenvalues --	0.55282	0.55314	0.55430	0.55548	0.55792
Alpha virt. eigenvalues --	0.55873	0.56031	0.56096	0.56248	0.56623
Alpha virt. eigenvalues --	0.56747	0.56774	0.56830	0.56979	0.57099
Alpha virt. eigenvalues --	0.57369	0.57405	0.57828	0.58614	0.58616
Alpha virt. eigenvalues --	0.58846	0.58950	0.59661	0.59844	0.59976
Alpha virt. eigenvalues --	0.60001	0.60333	0.60571	0.60766	0.60873
Alpha virt. eigenvalues --	0.60948	0.60990	0.61158	0.61220	0.61472
Alpha virt. eigenvalues --	0.61848	0.61973	0.61978	0.62115	0.62125
Alpha virt. eigenvalues --	0.62226	0.62234	0.62540	0.62547	0.62866
Alpha virt. eigenvalues --	0.63287	0.63345	0.63506	0.63512	0.63691
Alpha virt. eigenvalues --	0.63755	0.63805	0.63853	0.63874	0.63936
Alpha virt. eigenvalues --	0.64004	0.64149	0.64343	0.64479	0.64522
Alpha virt. eigenvalues --	0.64725	0.64803	0.64877	0.64916	0.65040
Alpha virt. eigenvalues --	0.65104	0.65524	0.65576	0.65631	0.65650
Alpha virt. eigenvalues --	0.66357	0.66467	0.66500	0.66593	0.66754
Alpha virt. eigenvalues --	0.66767	0.66937	0.66944	0.67029	0.67031
Alpha virt. eigenvalues --	0.67118	0.67296	0.67401	0.67691	0.67826
Alpha virt. eigenvalues --	0.67948	0.68081	0.68142	0.68281	0.68344
Alpha virt. eigenvalues --	0.68536	0.68587	0.68670	0.68731	0.68899
Alpha virt. eigenvalues --	0.68973	0.69171	0.69390	0.69473	0.69926
Alpha virt. eigenvalues --	0.70048	0.70145	0.70445	0.70618	0.70626
Alpha virt. eigenvalues --	0.71138	0.71315	0.71767	0.72074	0.72099
Alpha virt. eigenvalues --	0.72262	0.72544	0.72563	0.72943	0.73015
Alpha virt. eigenvalues --	0.73215	0.73291	0.73315	0.73862	0.74068
Alpha virt. eigenvalues --	0.74371	0.74531	0.74567	0.74747	0.74841
Alpha virt. eigenvalues --	0.75124	0.75159	0.75260	0.75444	0.75597
Alpha virt. eigenvalues --	0.75723	0.75957	0.76000	0.76168	0.76185
Alpha virt. eigenvalues --	0.76445	0.76507	0.76540	0.76721	0.76730
Alpha virt. eigenvalues --	0.76931	0.77060	0.77155	0.77327	0.77767
Alpha virt. eigenvalues --	0.77812	0.78148	0.78536	0.78730	0.78910
Alpha virt. eigenvalues --	0.79434	0.81142	0.81403	0.81636	0.81694
Alpha virt. eigenvalues --	0.81821	0.82684	0.83125	0.83410	0.84250
Alpha virt. eigenvalues --	0.84566	0.85037	0.85231	0.85415	0.85999
Alpha virt. eigenvalues --	0.86351	0.86657	0.87616	0.87655	0.87693
Alpha virt. eigenvalues --	0.87757	0.87828	0.88040	0.88091	0.88300
Alpha virt. eigenvalues --	0.88482	0.88523	0.88557	0.88571	0.89219
Alpha virt. eigenvalues --	0.90062	0.90960	0.91153	0.91419	0.91583
Alpha virt. eigenvalues --	0.91645	0.91736	0.91867	0.91976	0.92292
Alpha virt. eigenvalues --	0.92391	0.92826	0.93119	0.93256	0.93539

Alpha virt. eigenvalues --	0.94149	0.94311	0.94634	0.94887	0.95075
Alpha virt. eigenvalues --	0.95850	0.95875	0.96028	0.96291	0.96349
Alpha virt. eigenvalues --	0.97184	0.97394	0.97833	0.97941	0.98363
Alpha virt. eigenvalues --	0.98401	0.99041	0.99057	0.99793	0.99841
Alpha virt. eigenvalues --	0.99856	0.99971	1.00190	1.00512	1.00587
Alpha virt. eigenvalues --	1.00805	1.00928	1.01092	1.01501	1.01588
Alpha virt. eigenvalues --	1.01819	1.02261	1.02409	1.02873	1.03098
Alpha virt. eigenvalues --	1.03185	1.03503	1.03561	1.04171	1.04355
Alpha virt. eigenvalues --	1.04404	1.04621	1.05573	1.05941	1.06894
Alpha virt. eigenvalues --	1.07146	1.07575	1.07862	1.08038	1.08084
Alpha virt. eigenvalues --	1.08866	1.09076	1.09231	1.09646	1.09886
Alpha virt. eigenvalues --	1.10528	1.10888	1.10893	1.11273	1.11696
Alpha virt. eigenvalues --	1.12289	1.12554	1.12596	1.13296	1.13546
Alpha virt. eigenvalues --	1.13562	1.14374	1.15028	1.15366	1.15967
Alpha virt. eigenvalues --	1.16409	1.16548	1.16599	1.16873	1.17032
Alpha virt. eigenvalues --	1.17061	1.17608	1.17880	1.18726	1.19443
Alpha virt. eigenvalues --	1.19476	1.19646	1.19680	1.19797	1.20006
Alpha virt. eigenvalues --	1.20766	1.20907	1.20978	1.21032	1.21608
Alpha virt. eigenvalues --	1.21675	1.21802	1.22048	1.22183	1.22855
Alpha virt. eigenvalues --	1.23056	1.23467	1.24040	1.24125	1.24367
Alpha virt. eigenvalues --	1.24459	1.25075	1.25181	1.25848	1.25856
Alpha virt. eigenvalues --	1.26176	1.26272	1.26874	1.27194	1.27369
Alpha virt. eigenvalues --	1.27375	1.27603	1.27648	1.28128	1.28435
Alpha virt. eigenvalues --	1.29112	1.29284	1.29700	1.29835	1.30524
Alpha virt. eigenvalues --	1.30556	1.30776	1.30789	1.31544	1.31566
Alpha virt. eigenvalues --	1.32007	1.32083	1.32440	1.32657	1.33369
Alpha virt. eigenvalues --	1.33798	1.34318	1.34592	1.34613	1.34745
Alpha virt. eigenvalues --	1.34783	1.35760	1.35846	1.36176	1.36498
Alpha virt. eigenvalues --	1.36771	1.36917	1.37113	1.37228	1.38245
Alpha virt. eigenvalues --	1.38527	1.38810	1.38952	1.39264	1.39526
Alpha virt. eigenvalues --	1.39704	1.40217	1.40552	1.40892	1.41066
Alpha virt. eigenvalues --	1.41120	1.41157	1.41222	1.41367	1.41452
Alpha virt. eigenvalues --	1.41458	1.41478	1.41508	1.41573	1.41852
Alpha virt. eigenvalues --	1.42098	1.42180	1.42487	1.42568	1.42972
Alpha virt. eigenvalues --	1.43062	1.43564	1.43928	1.44163	1.44210
Alpha virt. eigenvalues --	1.44524	1.44618	1.44632	1.45140	1.45193
Alpha virt. eigenvalues --	1.45303	1.45512	1.45654	1.45865	1.45938
Alpha virt. eigenvalues --	1.46239	1.46578	1.46641	1.46868	1.47177
Alpha virt. eigenvalues --	1.47320	1.47609	1.47735	1.47836	1.48397
Alpha virt. eigenvalues --	1.48695	1.49122	1.49243	1.49259	1.49291
Alpha virt. eigenvalues --	1.49441	1.50042	1.50684	1.50765	1.51089
Alpha virt. eigenvalues --	1.51130	1.51689	1.51824	1.52741	1.52792
Alpha virt. eigenvalues --	1.52934	1.52942	1.53207	1.53398	1.53576
Alpha virt. eigenvalues --	1.53890	1.53937	1.54625	1.55073	1.55737
Alpha virt. eigenvalues --	1.55862	1.56200	1.56298	1.56555	1.56664
Alpha virt. eigenvalues --	1.56711	1.56994	1.57212	1.57544	1.57671
Alpha virt. eigenvalues --	1.57949	1.57989	1.58278	1.58583	1.58684
Alpha virt. eigenvalues --	1.58742	1.58858	1.58983	1.59264	1.59381

Alpha virt. eigenvalues --	1.59900	1.60016	1.60016	1.60248	1.60804
Alpha virt. eigenvalues --	1.60870	1.61324	1.61525	1.61697	1.61786
Alpha virt. eigenvalues --	1.61982	1.62124	1.62260	1.62602	1.62602
Alpha virt. eigenvalues --	1.62771	1.62789	1.62891	1.62929	1.63069
Alpha virt. eigenvalues --	1.63139	1.63167	1.63592	1.63600	1.63977
Alpha virt. eigenvalues --	1.64058	1.64111	1.64163	1.64290	1.64354
Alpha virt. eigenvalues --	1.64427	1.64941	1.65116	1.65492	1.65498
Alpha virt. eigenvalues --	1.65500	1.65690	1.65793	1.65997	1.66245
Alpha virt. eigenvalues --	1.66881	1.67002	1.67484	1.67574	1.67863
Alpha virt. eigenvalues --	1.67880	1.68170	1.68469	1.68593	1.68935
Alpha virt. eigenvalues --	1.69117	1.69218	1.69523	1.69562	1.69865
Alpha virt. eigenvalues --	1.69866	1.70296	1.70376	1.70863	1.70984
Alpha virt. eigenvalues --	1.71160	1.71463	1.71637	1.71648	1.71871
Alpha virt. eigenvalues --	1.72143	1.72153	1.72236	1.72330	1.72684
Alpha virt. eigenvalues --	1.72807	1.72941	1.73211	1.73405	1.73734
Alpha virt. eigenvalues --	1.73872	1.74362	1.74417	1.74531	1.74642
Alpha virt. eigenvalues --	1.75018	1.75098	1.75399	1.75536	1.75616
Alpha virt. eigenvalues --	1.75901	1.76070	1.76181	1.76623	1.76801
Alpha virt. eigenvalues --	1.76843	1.77074	1.77533	1.77578	1.77871
Alpha virt. eigenvalues --	1.78231	1.78352	1.78624	1.78811	1.78877
Alpha virt. eigenvalues --	1.79188	1.79297	1.79715	1.79721	1.80062
Alpha virt. eigenvalues --	1.80156	1.80304	1.80682	1.81636	1.81694
Alpha virt. eigenvalues --	1.82312	1.82362	1.82501	1.82530	1.82818
Alpha virt. eigenvalues --	1.82864	1.83236	1.83248	1.83472	1.84067
Alpha virt. eigenvalues --	1.84269	1.84417	1.84545	1.84855	1.85241
Alpha virt. eigenvalues --	1.85650	1.85800	1.85919	1.86227	1.86340
Alpha virt. eigenvalues --	1.86941	1.86956	1.87096	1.87180	1.87292
Alpha virt. eigenvalues --	1.87456	1.87536	1.87742	1.87924	1.88071
Alpha virt. eigenvalues --	1.88541	1.88953	1.89279	1.89424	1.89800
Alpha virt. eigenvalues --	1.90070	1.90439	1.90740	1.91178	1.91290
Alpha virt. eigenvalues --	1.91779	1.92026	1.92636	1.93468	1.93780
Alpha virt. eigenvalues --	1.93843	1.94061	1.94209	1.94323	1.94930
Alpha virt. eigenvalues --	1.95097	1.96243	1.96301	1.96602	1.96800
Alpha virt. eigenvalues --	1.96966	1.97859	1.98323	1.98487	1.98633
Alpha virt. eigenvalues --	1.98783	1.98785	1.98934	1.99146	1.99147
Alpha virt. eigenvalues --	1.99741	1.99841	2.00274	2.00287	2.00303
Alpha virt. eigenvalues --	2.00386	2.00560	2.00603	2.01360	2.01409
Alpha virt. eigenvalues --	2.01971	2.02092	2.02346	2.03089	2.03328
Alpha virt. eigenvalues --	2.03345	2.03537	2.03554	2.03669	2.04302
Alpha virt. eigenvalues --	2.04377	2.05034	2.05234	2.05851	2.06873
Alpha virt. eigenvalues --	2.06968	2.07192	2.07287	2.07834	2.07881
Alpha virt. eigenvalues --	2.08047	2.08293	2.08706	2.09524	2.09599
Alpha virt. eigenvalues --	2.09704	2.10083	2.10267	2.10485	2.10918
Alpha virt. eigenvalues --	2.11117	2.11185	2.12537	2.12579	2.12896
Alpha virt. eigenvalues --	2.13064	2.13129	2.13283	2.13613	2.14184
Alpha virt. eigenvalues --	2.14373	2.14736	2.14766	2.14935	2.15041
Alpha virt. eigenvalues --	2.15228	2.15938	2.16868	2.18248	2.18259
Alpha virt. eigenvalues --	2.18378	2.19024	2.19323	2.19448	2.19817

Alpha virt. eigenvalues --	2.19862	2.20020	2.20229	2.21362	2.21776
Alpha virt. eigenvalues --	2.22019	2.22071	2.22500	2.22664	2.22945
Alpha virt. eigenvalues --	2.23328	2.23364	2.23546	2.24665	2.24749
Alpha virt. eigenvalues --	2.26704	2.26758	2.27089	2.27267	2.27892
Alpha virt. eigenvalues --	2.28127	2.28143	2.28245	2.29039	2.29109
Alpha virt. eigenvalues --	2.29656	2.30591	2.30650	2.30663	2.31016
Alpha virt. eigenvalues --	2.32262	2.32701	2.32946	2.33783	2.34513
Alpha virt. eigenvalues --	2.34741	2.34794	2.34964	2.35581	2.35778
Alpha virt. eigenvalues --	2.37405	2.38119	2.38365	2.39479	2.39624
Alpha virt. eigenvalues --	2.39708	2.39743	2.39820	2.40003	2.41603
Alpha virt. eigenvalues --	2.42100	2.42313	2.42551	2.42615	2.42687
Alpha virt. eigenvalues --	2.42782	2.42990	2.43351	2.43486	2.43728
Alpha virt. eigenvalues --	2.43830	2.43842	2.43987	2.44049	2.44136
Alpha virt. eigenvalues --	2.44206	2.44231	2.44590	2.45089	2.45089
Alpha virt. eigenvalues --	2.45231	2.45649	2.45659	2.45824	2.45973
Alpha virt. eigenvalues --	2.46198	2.46480	2.47209	2.47520	2.47930
Alpha virt. eigenvalues --	2.47987	2.48020	2.48234	2.48858	2.49041
Alpha virt. eigenvalues --	2.49372	2.49381	2.49583	2.49646	2.49929
Alpha virt. eigenvalues --	2.49929	2.50110	2.50187	2.50477	2.50581
Alpha virt. eigenvalues --	2.51183	2.51217	2.52107	2.52283	2.53418
Alpha virt. eigenvalues --	2.53420	2.53654	2.54000	2.55278	2.55412
Alpha virt. eigenvalues --	2.55412	2.55983	2.56104	2.56157	2.56389
Alpha virt. eigenvalues --	2.56531	2.56625	2.56855	2.58293	2.58383
Alpha virt. eigenvalues --	2.58384	2.58938	2.59867	2.60048	2.61255
Alpha virt. eigenvalues --	2.61353	2.61959	2.64229	2.65760	2.66081
Alpha virt. eigenvalues --	2.68528	2.68939	2.69886	2.70152	2.71569
Alpha virt. eigenvalues --	2.72025	2.73644	2.73808	2.76302	2.76751
Alpha virt. eigenvalues --	2.80065	2.80242	2.82519	2.82763	2.84107
Alpha virt. eigenvalues --	2.84454	2.85911	2.86149	2.91720	2.91770
Alpha virt. eigenvalues --	2.92619	2.92634	2.94974	2.95223	2.95272
Alpha virt. eigenvalues --	2.95364	2.96779	2.96850	2.98382	2.98491
Alpha virt. eigenvalues --	2.99231	2.99233	2.99260	2.99320	2.99552
Alpha virt. eigenvalues --	2.99582	3.00033	3.00143	3.00869	3.01117
Alpha virt. eigenvalues --	3.02923	3.02925	3.03037	3.03087	3.05128
Alpha virt. eigenvalues --	3.05178	3.05615	3.05841	3.08338	3.08339
Alpha virt. eigenvalues --	3.08380	3.08413	3.09013	3.09013	3.09080
Alpha virt. eigenvalues --	3.09081	3.11165	3.11166	3.11337	3.11400
Alpha virt. eigenvalues --	3.12676	3.13443	3.13476	3.14541	3.14547
Alpha virt. eigenvalues --	3.14712	3.15238	3.15335	3.24560	3.24560
Alpha virt. eigenvalues --	3.24654	3.24736	3.26679	3.26679	3.26822
Alpha virt. eigenvalues --	3.26867	3.32221	3.32241	3.32395	3.32485
Alpha virt. eigenvalues --	3.36009	3.36150	3.37587	3.37606	3.37617
Alpha virt. eigenvalues --	3.37669	3.37698	3.37714	3.37953	3.37972
Alpha virt. eigenvalues --	3.41220	3.41612	3.42420	3.42801	3.43923
Alpha virt. eigenvalues --	3.44450	3.45863	3.46121	3.51812	3.52496
Alpha virt. eigenvalues --	3.53071	3.53741			

Cation/Polaron

Alpha occ. eigenvalues -- -89.17379 -89.17379 -89.12436 -89.12436 -89.11026
Alpha occ. eigenvalues -- -89.11026 -19.29514 -19.29514 -19.29103 -19.29103
Alpha occ. eigenvalues -- -19.28296 -19.28296 -19.27001 -19.27001 -19.24655
Alpha occ. eigenvalues -- -19.24655 -19.24595 -19.24595 -19.24370 -19.24370
Alpha occ. eigenvalues -- -19.24260 -19.24260 -14.46357 -14.46357 -14.46244
Alpha occ. eigenvalues -- -14.46244 -10.34644 -10.34643 -10.34410 -10.34410
Alpha occ. eigenvalues -- -10.33134 -10.33134 -10.32793 -10.32755 -10.32640
Alpha occ. eigenvalues -- -10.32640 -10.32363 -10.32363 -10.32177 -10.32177
Alpha occ. eigenvalues -- -10.31989 -10.31989 -10.31543 -10.31543 -10.31472
Alpha occ. eigenvalues -- -10.31472 -10.30881 -10.30881 -10.30653 -10.30653
Alpha occ. eigenvalues -- -10.30443 -10.30443 -10.30394 -10.30394 -10.30370
Alpha occ. eigenvalues -- -10.30370 -10.30320 -10.30320 -10.30071 -10.30071
Alpha occ. eigenvalues -- -10.30025 -10.30025 -10.29998 -10.29998 -10.29009
Alpha occ. eigenvalues -- -10.29009 -10.28960 -10.28960 -10.28838 -10.28838
Alpha occ. eigenvalues -- -10.28730 -10.28730 -10.28576 -10.28576 -10.28374
Alpha occ. eigenvalues -- -10.28374 -10.27948 -10.27948 -10.27448 -10.27448
Alpha occ. eigenvalues -- -10.27299 -10.27299 -8.11365 -8.11365 -8.06731
Alpha occ. eigenvalues -- -8.06731 -8.05360 -8.05360 -6.05351 -6.05350
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Alpha occ. eigenvalues -- -6.00634 -6.00243 -6.00243 -5.99777 -5.99777
Alpha occ. eigenvalues -- -5.99239 -5.99239 -5.98865 -5.98865 -5.98472
Alpha occ. eigenvalues -- -5.98472 -1.14836 -1.14775 -1.13290 -1.13290
Alpha occ. eigenvalues -- -1.12352 -1.12324 -1.10645 -1.10645 -1.08819
Alpha occ. eigenvalues -- -1.08817 -1.08621 -1.08621 -1.08499 -1.08499
Alpha occ. eigenvalues -- -1.08296 -1.08296 -1.07411 -1.07411 -0.96422
Alpha occ. eigenvalues -- -0.95315 -0.94788 -0.94316 -0.93256 -0.93025
Alpha occ. eigenvalues -- -0.91211 -0.90883 -0.87546 -0.87508 -0.86792
Alpha occ. eigenvalues -- -0.86779 -0.85777 -0.84142 -0.81947 -0.80917
Alpha occ. eigenvalues -- -0.80833 -0.80153 -0.79115 -0.78933 -0.77980
Alpha occ. eigenvalues -- -0.77979 -0.77396 -0.77365 -0.75576 -0.75522
Alpha occ. eigenvalues -- -0.75211 -0.75211 -0.74991 -0.73963 -0.73591
Alpha occ. eigenvalues -- -0.73141 -0.72661 -0.72529 -0.72487 -0.71303
Alpha occ. eigenvalues -- -0.69633 -0.69422 -0.69316 -0.69016 -0.68984
Alpha occ. eigenvalues -- -0.68706 -0.67289 -0.66248 -0.66164 -0.65943
Alpha occ. eigenvalues -- -0.65488 -0.65412 -0.65196 -0.65181 -0.63750
Alpha occ. eigenvalues -- -0.63484 -0.62358 -0.62237 -0.61960 -0.61210
Alpha occ. eigenvalues -- -0.60876 -0.60759 -0.60355 -0.59668 -0.58859
Alpha occ. eigenvalues -- -0.58623 -0.56660 -0.55944 -0.55446 -0.55275
Alpha occ. eigenvalues -- -0.55007 -0.54900 -0.54652 -0.54552 -0.54125
Alpha occ. eigenvalues -- -0.54118 -0.54014 -0.53686 -0.53277 -0.53113
Alpha occ. eigenvalues -- -0.52812 -0.52736 -0.52395 -0.52372 -0.52309
Alpha occ. eigenvalues -- -0.51615 -0.51303 -0.51148 -0.51126 -0.50452
Alpha occ. eigenvalues -- -0.50117 -0.50066 -0.49798 -0.49782 -0.49654
Alpha occ. eigenvalues -- -0.49585 -0.49424 -0.49412 -0.49293 -0.49178
Alpha occ. eigenvalues -- -0.49169 -0.48884 -0.48730 -0.48668 -0.48285
Alpha occ. eigenvalues -- -0.48200 -0.47963 -0.47861 -0.47632 -0.47470
Alpha occ. eigenvalues -- -0.47458 -0.47359 -0.46963 -0.46779 -0.46410

Alpha occ. eigenvalues --	-0.46178	-0.46081	-0.45549	-0.45212	-0.45147
Alpha occ. eigenvalues --	-0.45144	-0.44929	-0.44368	-0.43841	-0.43832
Alpha occ. eigenvalues --	-0.43722	-0.43693	-0.43386	-0.43122	-0.43021
Alpha occ. eigenvalues --	-0.42589	-0.42241	-0.42241	-0.41575	-0.41531
Alpha occ. eigenvalues --	-0.41344	-0.41253	-0.41131	-0.41049	-0.40826
Alpha occ. eigenvalues --	-0.40815	-0.40795	-0.40779	-0.40627	-0.40522
Alpha occ. eigenvalues --	-0.40439	-0.40124	-0.39996	-0.39753	-0.39610
Alpha occ. eigenvalues --	-0.39584	-0.39233	-0.38886	-0.38842	-0.38120
Alpha occ. eigenvalues --	-0.38101	-0.37948	-0.37488	-0.37447	-0.37219
Alpha occ. eigenvalues --	-0.37017	-0.36464	-0.36154	-0.35890	-0.35872
Alpha occ. eigenvalues --	-0.35493	-0.35315	-0.35313	-0.35053	-0.34745
Alpha occ. eigenvalues --	-0.34590	-0.34534	-0.34478	-0.34412	-0.34302
Alpha occ. eigenvalues --	-0.33973	-0.33970	-0.33481	-0.33416	-0.33370
Alpha occ. eigenvalues --	-0.33044	-0.33010	-0.32894	-0.31833	-0.31733
Alpha occ. eigenvalues --	-0.31105	-0.30451	-0.29599	-0.29566	-0.28912
Alpha occ. eigenvalues --	-0.28906	-0.28723	-0.28550	-0.28549	-0.28008
Alpha occ. eigenvalues --	-0.28008	-0.27710	-0.27709	-0.26210	-0.26169
Alpha occ. eigenvalues --	-0.25558	-0.24548	-0.24547	-0.23150	-0.21448
Alpha virt. eigenvalues --	-0.12128	-0.10846	-0.07420	-0.04867	-0.03860
Alpha virt. eigenvalues --	-0.02098	-0.00868	-0.00445	0.00341	0.00393
Alpha virt. eigenvalues --	0.01114	0.01584	0.01787	0.02585	0.03318
Alpha virt. eigenvalues --	0.03394	0.03796	0.04502	0.05178	0.05518
Alpha virt. eigenvalues --	0.05533	0.05716	0.06053	0.06397	0.06456
Alpha virt. eigenvalues --	0.06863	0.07135	0.07336	0.07357	0.07438
Alpha virt. eigenvalues --	0.07448	0.07909	0.08207	0.08483	0.08862
Alpha virt. eigenvalues --	0.09033	0.09041	0.09214	0.09280	0.09326
Alpha virt. eigenvalues --	0.09437	0.09536	0.09655	0.09926	0.10008
Alpha virt. eigenvalues --	0.10401	0.10646	0.10814	0.11019	0.11033
Alpha virt. eigenvalues --	0.11228	0.11689	0.11922	0.12195	0.12228
Alpha virt. eigenvalues --	0.12385	0.12596	0.12715	0.12737	0.12913
Alpha virt. eigenvalues --	0.12992	0.13175	0.13230	0.13237	0.13302
Alpha virt. eigenvalues --	0.13320	0.13353	0.13406	0.13518	0.13583
Alpha virt. eigenvalues --	0.13599	0.14136	0.14139	0.14153	0.14161
Alpha virt. eigenvalues --	0.14329	0.14353	0.14578	0.14653	0.15037
Alpha virt. eigenvalues --	0.15092	0.15106	0.15758	0.15907	0.15949
Alpha virt. eigenvalues --	0.15953	0.16065	0.16111	0.16199	0.16377
Alpha virt. eigenvalues --	0.16444	0.16975	0.17287	0.17313	0.17579
Alpha virt. eigenvalues --	0.17723	0.17733	0.18674	0.19022	0.19110
Alpha virt. eigenvalues --	0.19624	0.19686	0.19811	0.19940	0.19985
Alpha virt. eigenvalues --	0.20339	0.20578	0.20637	0.20857	0.21179
Alpha virt. eigenvalues --	0.21556	0.21662	0.21924	0.22053	0.22069
Alpha virt. eigenvalues --	0.22240	0.22510	0.22548	0.22735	0.22763
Alpha virt. eigenvalues --	0.23120	0.23138	0.23878	0.24381	0.24649
Alpha virt. eigenvalues --	0.24907	0.24927	0.25401	0.25493	0.25851
Alpha virt. eigenvalues --	0.25898	0.26122	0.26394	0.26663	0.26896
Alpha virt. eigenvalues --	0.27184	0.27268	0.27398	0.27606	0.27688
Alpha virt. eigenvalues --	0.27934	0.28591	0.28902	0.28978	0.28978
Alpha virt. eigenvalues --	0.29243	0.29267	0.30100	0.30820	0.30908

Alpha virt. eigenvalues --	0.31439	0.31794	0.33116	0.34356	0.34691
Alpha virt. eigenvalues --	0.34927	0.35129	0.35578	0.36071	0.37328
Alpha virt. eigenvalues --	0.37982	0.38654	0.38831	0.38973	0.40378
Alpha virt. eigenvalues --	0.40468	0.40934	0.41065	0.41290	0.41414
Alpha virt. eigenvalues --	0.41536	0.41896	0.42204	0.42303	0.42338
Alpha virt. eigenvalues --	0.42466	0.42536	0.42945	0.42976	0.43236
Alpha virt. eigenvalues --	0.43301	0.43520	0.43531	0.43595	0.44125
Alpha virt. eigenvalues --	0.44285	0.44374	0.44572	0.44707	0.45088
Alpha virt. eigenvalues --	0.45147	0.45189	0.45309	0.45398	0.45489
Alpha virt. eigenvalues --	0.45702	0.45835	0.45878	0.45968	0.46062
Alpha virt. eigenvalues --	0.46094	0.46209	0.46352	0.46402	0.46518
Alpha virt. eigenvalues --	0.46534	0.46584	0.46626	0.46827	0.46833
Alpha virt. eigenvalues --	0.46977	0.47074	0.47169	0.47221	0.47319
Alpha virt. eigenvalues --	0.47423	0.47550	0.47680	0.47710	0.47825
Alpha virt. eigenvalues --	0.47864	0.48105	0.48155	0.48309	0.48360
Alpha virt. eigenvalues --	0.48583	0.48608	0.48686	0.48798	0.48873
Alpha virt. eigenvalues --	0.49248	0.49392	0.49491	0.49585	0.49904
Alpha virt. eigenvalues --	0.50025	0.50054	0.50158	0.50199	0.50448
Alpha virt. eigenvalues --	0.50559	0.50721	0.50938	0.51067	0.51275
Alpha virt. eigenvalues --	0.51452	0.51607	0.51789	0.51885	0.52007
Alpha virt. eigenvalues --	0.52095	0.52999	0.53305	0.53338	0.53618
Alpha virt. eigenvalues --	0.53774	0.53851	0.53957	0.53968	0.54198
Alpha virt. eigenvalues --	0.54350	0.54481	0.54551	0.54839	0.54848
Alpha virt. eigenvalues --	0.55116	0.55123	0.55328	0.55476	0.55731
Alpha virt. eigenvalues --	0.55791	0.56032	0.56189	0.57045	0.57107
Alpha virt. eigenvalues --	0.57154	0.57163	0.57972	0.57999	0.58237
Alpha virt. eigenvalues --	0.58392	0.58898	0.59012	0.59200	0.59227
Alpha virt. eigenvalues --	0.59534	0.59610	0.59871	0.60004	0.60093
Alpha virt. eigenvalues --	0.60333	0.60563	0.60809	0.60952	0.61098
Alpha virt. eigenvalues --	0.61205	0.61214	0.61373	0.61471	0.61509
Alpha virt. eigenvalues --	0.61852	0.62100	0.62356	0.62421	0.62431
Alpha virt. eigenvalues --	0.62690	0.62717	0.62747	0.62775	0.62864
Alpha virt. eigenvalues --	0.62884	0.63120	0.63146	0.63310	0.63353
Alpha virt. eigenvalues --	0.63503	0.63675	0.63925	0.63960	0.64244
Alpha virt. eigenvalues --	0.64247	0.64455	0.64521	0.64639	0.64718
Alpha virt. eigenvalues --	0.64810	0.64986	0.65149	0.65181	0.65480
Alpha virt. eigenvalues --	0.65560	0.65582	0.65773	0.65821	0.65997
Alpha virt. eigenvalues --	0.66090	0.66153	0.66268	0.66400	0.66644
Alpha virt. eigenvalues --	0.66662	0.66866	0.66907	0.67105	0.67273
Alpha virt. eigenvalues --	0.67283	0.67395	0.67405	0.67688	0.67768
Alpha virt. eigenvalues --	0.67977	0.67979	0.68283	0.68310	0.68486
Alpha virt. eigenvalues --	0.68686	0.69054	0.69061	0.69328	0.69344
Alpha virt. eigenvalues --	0.69682	0.69911	0.70282	0.70322	0.70594
Alpha virt. eigenvalues --	0.70627	0.71230	0.71373	0.71468	0.71597
Alpha virt. eigenvalues --	0.71721	0.72305	0.72371	0.72479	0.72604
Alpha virt. eigenvalues --	0.72968	0.73178	0.73185	0.73392	0.73550
Alpha virt. eigenvalues --	0.73713	0.73724	0.73750	0.74208	0.74289
Alpha virt. eigenvalues --	0.74433	0.74553	0.74737	0.74868	0.75021

Alpha virt. eigenvalues --	0.75198	0.75306	0.75354	0.75427	0.75507
Alpha virt. eigenvalues --	0.75704	0.75775	0.75787	0.75809	0.75984
Alpha virt. eigenvalues --	0.76077	0.76670	0.77004	0.77159	0.77244
Alpha virt. eigenvalues --	0.77411	0.78889	0.79940	0.80124	0.80210
Alpha virt. eigenvalues --	0.80578	0.80687	0.81442	0.81745	0.82410
Alpha virt. eigenvalues --	0.82851	0.83060	0.83321	0.83724	0.84066
Alpha virt. eigenvalues --	0.84071	0.84775	0.85429	0.85544	0.85832
Alpha virt. eigenvalues --	0.86088	0.86523	0.86768	0.87034	0.87040
Alpha virt. eigenvalues --	0.87141	0.87167	0.87346	0.87580	0.87781
Alpha virt. eigenvalues --	0.88133	0.89192	0.89359	0.89779	0.90278
Alpha virt. eigenvalues --	0.90294	0.90689	0.90796	0.90836	0.90907
Alpha virt. eigenvalues --	0.91157	0.91340	0.91506	0.91543	0.91683
Alpha virt. eigenvalues --	0.92406	0.92625	0.92828	0.93231	0.93277
Alpha virt. eigenvalues --	0.94070	0.94154	0.94264	0.94314	0.94694
Alpha virt. eigenvalues --	0.95209	0.95877	0.96498	0.96682	0.96726
Alpha virt. eigenvalues --	0.96794	0.96998	0.97199	0.98199	0.98233
Alpha virt. eigenvalues --	0.98384	0.98539	0.98600	0.98919	0.99145
Alpha virt. eigenvalues --	0.99246	0.99447	0.99521	0.99672	0.99708
Alpha virt. eigenvalues --	1.00130	1.00159	1.00546	1.01130	1.01262
Alpha virt. eigenvalues --	1.01471	1.01953	1.02143	1.02562	1.02685
Alpha virt. eigenvalues --	1.02799	1.02832	1.03574	1.03627	1.05052
Alpha virt. eigenvalues --	1.05338	1.05503	1.05838	1.06130	1.06173
Alpha virt. eigenvalues --	1.06895	1.07253	1.07383	1.07631	1.08314
Alpha virt. eigenvalues --	1.08573	1.08743	1.09038	1.09195	1.09644
Alpha virt. eigenvalues --	1.10333	1.10601	1.10636	1.11190	1.12113
Alpha virt. eigenvalues --	1.12519	1.12520	1.13381	1.13724	1.14339
Alpha virt. eigenvalues --	1.14771	1.14974	1.15173	1.15336	1.15601
Alpha virt. eigenvalues --	1.15612	1.16138	1.16439	1.17192	1.17416
Alpha virt. eigenvalues --	1.17913	1.18495	1.18625	1.18755	1.18815
Alpha virt. eigenvalues --	1.19090	1.19205	1.19373	1.19461	1.19856
Alpha virt. eigenvalues --	1.19869	1.20187	1.20733	1.20943	1.21368
Alpha virt. eigenvalues --	1.21540	1.22045	1.22808	1.22920	1.23018
Alpha virt. eigenvalues --	1.23031	1.23395	1.23762	1.24240	1.24270
Alpha virt. eigenvalues --	1.24711	1.24821	1.25097	1.25748	1.25895
Alpha virt. eigenvalues --	1.26128	1.26311	1.26585	1.26811	1.26825
Alpha virt. eigenvalues --	1.27372	1.27514	1.27880	1.28104	1.28674
Alpha virt. eigenvalues --	1.28853	1.29138	1.29191	1.29889	1.29963
Alpha virt. eigenvalues --	1.30394	1.30636	1.30875	1.30975	1.31173
Alpha virt. eigenvalues --	1.32254	1.32594	1.32961	1.33141	1.33561
Alpha virt. eigenvalues --	1.33570	1.34184	1.34342	1.34650	1.34915
Alpha virt. eigenvalues --	1.35185	1.35322	1.35621	1.35903	1.36452
Alpha virt. eigenvalues --	1.37064	1.37231	1.37271	1.37548	1.37744
Alpha virt. eigenvalues --	1.38094	1.38666	1.38983	1.39590	1.39679
Alpha virt. eigenvalues --	1.39693	1.40158	1.40304	1.40310	1.40481
Alpha virt. eigenvalues --	1.40485	1.40690	1.40735	1.40765	1.40856
Alpha virt. eigenvalues --	1.40925	1.40926	1.41012	1.41383	1.41453
Alpha virt. eigenvalues --	1.41549	1.42114	1.42200	1.42427	1.42561
Alpha virt. eigenvalues --	1.43062	1.43436	1.43562	1.43664	1.43961

Alpha virt. eigenvalues --	1.44097	1.44098	1.44156	1.44327	1.44385
Alpha virt. eigenvalues --	1.44461	1.44947	1.45090	1.45305	1.45424
Alpha virt. eigenvalues --	1.46008	1.46284	1.46431	1.46707	1.46770
Alpha virt. eigenvalues --	1.46888	1.47269	1.47350	1.47367	1.47842
Alpha virt. eigenvalues --	1.47968	1.48511	1.48821	1.48933	1.49106
Alpha virt. eigenvalues --	1.49453	1.50331	1.50572	1.51306	1.51316
Alpha virt. eigenvalues --	1.51518	1.51841	1.51920	1.51947	1.52138
Alpha virt. eigenvalues --	1.52300	1.52562	1.52761	1.53426	1.53703
Alpha virt. eigenvalues --	1.54127	1.54565	1.55114	1.55230	1.55360
Alpha virt. eigenvalues --	1.55427	1.55686	1.55761	1.56067	1.56274
Alpha virt. eigenvalues --	1.56688	1.56816	1.56865	1.57089	1.57471
Alpha virt. eigenvalues --	1.57658	1.57824	1.57984	1.58020	1.58061
Alpha virt. eigenvalues --	1.58178	1.58566	1.58780	1.58809	1.59169
Alpha virt. eigenvalues --	1.59247	1.59623	1.59908	1.60094	1.60192
Alpha virt. eigenvalues --	1.60676	1.60804	1.60971	1.61204	1.61294
Alpha virt. eigenvalues --	1.61399	1.61814	1.61822	1.61943	1.61971
Alpha virt. eigenvalues --	1.62174	1.62217	1.62348	1.62363	1.62572
Alpha virt. eigenvalues --	1.62703	1.62908	1.63004	1.63065	1.63355
Alpha virt. eigenvalues --	1.63474	1.63541	1.63593	1.64098	1.64277
Alpha virt. eigenvalues --	1.64554	1.64616	1.64705	1.64821	1.64936
Alpha virt. eigenvalues --	1.65498	1.65618	1.65842	1.65920	1.66189
Alpha virt. eigenvalues --	1.66336	1.66666	1.67032	1.67391	1.67755
Alpha virt. eigenvalues --	1.67871	1.68077	1.68183	1.68316	1.68361
Alpha virt. eigenvalues --	1.68364	1.68650	1.68916	1.69386	1.69432
Alpha virt. eigenvalues --	1.69695	1.69779	1.70000	1.70132	1.70353
Alpha virt. eigenvalues --	1.71098	1.71151	1.71265	1.71389	1.71420
Alpha virt. eigenvalues --	1.71562	1.71588	1.71755	1.71777	1.72195
Alpha virt. eigenvalues --	1.72275	1.72684	1.72760	1.73048	1.73115
Alpha virt. eigenvalues --	1.73589	1.73731	1.73925	1.73969	1.74022
Alpha virt. eigenvalues --	1.74452	1.74491	1.74675	1.75239	1.75266
Alpha virt. eigenvalues --	1.75498	1.75557	1.76075	1.76172	1.76491
Alpha virt. eigenvalues --	1.76882	1.76938	1.77047	1.77383	1.77598
Alpha virt. eigenvalues --	1.77953	1.78087	1.78590	1.78616	1.78750
Alpha virt. eigenvalues --	1.78863	1.78903	1.79083	1.79923	1.79971
Alpha virt. eigenvalues --	1.80589	1.80839	1.80921	1.80995	1.81577
Alpha virt. eigenvalues --	1.81588	1.82077	1.82327	1.82383	1.82726
Alpha virt. eigenvalues --	1.82784	1.83129	1.83347	1.83499	1.83510
Alpha virt. eigenvalues --	1.84173	1.84372	1.84402	1.84652	1.85042
Alpha virt. eigenvalues --	1.85610	1.85748	1.85907	1.85967	1.85999
Alpha virt. eigenvalues --	1.86190	1.86242	1.86275	1.86555	1.86898
Alpha virt. eigenvalues --	1.87005	1.87419	1.87815	1.88045	1.88330
Alpha virt. eigenvalues --	1.88378	1.88570	1.88851	1.89081	1.89503
Alpha virt. eigenvalues --	1.89916	1.90347	1.90711	1.91662	1.91868
Alpha virt. eigenvalues --	1.91952	1.92285	1.92408	1.92668	1.93247
Alpha virt. eigenvalues --	1.93561	1.93946	1.94237	1.94749	1.95045
Alpha virt. eigenvalues --	1.95256	1.96056	1.96643	1.96737	1.96936
Alpha virt. eigenvalues --	1.97062	1.97115	1.97166	1.97349	1.97395
Alpha virt. eigenvalues --	1.98630	1.98801	1.99007	1.99026	1.99134

Alpha virt. eigenvalues --	1.99453	1.99501	1.99651	1.99762	1.99815
Alpha virt. eigenvalues --	2.00267	2.00757	2.00906	2.01312	2.01375
Alpha virt. eigenvalues --	2.02122	2.02517	2.02790	2.02800	2.02827
Alpha virt. eigenvalues --	2.03227	2.03240	2.03358	2.04474	2.05484
Alpha virt. eigenvalues --	2.05543	2.06242	2.06270	2.06713	2.06829
Alpha virt. eigenvalues --	2.06830	2.07175	2.07325	2.08176	2.08227
Alpha virt. eigenvalues --	2.08450	2.08683	2.08688	2.09020	2.09387
Alpha virt. eigenvalues --	2.09890	2.09932	2.10544	2.10766	2.11276
Alpha virt. eigenvalues --	2.12042	2.12043	2.12353	2.12375	2.12518
Alpha virt. eigenvalues --	2.12585	2.13244	2.13650	2.13688	2.13996
Alpha virt. eigenvalues --	2.14161	2.14305	2.14898	2.17007	2.17226
Alpha virt. eigenvalues --	2.17420	2.17426	2.17527	2.17764	2.18372
Alpha virt. eigenvalues --	2.18512	2.18742	2.18743	2.19380	2.19570
Alpha virt. eigenvalues --	2.20285	2.20360	2.21265	2.21346	2.21631
Alpha virt. eigenvalues --	2.21987	2.22073	2.22105	2.23190	2.23224
Alpha virt. eigenvalues --	2.25010	2.25294	2.25780	2.25839	2.26084
Alpha virt. eigenvalues --	2.26116	2.26427	2.26557	2.27287	2.27782
Alpha virt. eigenvalues --	2.28021	2.29456	2.29715	2.29839	2.29872
Alpha virt. eigenvalues --	2.30598	2.31454	2.31502	2.32131	2.32978
Alpha virt. eigenvalues --	2.33648	2.33776	2.33784	2.34051	2.34165
Alpha virt. eigenvalues --	2.35760	2.36292	2.36611	2.37948	2.38105
Alpha virt. eigenvalues --	2.38303	2.38432	2.38786	2.38792	2.40057
Alpha virt. eigenvalues --	2.40415	2.40555	2.41048	2.41759	2.41765
Alpha virt. eigenvalues --	2.41984	2.41989	2.42057	2.42077	2.42160
Alpha virt. eigenvalues --	2.42352	2.42746	2.42798	2.42965	2.43061
Alpha virt. eigenvalues --	2.43213	2.43260	2.43493	2.43955	2.44019
Alpha virt. eigenvalues --	2.44102	2.44847	2.44867	2.44938	2.45022
Alpha virt. eigenvalues --	2.45198	2.45371	2.46070	2.46311	2.46353
Alpha virt. eigenvalues --	2.46650	2.47104	2.47112	2.47642	2.47839
Alpha virt. eigenvalues --	2.48088	2.48098	2.48115	2.48158	2.49047
Alpha virt. eigenvalues --	2.49095	2.49239	2.49241	2.49319	2.49454
Alpha virt. eigenvalues --	2.50137	2.50210	2.50773	2.50894	2.51435
Alpha virt. eigenvalues --	2.52378	2.52591	2.52714	2.53217	2.53843
Alpha virt. eigenvalues --	2.53984	2.54612	2.54965	2.54993	2.55343
Alpha virt. eigenvalues --	2.55411	2.55784	2.55792	2.57044	2.57532
Alpha virt. eigenvalues --	2.57560	2.57573	2.58084	2.58218	2.59640
Alpha virt. eigenvalues --	2.60153	2.60501	2.61987	2.63849	2.64157
Alpha virt. eigenvalues --	2.66756	2.67387	2.68416	2.68593	2.69932
Alpha virt. eigenvalues --	2.70400	2.71678	2.71805	2.74070	2.74485
Alpha virt. eigenvalues --	2.77847	2.78013	2.80077	2.80317	2.82000
Alpha virt. eigenvalues --	2.82474	2.83858	2.83995	2.89349	2.89438
Alpha virt. eigenvalues --	2.90984	2.90987	2.92841	2.93134	2.93922
Alpha virt. eigenvalues --	2.93934	2.94887	2.95006	2.96576	2.96772
Alpha virt. eigenvalues --	2.98132	2.98214	2.98372	2.98387	2.98563
Alpha virt. eigenvalues --	2.98567	2.98952	2.99102	2.99569	2.99651
Alpha virt. eigenvalues --	3.01848	3.01874	3.02181	3.02181	3.03290
Alpha virt. eigenvalues --	3.03496	3.04036	3.04050	3.07355	3.07420
Alpha virt. eigenvalues --	3.07681	3.07682	3.08074	3.08076	3.08363

Alpha virt. eigenvalues --	3.08363	3.09233	3.09847	3.10135	3.10135
Alpha virt. eigenvalues --	3.10716	3.12104	3.12299	3.12357	3.12846
Alpha virt. eigenvalues --	3.12919	3.13326	3.13360	3.23633	3.23714
Alpha virt. eigenvalues --	3.23891	3.23891	3.25730	3.25789	3.25997
Alpha virt. eigenvalues --	3.25998	3.29961	3.30058	3.31004	3.31005
Alpha virt. eigenvalues --	3.33789	3.33953	3.36394	3.36527	3.36687
Alpha virt. eigenvalues --	3.36701	3.36915	3.36915	3.37075	3.37084
Alpha virt. eigenvalues --	3.38854	3.39523	3.40926	3.41250	3.42140
Alpha virt. eigenvalues --	3.42569	3.43748	3.43776	3.49252	3.50406
Alpha virt. eigenvalues --	3.51488	3.51675			
Beta occ. eigenvalues --	-89.17386	-89.17386	-89.12454	-89.12454	-89.11029
Beta occ. eigenvalues --	-89.11029	-19.29456	-19.29456	-19.29099	-19.29098
Beta occ. eigenvalues --	-19.28253	-19.28253	-19.27008	-19.27008	-19.24655
Beta occ. eigenvalues --	-19.24655	-19.24594	-19.24594	-19.24369	-19.24369
Beta occ. eigenvalues --	-19.24260	-19.24260	-14.46287	-14.46287	-14.46277
Beta occ. eigenvalues --	-14.46277	-10.34539	-10.34538	-10.34444	-10.34444
Beta occ. eigenvalues --	-10.33032	-10.33032	-10.32652	-10.32613	-10.32333
Beta occ. eigenvalues --	-10.32333	-10.32320	-10.32320	-10.32211	-10.32211
Beta occ. eigenvalues --	-10.32035	-10.32035	-10.31540	-10.31540	-10.31473
Beta occ. eigenvalues --	-10.31473	-10.30880	-10.30880	-10.30471	-10.30471
Beta occ. eigenvalues --	-10.30444	-10.30444	-10.30400	-10.30399	-10.30394
Beta occ. eigenvalues --	-10.30394	-10.30370	-10.30370	-10.30093	-10.30093
Beta occ. eigenvalues --	-10.30025	-10.30025	-10.29998	-10.29998	-10.29009
Beta occ. eigenvalues --	-10.29009	-10.28960	-10.28960	-10.28838	-10.28838
Beta occ. eigenvalues --	-10.28730	-10.28730	-10.28450	-10.28450	-10.28207
Beta occ. eigenvalues --	-10.28207	-10.27946	-10.27946	-10.27534	-10.27534
Beta occ. eigenvalues --	-10.27298	-10.27298	-8.11372	-8.11372	-8.06749
Beta occ. eigenvalues --	-8.06749	-8.05364	-8.05364	-6.05355	-6.05355
Beta occ. eigenvalues --	-6.04768	-6.04768	-6.04534	-6.04534	-6.00657
Beta occ. eigenvalues --	-6.00657	-6.00264	-6.00264	-5.99816	-5.99816
Beta occ. eigenvalues --	-5.99243	-5.99243	-5.98869	-5.98869	-5.98480
Beta occ. eigenvalues --	-5.98480	-1.14759	-1.14703	-1.13226	-1.13226
Beta occ. eigenvalues --	-1.12287	-1.12257	-1.10629	-1.10629	-1.08817
Beta occ. eigenvalues --	-1.08816	-1.08620	-1.08620	-1.08498	-1.08498
Beta occ. eigenvalues --	-1.08295	-1.08295	-1.07388	-1.07388	-0.96114
Beta occ. eigenvalues --	-0.95166	-0.94705	-0.94104	-0.93130	-0.92886
Beta occ. eigenvalues --	-0.91055	-0.90722	-0.87524	-0.87494	-0.86780
Beta occ. eigenvalues --	-0.86771	-0.85443	-0.83909	-0.81751	-0.80874
Beta occ. eigenvalues --	-0.80760	-0.79939	-0.79060	-0.78865	-0.77869
Beta occ. eigenvalues --	-0.77867	-0.77363	-0.77326	-0.75569	-0.75519
Beta occ. eigenvalues --	-0.75211	-0.75210	-0.74932	-0.73841	-0.73574
Beta occ. eigenvalues --	-0.73124	-0.72630	-0.72506	-0.72478	-0.71026
Beta occ. eigenvalues --	-0.69576	-0.69419	-0.69238	-0.69008	-0.68965
Beta occ. eigenvalues --	-0.68621	-0.67194	-0.66165	-0.66086	-0.65847
Beta occ. eigenvalues --	-0.65485	-0.65394	-0.65194	-0.65176	-0.63612
Beta occ. eigenvalues --	-0.63365	-0.62288	-0.62179	-0.61911	-0.61180
Beta occ. eigenvalues --	-0.60836	-0.60728	-0.60290	-0.59603	-0.58814
Beta occ. eigenvalues --	-0.58532	-0.56613	-0.55888	-0.55380	-0.55220

Beta occ. eigenvalues --	-0.54927	-0.54844	-0.54622	-0.54532	-0.54082
Beta occ. eigenvalues --	-0.54058	-0.53975	-0.53639	-0.53214	-0.53085
Beta occ. eigenvalues --	-0.52796	-0.52707	-0.52351	-0.52288	-0.52252
Beta occ. eigenvalues --	-0.51554	-0.51238	-0.51106	-0.51080	-0.50384
Beta occ. eigenvalues --	-0.50034	-0.49991	-0.49785	-0.49774	-0.49526
Beta occ. eigenvalues --	-0.49444	-0.49418	-0.49409	-0.49222	-0.49141
Beta occ. eigenvalues --	-0.49126	-0.48785	-0.48671	-0.48580	-0.48229
Beta occ. eigenvalues --	-0.48136	-0.47945	-0.47828	-0.47606	-0.47454
Beta occ. eigenvalues --	-0.47446	-0.47332	-0.46929	-0.46739	-0.46341
Beta occ. eigenvalues --	-0.46107	-0.45915	-0.45475	-0.45142	-0.45079
Beta occ. eigenvalues --	-0.44926	-0.44821	-0.44049	-0.43784	-0.43782
Beta occ. eigenvalues --	-0.43589	-0.43583	-0.43205	-0.43067	-0.42865
Beta occ. eigenvalues --	-0.42538	-0.42186	-0.42185	-0.41546	-0.41447
Beta occ. eigenvalues --	-0.41246	-0.41227	-0.41110	-0.41041	-0.40808
Beta occ. eigenvalues --	-0.40772	-0.40715	-0.40710	-0.40599	-0.40352
Beta occ. eigenvalues --	-0.40258	-0.40082	-0.39891	-0.39588	-0.39518
Beta occ. eigenvalues --	-0.39488	-0.39049	-0.38787	-0.38755	-0.38017
Beta occ. eigenvalues --	-0.37903	-0.37814	-0.37403	-0.37392	-0.37018
Beta occ. eigenvalues --	-0.36796	-0.36428	-0.36119	-0.35843	-0.35837
Beta occ. eigenvalues --	-0.35457	-0.35303	-0.35301	-0.34995	-0.34650
Beta occ. eigenvalues --	-0.34575	-0.34508	-0.34445	-0.34402	-0.34210
Beta occ. eigenvalues --	-0.33962	-0.33958	-0.33393	-0.33353	-0.33140
Beta occ. eigenvalues --	-0.32999	-0.32757	-0.32622	-0.31706	-0.31635
Beta occ. eigenvalues --	-0.30766	-0.29951	-0.29515	-0.29515	-0.28907
Beta occ. eigenvalues --	-0.28899	-0.28545	-0.28545	-0.28007	-0.28007
Beta occ. eigenvalues --	-0.27796	-0.27709	-0.27707	-0.25954	-0.25784
Beta occ. eigenvalues --	-0.24411	-0.24407	-0.24406	-0.22180	
Beta virt. eigenvalues --	-0.17057	-0.11513	-0.10441	-0.06744	-0.04515
Beta virt. eigenvalues --	-0.03332	-0.01430	-0.00458	-0.00077	0.00372
Beta virt. eigenvalues --	0.00409	0.01556	0.01735	0.01881	0.02968
Beta virt. eigenvalues --	0.03381	0.03668	0.03884	0.04800	0.05294
Beta virt. eigenvalues --	0.05569	0.05580	0.05761	0.06146	0.06442
Beta virt. eigenvalues --	0.06687	0.06916	0.07339	0.07362	0.07435
Beta virt. eigenvalues --	0.07457	0.07587	0.08236	0.08550	0.08663
Beta virt. eigenvalues --	0.08916	0.09039	0.09103	0.09217	0.09290
Beta virt. eigenvalues --	0.09351	0.09474	0.09556	0.09668	0.09968
Beta virt. eigenvalues --	0.10053	0.10450	0.10682	0.10836	0.11035
Beta virt. eigenvalues --	0.11049	0.11277	0.11724	0.11943	0.12211
Beta virt. eigenvalues --	0.12241	0.12400	0.12610	0.12738	0.12760
Beta virt. eigenvalues --	0.12927	0.13011	0.13190	0.13236	0.13242
Beta virt. eigenvalues --	0.13305	0.13330	0.13356	0.13416	0.13537
Beta virt. eigenvalues --	0.13588	0.13608	0.14144	0.14148	0.14163
Beta virt. eigenvalues --	0.14173	0.14334	0.14356	0.14604	0.14674
Beta virt. eigenvalues --	0.15084	0.15111	0.15124	0.15773	0.15934
Beta virt. eigenvalues --	0.15986	0.16016	0.16166	0.16239	0.16324
Beta virt. eigenvalues --	0.16430	0.16490	0.17032	0.17338	0.17348
Beta virt. eigenvalues --	0.17657	0.17804	0.17821	0.18751	0.19079
Beta virt. eigenvalues --	0.19170	0.19651	0.19713	0.19824	0.19949

Beta virt. eigenvalues --	0.20025	0.20379	0.20616	0.20696	0.20908
Beta virt. eigenvalues --	0.21222	0.21579	0.21688	0.21960	0.22074
Beta virt. eigenvalues --	0.22109	0.22249	0.22529	0.22569	0.22748
Beta virt. eigenvalues --	0.22777	0.23130	0.23153	0.24052	0.24396
Beta virt. eigenvalues --	0.24686	0.24961	0.24963	0.25421	0.25517
Beta virt. eigenvalues --	0.25890	0.25930	0.26164	0.26485	0.26722
Beta virt. eigenvalues --	0.26960	0.27203	0.27280	0.27423	0.27647
Beta virt. eigenvalues --	0.27713	0.27952	0.28636	0.28938	0.29005
Beta virt. eigenvalues --	0.29006	0.29261	0.29290	0.30174	0.30884
Beta virt. eigenvalues --	0.30961	0.31499	0.31831	0.33187	0.34410
Beta virt. eigenvalues --	0.34738	0.34994	0.35201	0.35679	0.36227
Beta virt. eigenvalues --	0.37410	0.38112	0.38689	0.38916	0.39006
Beta virt. eigenvalues --	0.40457	0.40532	0.40981	0.41151	0.41322
Beta virt. eigenvalues --	0.41444	0.41560	0.41952	0.42236	0.42336
Beta virt. eigenvalues --	0.42426	0.42523	0.42567	0.43089	0.43094
Beta virt. eigenvalues --	0.43386	0.43387	0.43608	0.43610	0.43748
Beta virt. eigenvalues --	0.44185	0.44342	0.44413	0.44625	0.44742
Beta virt. eigenvalues --	0.45179	0.45207	0.45300	0.45397	0.45449
Beta virt. eigenvalues --	0.45582	0.45796	0.45907	0.45914	0.46043
Beta virt. eigenvalues --	0.46091	0.46158	0.46228	0.46376	0.46475
Beta virt. eigenvalues --	0.46572	0.46605	0.46621	0.46763	0.46872
Beta virt. eigenvalues --	0.46906	0.47062	0.47103	0.47195	0.47263
Beta virt. eigenvalues --	0.47401	0.47476	0.47581	0.47731	0.47788
Beta virt. eigenvalues --	0.47926	0.47974	0.48193	0.48245	0.48407
Beta virt. eigenvalues --	0.48465	0.48708	0.48719	0.48777	0.48857
Beta virt. eigenvalues --	0.49007	0.49294	0.49441	0.49575	0.49657
Beta virt. eigenvalues --	0.50060	0.50135	0.50233	0.50367	0.50415
Beta virt. eigenvalues --	0.50609	0.50638	0.50830	0.51038	0.51170
Beta virt. eigenvalues --	0.51339	0.51522	0.51699	0.51856	0.51943
Beta virt. eigenvalues --	0.52077	0.52215	0.53046	0.53370	0.53389
Beta virt. eigenvalues --	0.53739	0.53800	0.53915	0.53992	0.53995
Beta virt. eigenvalues --	0.54261	0.54414	0.54553	0.54660	0.54867
Beta virt. eigenvalues --	0.54873	0.55115	0.55135	0.55370	0.55536
Beta virt. eigenvalues --	0.55760	0.55829	0.56114	0.56251	0.57081
Beta virt. eigenvalues --	0.57132	0.57239	0.57258	0.58076	0.58111
Beta virt. eigenvalues --	0.58263	0.58486	0.58950	0.59110	0.59235
Beta virt. eigenvalues --	0.59299	0.59576	0.59656	0.59951	0.60051
Beta virt. eigenvalues --	0.60173	0.60422	0.60676	0.60851	0.60983
Beta virt. eigenvalues --	0.61114	0.61262	0.61273	0.61395	0.61474
Beta virt. eigenvalues --	0.61522	0.61939	0.62126	0.62389	0.62443
Beta virt. eigenvalues --	0.62488	0.62724	0.62738	0.62775	0.62807
Beta virt. eigenvalues --	0.62915	0.62918	0.63138	0.63206	0.63347
Beta virt. eigenvalues --	0.63382	0.63610	0.63703	0.63942	0.63968
Beta virt. eigenvalues --	0.64249	0.64252	0.64485	0.64535	0.64664
Beta virt. eigenvalues --	0.64730	0.64855	0.65026	0.65218	0.65223
Beta virt. eigenvalues --	0.65530	0.65590	0.65609	0.65813	0.65841
Beta virt. eigenvalues --	0.66033	0.66111	0.66186	0.66278	0.66446
Beta virt. eigenvalues --	0.66674	0.66687	0.66877	0.66940	0.67156

Beta virt. eigenvalues --	0.67295	0.67304	0.67436	0.67448	0.67716
Beta virt. eigenvalues --	0.67785	0.67984	0.67987	0.68310	0.68335
Beta virt. eigenvalues --	0.68519	0.68721	0.69106	0.69127	0.69358
Beta virt. eigenvalues --	0.69407	0.69719	0.69946	0.70357	0.70374
Beta virt. eigenvalues --	0.70662	0.70673	0.71281	0.71392	0.71551
Beta virt. eigenvalues --	0.71644	0.71779	0.72344	0.72382	0.72521
Beta virt. eigenvalues --	0.72641	0.72989	0.73214	0.73228	0.73444
Beta virt. eigenvalues --	0.73569	0.73738	0.73758	0.73786	0.74239
Beta virt. eigenvalues --	0.74342	0.74523	0.74570	0.74751	0.74942
Beta virt. eigenvalues --	0.75091	0.75236	0.75356	0.75413	0.75470
Beta virt. eigenvalues --	0.75540	0.75722	0.75797	0.75828	0.75833
Beta virt. eigenvalues --	0.76026	0.76167	0.76731	0.77046	0.77229
Beta virt. eigenvalues --	0.77331	0.77548	0.79009	0.80029	0.80177
Beta virt. eigenvalues --	0.80355	0.80597	0.80755	0.81555	0.81825
Beta virt. eigenvalues --	0.82504	0.82995	0.83239	0.83350	0.83752
Beta virt. eigenvalues --	0.84166	0.84205	0.84898	0.85618	0.85733
Beta virt. eigenvalues --	0.86006	0.86177	0.86547	0.86796	0.87076
Beta virt. eigenvalues --	0.87093	0.87151	0.87187	0.87396	0.87613
Beta virt. eigenvalues --	0.87804	0.88267	0.89294	0.89440	0.89838
Beta virt. eigenvalues --	0.90328	0.90367	0.90774	0.90822	0.90874
Beta virt. eigenvalues --	0.90978	0.91222	0.91390	0.91531	0.91568
Beta virt. eigenvalues --	0.91862	0.92557	0.92693	0.92935	0.93337
Beta virt. eigenvalues --	0.93339	0.94152	0.94223	0.94319	0.94398
Beta virt. eigenvalues --	0.94758	0.95409	0.95913	0.96565	0.96735
Beta virt. eigenvalues --	0.96796	0.96835	0.97050	0.97322	0.98251
Beta virt. eigenvalues --	0.98274	0.98425	0.98671	0.98675	0.98981
Beta virt. eigenvalues --	0.99190	0.99272	0.99477	0.99563	0.99728
Beta virt. eigenvalues --	0.99765	1.00187	1.00251	1.00643	1.01229
Beta virt. eigenvalues --	1.01311	1.01542	1.02014	1.02189	1.02610
Beta virt. eigenvalues --	1.02728	1.02871	1.02913	1.03652	1.03778
Beta virt. eigenvalues --	1.05127	1.05396	1.05583	1.05905	1.06184
Beta virt. eigenvalues --	1.06233	1.06976	1.07357	1.07541	1.07703
Beta virt. eigenvalues --	1.08353	1.08645	1.08889	1.09111	1.09309
Beta virt. eigenvalues --	1.09723	1.10429	1.10686	1.10734	1.11285
Beta virt. eigenvalues --	1.12258	1.12568	1.12569	1.13445	1.13795
Beta virt. eigenvalues --	1.14408	1.14853	1.15054	1.15226	1.15382
Beta virt. eigenvalues --	1.15623	1.15651	1.16195	1.16493	1.17238
Beta virt. eigenvalues --	1.17619	1.17971	1.18518	1.18642	1.18788
Beta virt. eigenvalues --	1.18887	1.19150	1.19292	1.19428	1.19515
Beta virt. eigenvalues --	1.19937	1.19953	1.20232	1.20792	1.21006
Beta virt. eigenvalues --	1.21403	1.21594	1.22091	1.22857	1.22965
Beta virt. eigenvalues --	1.23052	1.23061	1.23456	1.23796	1.24279
Beta virt. eigenvalues --	1.24322	1.24764	1.24875	1.25175	1.25798
Beta virt. eigenvalues --	1.25936	1.26172	1.26374	1.26604	1.26873
Beta virt. eigenvalues --	1.26913	1.27442	1.27630	1.27998	1.28143
Beta virt. eigenvalues --	1.28771	1.28935	1.29233	1.29278	1.29986
Beta virt. eigenvalues --	1.30027	1.30484	1.30717	1.30943	1.31051
Beta virt. eigenvalues --	1.31317	1.32337	1.32681	1.33041	1.33206

Beta virt. eigenvalues --	1.33591	1.33601	1.34264	1.34454	1.34709
Beta virt. eigenvalues --	1.34975	1.35225	1.35384	1.35727	1.35948
Beta virt. eigenvalues --	1.36582	1.37128	1.37284	1.37340	1.37640
Beta virt. eigenvalues --	1.37838	1.38186	1.38714	1.39079	1.39659
Beta virt. eigenvalues --	1.39715	1.39778	1.40223	1.40336	1.40346
Beta virt. eigenvalues --	1.40495	1.40503	1.40696	1.40744	1.40774
Beta virt. eigenvalues --	1.40910	1.40927	1.40937	1.41061	1.41421
Beta virt. eigenvalues --	1.41507	1.41609	1.42167	1.42264	1.42479
Beta virt. eigenvalues --	1.42633	1.43096	1.43473	1.43587	1.43741
Beta virt. eigenvalues --	1.44029	1.44127	1.44146	1.44184	1.44378
Beta virt. eigenvalues --	1.44436	1.44509	1.44988	1.45140	1.45351
Beta virt. eigenvalues --	1.45476	1.46042	1.46308	1.46471	1.46731
Beta virt. eigenvalues --	1.46814	1.46953	1.47351	1.47440	1.47452
Beta virt. eigenvalues --	1.47881	1.48013	1.48556	1.48885	1.49040
Beta virt. eigenvalues --	1.49214	1.49487	1.50370	1.50609	1.51348
Beta virt. eigenvalues --	1.51362	1.51558	1.51874	1.51964	1.52000
Beta virt. eigenvalues --	1.52176	1.52349	1.52590	1.52821	1.53472
Beta virt. eigenvalues --	1.53750	1.54187	1.54649	1.55173	1.55276
Beta virt. eigenvalues --	1.55406	1.55477	1.55733	1.55790	1.56116
Beta virt. eigenvalues --	1.56311	1.56741	1.56836	1.56889	1.57124
Beta virt. eigenvalues --	1.57492	1.57694	1.57864	1.57994	1.58031
Beta virt. eigenvalues --	1.58120	1.58239	1.58638	1.58822	1.58842
Beta virt. eigenvalues --	1.59267	1.59327	1.59720	1.59942	1.60187
Beta virt. eigenvalues --	1.60256	1.60715	1.60862	1.61015	1.61240
Beta virt. eigenvalues --	1.61324	1.61451	1.61837	1.61838	1.61962
Beta virt. eigenvalues --	1.61995	1.62205	1.62253	1.62390	1.62399
Beta virt. eigenvalues --	1.62607	1.62743	1.62936	1.63052	1.63110
Beta virt. eigenvalues --	1.63379	1.63529	1.63552	1.63603	1.64141
Beta virt. eigenvalues --	1.64332	1.64566	1.64648	1.64714	1.64841
Beta virt. eigenvalues --	1.64962	1.65551	1.65671	1.65895	1.65954
Beta virt. eigenvalues --	1.66239	1.66387	1.66708	1.67081	1.67425
Beta virt. eigenvalues --	1.67786	1.67908	1.68120	1.68216	1.68355
Beta virt. eigenvalues --	1.68399	1.68414	1.68698	1.68958	1.69426
Beta virt. eigenvalues --	1.69503	1.69751	1.69869	1.70068	1.70159
Beta virt. eigenvalues --	1.70424	1.71120	1.71171	1.71300	1.71411
Beta virt. eigenvalues --	1.71442	1.71590	1.71612	1.71802	1.71855
Beta virt. eigenvalues --	1.72232	1.72318	1.72763	1.72817	1.73095
Beta virt. eigenvalues --	1.73155	1.73674	1.73788	1.73965	1.74042
Beta virt. eigenvalues --	1.74066	1.74523	1.74537	1.74719	1.75288
Beta virt. eigenvalues --	1.75315	1.75547	1.75626	1.76140	1.76208
Beta virt. eigenvalues --	1.76533	1.76936	1.77004	1.77101	1.77428
Beta virt. eigenvalues --	1.77627	1.77980	1.78118	1.78620	1.78654
Beta virt. eigenvalues --	1.78783	1.78915	1.78944	1.79130	1.79976
Beta virt. eigenvalues --	1.80038	1.80683	1.80905	1.81007	1.81040
Beta virt. eigenvalues --	1.81602	1.81624	1.82126	1.82350	1.82402
Beta virt. eigenvalues --	1.82824	1.82859	1.83156	1.83362	1.83541
Beta virt. eigenvalues --	1.83562	1.84233	1.84422	1.84469	1.84696
Beta virt. eigenvalues --	1.85090	1.85740	1.85794	1.85951	1.85986

Beta virt. eigenvalues --	1.86033	1.86213	1.86258	1.86322	1.86645
Beta virt. eigenvalues --	1.86921	1.87042	1.87464	1.87876	1.88088
Beta virt. eigenvalues --	1.88383	1.88486	1.88639	1.88949	1.89227
Beta virt. eigenvalues --	1.89564	1.90017	1.90401	1.90821	1.91742
Beta virt. eigenvalues --	1.91995	1.92077	1.92425	1.92470	1.92785
Beta virt. eigenvalues --	1.93361	1.93657	1.94122	1.94306	1.94848
Beta virt. eigenvalues --	1.95178	1.95347	1.96225	1.96728	1.96813
Beta virt. eigenvalues --	1.97033	1.97146	1.97160	1.97244	1.97393
Beta virt. eigenvalues --	1.97475	1.98676	1.98851	1.99097	1.99114
Beta virt. eigenvalues --	1.99213	1.99462	1.99512	1.99662	1.99798
Beta virt. eigenvalues --	1.99834	2.00311	2.00816	2.00977	2.01413
Beta virt. eigenvalues --	2.01509	2.02154	2.02527	2.02802	2.02810
Beta virt. eigenvalues --	2.02900	2.03258	2.03266	2.03406	2.04504
Beta virt. eigenvalues --	2.05505	2.05588	2.06270	2.06289	2.06759
Beta virt. eigenvalues --	2.06854	2.06877	2.07206	2.07354	2.08213
Beta virt. eigenvalues --	2.08314	2.08474	2.08706	2.08748	2.09066
Beta virt. eigenvalues --	2.09431	2.09936	2.09983	2.10672	2.10871
Beta virt. eigenvalues --	2.11410	2.12073	2.12096	2.12374	2.12399
Beta virt. eigenvalues --	2.12540	2.12699	2.13318	2.13671	2.13743
Beta virt. eigenvalues --	2.14014	2.14166	2.14322	2.14980	2.17038
Beta virt. eigenvalues --	2.17275	2.17428	2.17441	2.17571	2.17836
Beta virt. eigenvalues --	2.18412	2.18562	2.18771	2.18776	2.19469
Beta virt. eigenvalues --	2.19623	2.20351	2.20429	2.21298	2.21371
Beta virt. eigenvalues --	2.21651	2.22022	2.22096	2.22127	2.23223
Beta virt. eigenvalues --	2.23263	2.25068	2.25332	2.25860	2.25881
Beta virt. eigenvalues --	2.26157	2.26225	2.26444	2.26592	2.27345
Beta virt. eigenvalues --	2.27809	2.28059	2.29484	2.29728	2.29848
Beta virt. eigenvalues --	2.29880	2.30708	2.31511	2.31538	2.32174
Beta virt. eigenvalues --	2.33043	2.33658	2.33813	2.33821	2.34084
Beta virt. eigenvalues --	2.34217	2.35831	2.36382	2.36708	2.38009
Beta virt. eigenvalues --	2.38147	2.38331	2.38486	2.38812	2.38816
Beta virt. eigenvalues --	2.40093	2.40452	2.40601	2.41156	2.41803
Beta virt. eigenvalues --	2.41818	2.42023	2.42053	2.42072	2.42102
Beta virt. eigenvalues --	2.42230	2.42405	2.42752	2.42810	2.42991
Beta virt. eigenvalues --	2.43081	2.43221	2.43271	2.43516	2.43992
Beta virt. eigenvalues --	2.44050	2.44129	2.44853	2.44883	2.44950
Beta virt. eigenvalues --	2.45026	2.45214	2.45404	2.46094	2.46339
Beta virt. eigenvalues --	2.46381	2.46674	2.47117	2.47125	2.47661
Beta virt. eigenvalues --	2.47850	2.48100	2.48110	2.48125	2.48191
Beta virt. eigenvalues --	2.49054	2.49108	2.49242	2.49244	2.49345
Beta virt. eigenvalues --	2.49470	2.50163	2.50235	2.50804	2.50916
Beta virt. eigenvalues --	2.51535	2.52406	2.52604	2.52736	2.53298
Beta virt. eigenvalues --	2.53887	2.54023	2.54688	2.54990	2.55017
Beta virt. eigenvalues --	2.55346	2.55422	2.55786	2.55795	2.57053
Beta virt. eigenvalues --	2.57558	2.57567	2.57580	2.58099	2.58235
Beta virt. eigenvalues --	2.59663	2.60186	2.60530	2.62028	2.63883
Beta virt. eigenvalues --	2.64191	2.66824	2.67434	2.68443	2.68620
Beta virt. eigenvalues --	2.69968	2.70443	2.71742	2.71867	2.74151

Beta virt. eigenvalues --	2.74557	2.77885	2.78055	2.80154	2.80391
Beta virt. eigenvalues --	2.82061	2.82535	2.83907	2.84048	2.89431
Beta virt. eigenvalues --	2.89504	2.91039	2.91041	2.92907	2.93217
Beta virt. eigenvalues --	2.93961	2.93972	2.94925	2.95041	2.96638
Beta virt. eigenvalues --	2.96826	2.98143	2.98224	2.98394	2.98405
Beta virt. eigenvalues --	2.98569	2.98573	2.98964	2.99116	2.99590
Beta virt. eigenvalues --	2.99677	3.01860	3.01891	3.02183	3.02184
Beta virt. eigenvalues --	3.03349	3.03557	3.04084	3.04098	3.07360
Beta virt. eigenvalues --	3.07422	3.07683	3.07683	3.08076	3.08078
Beta virt. eigenvalues --	3.08363	3.08363	3.09311	3.09883	3.10172
Beta virt. eigenvalues --	3.10172	3.10769	3.12180	3.12311	3.12409
Beta virt. eigenvalues --	3.12876	3.12963	3.13380	3.13416	3.23636
Beta virt. eigenvalues --	3.23717	3.23893	3.23893	3.25735	3.25792
Beta virt. eigenvalues --	3.25999	3.25999	3.30014	3.30108	3.31031
Beta virt. eigenvalues --	3.31032	3.33836	3.34001	3.36403	3.36535
Beta virt. eigenvalues --	3.36689	3.36705	3.36916	3.36916	3.37079
Beta virt. eigenvalues --	3.37089	3.38881	3.39546	3.40943	3.41267
Beta virt. eigenvalues --	3.42159	3.42594	3.43782	3.43813	3.49303
Beta virt. eigenvalues --	3.50455	3.51513	3.51708		

Dication/Bipolaron

Alpha occ. eigenvalues --	-89.19262	-89.19262	-89.14921	-89.14921	-89.13009
Alpha occ. eigenvalues --	-89.13009	-19.31727	-19.31726	-19.31248	-19.31248
Alpha occ. eigenvalues --	-19.30376	-19.30376	-19.28453	-19.28453	-19.25532
Alpha occ. eigenvalues --	-19.25532	-19.25484	-19.25484	-19.25112	-19.25112
Alpha occ. eigenvalues --	-19.24926	-19.24926	-14.48359	-14.48359	-14.48230
Alpha occ. eigenvalues --	-14.48230	-10.37453	-10.37453	-10.37222	-10.37222
Alpha occ. eigenvalues --	-10.36034	-10.36013	-10.36013	-10.35995	-10.35701
Alpha occ. eigenvalues --	-10.35701	-10.34492	-10.34492	-10.34303	-10.34303
Alpha occ. eigenvalues --	-10.34011	-10.34011	-10.33681	-10.33681	-10.33175
Alpha occ. eigenvalues --	-10.33175	-10.32963	-10.32963	-10.32859	-10.32859
Alpha occ. eigenvalues --	-10.32700	-10.32700	-10.32107	-10.32107	-10.31467
Alpha occ. eigenvalues --	-10.31467	-10.31321	-10.31321	-10.31303	-10.31303
Alpha occ. eigenvalues --	-10.31110	-10.31110	-10.31105	-10.31105	-10.30782
Alpha occ. eigenvalues --	-10.30782	-10.30730	-10.30730	-10.29946	-10.29946
Alpha occ. eigenvalues --	-10.29746	-10.29746	-10.29716	-10.29716	-10.29475
Alpha occ. eigenvalues --	-10.29475	-10.29282	-10.29282	-10.29163	-10.29163
Alpha occ. eigenvalues --	-10.28277	-10.28277	-8.13228	-8.13228	-8.09235
Alpha occ. eigenvalues --	-8.09235	-8.07359	-8.07359	-6.07212	-6.07212
Alpha occ. eigenvalues --	-6.06619	-6.06619	-6.06387	-6.06387	-6.03147
Alpha occ. eigenvalues --	-6.03147	-6.02748	-6.02748	-6.02270	-6.02270
Alpha occ. eigenvalues --	-6.01242	-6.01242	-6.00860	-6.00860	-6.00460
Alpha occ. eigenvalues --	-6.00460	-1.16930	-1.16863	-1.15089	-1.15089
Alpha occ. eigenvalues --	-1.14425	-1.14395	-1.12208	-1.12208	-1.09707
Alpha occ. eigenvalues --	-1.09705	-1.09500	-1.09500	-1.09347	-1.09347
Alpha occ. eigenvalues --	-1.09229	-1.09229	-1.08980	-1.08980	-0.99030
Alpha occ. eigenvalues --	-0.97651	-0.96868	-0.96625	-0.95476	-0.95225
Alpha occ. eigenvalues --	-0.93572	-0.93258	-0.88890	-0.88839	-0.88320

Alpha occ. eigenvalues --	-0.87836	-0.87793	-0.86580	-0.84351	-0.83024
Alpha occ. eigenvalues --	-0.82966	-0.82359	-0.81342	-0.81159	-0.79917
Alpha occ. eigenvalues --	-0.79868	-0.79286	-0.79228	-0.76932	-0.76408
Alpha occ. eigenvalues --	-0.76308	-0.75954	-0.75913	-0.75725	-0.75173
Alpha occ. eigenvalues --	-0.74591	-0.74388	-0.73759	-0.73674	-0.73117
Alpha occ. eigenvalues --	-0.71536	-0.70826	-0.70514	-0.70412	-0.69884
Alpha occ. eigenvalues --	-0.69854	-0.69469	-0.68427	-0.68354	-0.68127
Alpha occ. eigenvalues --	-0.66397	-0.66299	-0.65994	-0.65888	-0.65794
Alpha occ. eigenvalues --	-0.65653	-0.64347	-0.64214	-0.63665	-0.62832
Alpha occ. eigenvalues --	-0.62354	-0.62249	-0.62088	-0.61448	-0.60556
Alpha occ. eigenvalues --	-0.60384	-0.58540	-0.57863	-0.57220	-0.57175
Alpha occ. eigenvalues --	-0.56521	-0.56508	-0.56271	-0.56210	-0.55763
Alpha occ. eigenvalues --	-0.55562	-0.55356	-0.55194	-0.55119	-0.54761
Alpha occ. eigenvalues --	-0.54594	-0.53928	-0.53753	-0.53699	-0.53558
Alpha occ. eigenvalues --	-0.53452	-0.53008	-0.52697	-0.52601	-0.52304
Alpha occ. eigenvalues --	-0.51676	-0.51496	-0.51298	-0.51276	-0.50817
Alpha occ. eigenvalues --	-0.50798	-0.50664	-0.50354	-0.50314	-0.50288
Alpha occ. eigenvalues --	-0.50252	-0.50130	-0.50118	-0.50111	-0.49416
Alpha occ. eigenvalues --	-0.49355	-0.49125	-0.49000	-0.48992	-0.48890
Alpha occ. eigenvalues --	-0.48365	-0.48353	-0.48230	-0.47985	-0.47926
Alpha occ. eigenvalues --	-0.47739	-0.47706	-0.47310	-0.47225	-0.46555
Alpha occ. eigenvalues --	-0.46502	-0.46501	-0.45774	-0.45528	-0.45491
Alpha occ. eigenvalues --	-0.45336	-0.45069	-0.44889	-0.44825	-0.44672
Alpha occ. eigenvalues --	-0.44369	-0.43520	-0.43400	-0.43321	-0.43110
Alpha occ. eigenvalues --	-0.42892	-0.42804	-0.42644	-0.42402	-0.42244
Alpha occ. eigenvalues --	-0.42229	-0.42024	-0.41954	-0.41845	-0.41772
Alpha occ. eigenvalues --	-0.41693	-0.41644	-0.41411	-0.41334	-0.41193
Alpha occ. eigenvalues --	-0.41102	-0.40855	-0.40735	-0.40647	-0.39643
Alpha occ. eigenvalues --	-0.39513	-0.39331	-0.38901	-0.38719	-0.38470
Alpha occ. eigenvalues --	-0.38434	-0.38270	-0.38048	-0.37189	-0.37037
Alpha occ. eigenvalues --	-0.36937	-0.36470	-0.36294	-0.36196	-0.36182
Alpha occ. eigenvalues --	-0.35979	-0.35787	-0.35773	-0.35449	-0.35446
Alpha occ. eigenvalues --	-0.35122	-0.35042	-0.35005	-0.34829	-0.34827
Alpha occ. eigenvalues --	-0.34601	-0.34595	-0.34308	-0.33373	-0.33294
Alpha occ. eigenvalues --	-0.32681	-0.32065	-0.31509	-0.31487	-0.30362
Alpha occ. eigenvalues --	-0.29880	-0.29856	-0.29298	-0.29297	-0.28863
Alpha occ. eigenvalues --	-0.28863	-0.28388	-0.28388	-0.28161	-0.28004
Alpha occ. eigenvalues --	-0.26978	-0.26180	-0.26177	-0.24395	
Alpha virt. eigenvalues --	-0.20404	-0.13983	-0.12639	-0.09266	-0.06753
Alpha virt. eigenvalues --	-0.05711	-0.04017	-0.02787	-0.02355	-0.01445
Alpha virt. eigenvalues --	-0.01332	-0.00801	-0.00506	-0.00367	0.00523
Alpha virt. eigenvalues --	0.01438	0.01443	0.01754	0.02843	0.03993
Alpha virt. eigenvalues --	0.04330	0.04380	0.04586	0.04588	0.04863
Alpha virt. eigenvalues --	0.05176	0.05204	0.05707	0.06217	0.06257
Alpha virt. eigenvalues --	0.06454	0.06478	0.06673	0.06737	0.06875
Alpha virt. eigenvalues --	0.07308	0.08002	0.08014	0.08213	0.08317
Alpha virt. eigenvalues --	0.08434	0.08487	0.08513	0.08567	0.08924
Alpha virt. eigenvalues --	0.09038	0.09144	0.09611	0.09785	0.10062

Alpha virt. eigenvalues --	0.10130	0.10186	0.10530	0.10804	0.11098
Alpha virt. eigenvalues --	0.11137	0.11283	0.11613	0.11691	0.11755
Alpha virt. eigenvalues --	0.11795	0.11866	0.12097	0.12375	0.12395
Alpha virt. eigenvalues --	0.12450	0.12536	0.12549	0.12569	0.12598
Alpha virt. eigenvalues --	0.12913	0.12916	0.13200	0.13268	0.13338
Alpha virt. eigenvalues --	0.13398	0.13410	0.13702	0.13726	0.13734
Alpha virt. eigenvalues --	0.13832	0.14082	0.14225	0.14433	0.14509
Alpha virt. eigenvalues --	0.14648	0.14886	0.15066	0.15116	0.15241
Alpha virt. eigenvalues --	0.15533	0.15573	0.15690	0.16128	0.16169
Alpha virt. eigenvalues --	0.16334	0.16639	0.16653	0.17040	0.17442
Alpha virt. eigenvalues --	0.17582	0.18100	0.18649	0.18880	0.18947
Alpha virt. eigenvalues --	0.19007	0.19152	0.19246	0.19258	0.19905
Alpha virt. eigenvalues --	0.20136	0.20289	0.20337	0.20661	0.20827
Alpha virt. eigenvalues --	0.20894	0.21109	0.21588	0.21603	0.21622
Alpha virt. eigenvalues --	0.21655	0.21875	0.22186	0.22189	0.23111
Alpha virt. eigenvalues --	0.23226	0.23368	0.23602	0.24103	0.24110
Alpha virt. eigenvalues --	0.24428	0.24478	0.24621	0.24644	0.24948
Alpha virt. eigenvalues --	0.25216	0.25629	0.25978	0.26011	0.26059
Alpha virt. eigenvalues --	0.26461	0.26785	0.27355	0.27512	0.27603
Alpha virt. eigenvalues --	0.27716	0.28165	0.28334	0.28519	0.28954
Alpha virt. eigenvalues --	0.29069	0.29742	0.29944	0.31035	0.32568
Alpha virt. eigenvalues --	0.33026	0.33198	0.33293	0.33757	0.34110
Alpha virt. eigenvalues --	0.35311	0.36003	0.36750	0.36966	0.37224
Alpha virt. eigenvalues --	0.38497	0.38539	0.39185	0.39387	0.39692
Alpha virt. eigenvalues --	0.39771	0.40064	0.40337	0.40547	0.40602
Alpha virt. eigenvalues --	0.40751	0.40982	0.41158	0.41266	0.41309
Alpha virt. eigenvalues --	0.41522	0.41695	0.41843	0.41905	0.41916
Alpha virt. eigenvalues --	0.42622	0.42672	0.42910	0.43029	0.43164
Alpha virt. eigenvalues --	0.43495	0.43634	0.43639	0.43706	0.43821
Alpha virt. eigenvalues --	0.43952	0.44087	0.44236	0.44525	0.44612
Alpha virt. eigenvalues --	0.44641	0.44757	0.44873	0.45035	0.45065
Alpha virt. eigenvalues --	0.45220	0.45221	0.45336	0.45499	0.45624
Alpha virt. eigenvalues --	0.45736	0.45872	0.45901	0.46013	0.46019
Alpha virt. eigenvalues --	0.46136	0.46157	0.46234	0.46315	0.46395
Alpha virt. eigenvalues --	0.46455	0.46483	0.46639	0.46679	0.46850
Alpha virt. eigenvalues --	0.46867	0.46961	0.47022	0.47070	0.47469
Alpha virt. eigenvalues --	0.47572	0.47808	0.47840	0.47965	0.48149
Alpha virt. eigenvalues --	0.48162	0.48197	0.48272	0.48492	0.48815
Alpha virt. eigenvalues --	0.48891	0.49117	0.49176	0.49508	0.49617
Alpha virt. eigenvalues --	0.49867	0.49868	0.49895	0.50226	0.50478
Alpha virt. eigenvalues --	0.50669	0.50682	0.51558	0.51757	0.51821
Alpha virt. eigenvalues --	0.52089	0.52285	0.52489	0.52535	0.52556
Alpha virt. eigenvalues --	0.52635	0.52656	0.52825	0.52914	0.53357
Alpha virt. eigenvalues --	0.53367	0.53684	0.53734	0.53879	0.54010
Alpha virt. eigenvalues --	0.54346	0.54521	0.54707	0.54825	0.55325
Alpha virt. eigenvalues --	0.55447	0.55706	0.55889	0.56287	0.56338
Alpha virt. eigenvalues --	0.56437	0.56749	0.57289	0.57389	0.57588
Alpha virt. eigenvalues --	0.57799	0.58167	0.58286	0.58435	0.58711

Alpha virt. eigenvalues --	0.58794	0.59047	0.59259	0.59686	0.59751
Alpha virt. eigenvalues --	0.59946	0.60092	0.60189	0.60289	0.60403
Alpha virt. eigenvalues --	0.60735	0.60742	0.60855	0.60929	0.61189
Alpha virt. eigenvalues --	0.61312	0.61574	0.61591	0.61639	0.61711
Alpha virt. eigenvalues --	0.61781	0.61801	0.62100	0.62114	0.62313
Alpha virt. eigenvalues --	0.62385	0.62467	0.62568	0.62878	0.63021
Alpha virt. eigenvalues --	0.63042	0.63421	0.63428	0.63563	0.63574
Alpha virt. eigenvalues --	0.63700	0.63701	0.63979	0.64019	0.64064
Alpha virt. eigenvalues --	0.64166	0.64255	0.64267	0.64453	0.64614
Alpha virt. eigenvalues --	0.64838	0.64971	0.65155	0.65215	0.65235
Alpha virt. eigenvalues --	0.65488	0.65558	0.65602	0.65868	0.65887
Alpha virt. eigenvalues --	0.66060	0.66177	0.66281	0.66361	0.66668
Alpha virt. eigenvalues --	0.66698	0.66916	0.67208	0.67227	0.67286
Alpha virt. eigenvalues --	0.67308	0.67434	0.67836	0.67947	0.68051
Alpha virt. eigenvalues --	0.68179	0.68416	0.68635	0.68688	0.69005
Alpha virt. eigenvalues --	0.69171	0.69209	0.69902	0.70084	0.70176
Alpha virt. eigenvalues --	0.70203	0.70403	0.70904	0.70991	0.71341
Alpha virt. eigenvalues --	0.71515	0.71732	0.71815	0.71875	0.72078
Alpha virt. eigenvalues --	0.72327	0.72339	0.72411	0.72441	0.72792
Alpha virt. eigenvalues --	0.72807	0.73162	0.73296	0.73434	0.73501
Alpha virt. eigenvalues --	0.73777	0.73859	0.73956	0.73994	0.74120
Alpha virt. eigenvalues --	0.74195	0.74589	0.74680	0.74692	0.74798
Alpha virt. eigenvalues --	0.74883	0.74908	0.75358	0.75707	0.75785
Alpha virt. eigenvalues --	0.75818	0.75873	0.76923	0.78259	0.78414
Alpha virt. eigenvalues --	0.78684	0.79379	0.79401	0.79867	0.80267
Alpha virt. eigenvalues --	0.80572	0.80982	0.81173	0.81771	0.82087
Alpha virt. eigenvalues --	0.82169	0.82259	0.82986	0.83431	0.83707
Alpha virt. eigenvalues --	0.84035	0.84251	0.85310	0.85423	0.85443
Alpha virt. eigenvalues --	0.85692	0.86084	0.86098	0.86247	0.86387
Alpha virt. eigenvalues --	0.86743	0.86768	0.87481	0.87695	0.87943
Alpha virt. eigenvalues --	0.88550	0.88772	0.88842	0.89559	0.89566
Alpha virt. eigenvalues --	0.89861	0.89967	0.90094	0.90287	0.90701
Alpha virt. eigenvalues --	0.90711	0.90759	0.91033	0.91337	0.91609
Alpha virt. eigenvalues --	0.91664	0.92243	0.92374	0.92685	0.92779
Alpha virt. eigenvalues --	0.92982	0.93399	0.94549	0.94694	0.94951
Alpha virt. eigenvalues --	0.95258	0.95407	0.95636	0.95725	0.96463
Alpha virt. eigenvalues --	0.96515	0.96646	0.96757	0.96861	0.97297
Alpha virt. eigenvalues --	0.97602	0.97775	0.98063	0.98066	0.98312
Alpha virt. eigenvalues --	0.98357	0.98608	0.98635	0.99174	0.99346
Alpha virt. eigenvalues --	0.99705	0.99762	1.00199	1.00507	1.00969
Alpha virt. eigenvalues --	1.01223	1.01326	1.01330	1.01764	1.01851
Alpha virt. eigenvalues --	1.03243	1.03507	1.03643	1.03849	1.04304
Alpha virt. eigenvalues --	1.04357	1.05253	1.05342	1.05572	1.05883
Alpha virt. eigenvalues --	1.06683	1.06684	1.06868	1.07205	1.07345
Alpha virt. eigenvalues --	1.07678	1.08726	1.08810	1.08969	1.09431
Alpha virt. eigenvalues --	1.10282	1.11342	1.11353	1.11636	1.12042
Alpha virt. eigenvalues --	1.12667	1.13166	1.13267	1.13691	1.14008
Alpha virt. eigenvalues --	1.14303	1.14360	1.14845	1.15041	1.15541

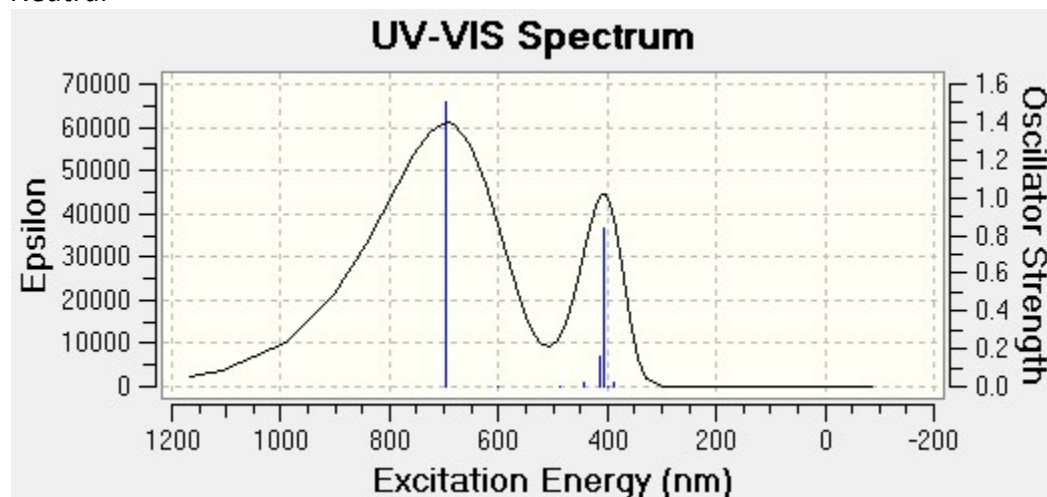
Alpha virt. eigenvalues --	1.15664	1.16468	1.17151	1.17284	1.17493
Alpha virt. eigenvalues --	1.17549	1.17632	1.17710	1.17974	1.18101
Alpha virt. eigenvalues --	1.18453	1.18527	1.18782	1.19241	1.19503
Alpha virt. eigenvalues --	1.20210	1.20305	1.20656	1.21220	1.21463
Alpha virt. eigenvalues --	1.21641	1.21860	1.22081	1.22462	1.22843
Alpha virt. eigenvalues --	1.22903	1.23446	1.23481	1.23574	1.24184
Alpha virt. eigenvalues --	1.24652	1.24776	1.25048	1.25245	1.25632
Alpha virt. eigenvalues --	1.25686	1.25828	1.25830	1.26272	1.26481
Alpha virt. eigenvalues --	1.27008	1.27263	1.27567	1.27589	1.28277
Alpha virt. eigenvalues --	1.28480	1.28789	1.29220	1.29503	1.29530
Alpha virt. eigenvalues --	1.29616	1.30668	1.31055	1.31451	1.31620
Alpha virt. eigenvalues --	1.32260	1.32277	1.32681	1.32698	1.33279
Alpha virt. eigenvalues --	1.33427	1.33731	1.33856	1.33949	1.34556
Alpha virt. eigenvalues --	1.35094	1.35520	1.35866	1.35873	1.36095
Alpha virt. eigenvalues --	1.36143	1.36659	1.37296	1.37463	1.38017
Alpha virt. eigenvalues --	1.38128	1.38396	1.38741	1.38901	1.38919
Alpha virt. eigenvalues --	1.39248	1.39554	1.39866	1.39867	1.39917
Alpha virt. eigenvalues --	1.40004	1.40026	1.40053	1.40329	1.40341
Alpha virt. eigenvalues --	1.40373	1.40380	1.40572	1.40693	1.40988
Alpha virt. eigenvalues --	1.41105	1.41518	1.41973	1.42061	1.42387
Alpha virt. eigenvalues --	1.42506	1.42684	1.42835	1.42870	1.43049
Alpha virt. eigenvalues --	1.43066	1.43252	1.43546	1.43633	1.43788
Alpha virt. eigenvalues --	1.43872	1.44414	1.45106	1.45126	1.45302
Alpha virt. eigenvalues --	1.45333	1.45522	1.45606	1.45883	1.45896
Alpha virt. eigenvalues --	1.46331	1.46580	1.46619	1.47084	1.47278
Alpha virt. eigenvalues --	1.47519	1.48159	1.49005	1.49333	1.49803
Alpha virt. eigenvalues --	1.49920	1.50254	1.50343	1.50593	1.50648
Alpha virt. eigenvalues --	1.50747	1.51014	1.51163	1.51332	1.51869
Alpha virt. eigenvalues --	1.51972	1.52504	1.52953	1.53576	1.53745
Alpha virt. eigenvalues --	1.53819	1.54021	1.54328	1.54670	1.54773
Alpha virt. eigenvalues --	1.55169	1.55434	1.55645	1.55700	1.55752
Alpha virt. eigenvalues --	1.56251	1.56260	1.56465	1.56746	1.56808
Alpha virt. eigenvalues --	1.56946	1.57027	1.57290	1.57579	1.57597
Alpha virt. eigenvalues --	1.57625	1.57770	1.57909	1.58315	1.58425
Alpha virt. eigenvalues --	1.58538	1.59253	1.59266	1.59587	1.59684
Alpha virt. eigenvalues --	1.60208	1.60240	1.60610	1.60679	1.60814
Alpha virt. eigenvalues --	1.60918	1.61020	1.61048	1.61148	1.61352
Alpha virt. eigenvalues --	1.61353	1.61548	1.61789	1.61911	1.61934
Alpha virt. eigenvalues --	1.62436	1.62463	1.62570	1.62871	1.62923
Alpha virt. eigenvalues --	1.63016	1.63385	1.63443	1.63745	1.63823
Alpha virt. eigenvalues --	1.63875	1.63884	1.64107	1.64318	1.64356
Alpha virt. eigenvalues --	1.64882	1.64882	1.65465	1.65677	1.65977
Alpha virt. eigenvalues --	1.66127	1.66556	1.66732	1.67074	1.67093
Alpha virt. eigenvalues --	1.67170	1.67208	1.67350	1.67622	1.67852
Alpha virt. eigenvalues --	1.67993	1.68025	1.68123	1.68567	1.68750
Alpha virt. eigenvalues --	1.68822	1.69645	1.69924	1.70112	1.70118
Alpha virt. eigenvalues --	1.70270	1.70424	1.70482	1.70720	1.70760
Alpha virt. eigenvalues --	1.70793	1.70949	1.71163	1.71212	1.71679

Alpha virt. eigenvalues --	1.71771	1.72029	1.72339	1.72436	1.72495
Alpha virt. eigenvalues --	1.72592	1.72928	1.73312	1.73384	1.73879
Alpha virt. eigenvalues --	1.74032	1.74121	1.74239	1.74746	1.74917
Alpha virt. eigenvalues --	1.75212	1.75505	1.75511	1.75714	1.76132
Alpha virt. eigenvalues --	1.76327	1.76680	1.76882	1.77212	1.77428
Alpha virt. eigenvalues --	1.77486	1.77550	1.77792	1.77825	1.78477
Alpha virt. eigenvalues --	1.78532	1.78867	1.79256	1.79466	1.79576
Alpha virt. eigenvalues --	1.80340	1.80414	1.80769	1.81164	1.81369
Alpha virt. eigenvalues --	1.81430	1.81433	1.81971	1.82165	1.82167
Alpha virt. eigenvalues --	1.82334	1.82817	1.82913	1.83031	1.83404
Alpha virt. eigenvalues --	1.83734	1.84032	1.84382	1.84469	1.84732
Alpha virt. eigenvalues --	1.84893	1.84934	1.85020	1.85316	1.85331
Alpha virt. eigenvalues --	1.85824	1.85873	1.86079	1.86443	1.86513
Alpha virt. eigenvalues --	1.86630	1.86901	1.87128	1.87169	1.87242
Alpha virt. eigenvalues --	1.87936	1.88148	1.88763	1.88946	1.89914
Alpha virt. eigenvalues --	1.89945	1.90271	1.90602	1.90758	1.91075
Alpha virt. eigenvalues --	1.91690	1.92068	1.92265	1.92344	1.92859
Alpha virt. eigenvalues --	1.93406	1.93731	1.94385	1.94822	1.94924
Alpha virt. eigenvalues --	1.95270	1.95385	1.95503	1.95612	1.95901
Alpha virt. eigenvalues --	1.95910	1.97070	1.97397	1.97477	1.97704
Alpha virt. eigenvalues --	1.97761	1.98533	1.98535	1.98695	1.98820
Alpha virt. eigenvalues --	1.98840	1.99026	1.99311	1.99401	1.99910
Alpha virt. eigenvalues --	1.99947	2.00540	2.01474	2.01512	2.01748
Alpha virt. eigenvalues --	2.01868	2.01869	2.02076	2.02095	2.03228
Alpha virt. eigenvalues --	2.04046	2.04094	2.05042	2.05114	2.05364
Alpha virt. eigenvalues --	2.05789	2.05791	2.06057	2.06187	2.06828
Alpha virt. eigenvalues --	2.06909	2.07203	2.07309	2.07550	2.07802
Alpha virt. eigenvalues --	2.08002	2.08565	2.08636	2.08722	2.08936
Alpha virt. eigenvalues --	2.09574	2.10358	2.10476	2.11315	2.11396
Alpha virt. eigenvalues --	2.11436	2.11714	2.11837	2.12241	2.12479
Alpha virt. eigenvalues --	2.12840	2.13209	2.13321	2.13339	2.15373
Alpha virt. eigenvalues --	2.15542	2.16150	2.16167	2.16530	2.16536
Alpha virt. eigenvalues --	2.16841	2.16983	2.17444	2.17472	2.17693
Alpha virt. eigenvalues --	2.17743	2.18666	2.18748	2.19883	2.19959
Alpha virt. eigenvalues --	2.20404	2.20691	2.20942	2.20985	2.21848
Alpha virt. eigenvalues --	2.21854	2.23104	2.23372	2.23828	2.24006
Alpha virt. eigenvalues --	2.24492	2.24650	2.25170	2.25290	2.25716
Alpha virt. eigenvalues --	2.26486	2.26643	2.28296	2.28671	2.28928
Alpha virt. eigenvalues --	2.28993	2.29148	2.30088	2.30166	2.30739
Alpha virt. eigenvalues --	2.31540	2.32306	2.32388	2.32536	2.33047
Alpha virt. eigenvalues --	2.33074	2.34114	2.34524	2.35019	2.36390
Alpha virt. eigenvalues --	2.36776	2.36814	2.37171	2.37752	2.37779
Alpha virt. eigenvalues --	2.38734	2.38791	2.38852	2.39338	2.39881
Alpha virt. eigenvalues --	2.39928	2.40517	2.41003	2.41113	2.41196
Alpha virt. eigenvalues --	2.41425	2.41429	2.41889	2.41941	2.42015
Alpha virt. eigenvalues --	2.42082	2.42340	2.42397	2.42543	2.42927
Alpha virt. eigenvalues --	2.43053	2.43083	2.43834	2.43847	2.44053
Alpha virt. eigenvalues --	2.44166	2.44243	2.44297	2.45005	2.45040

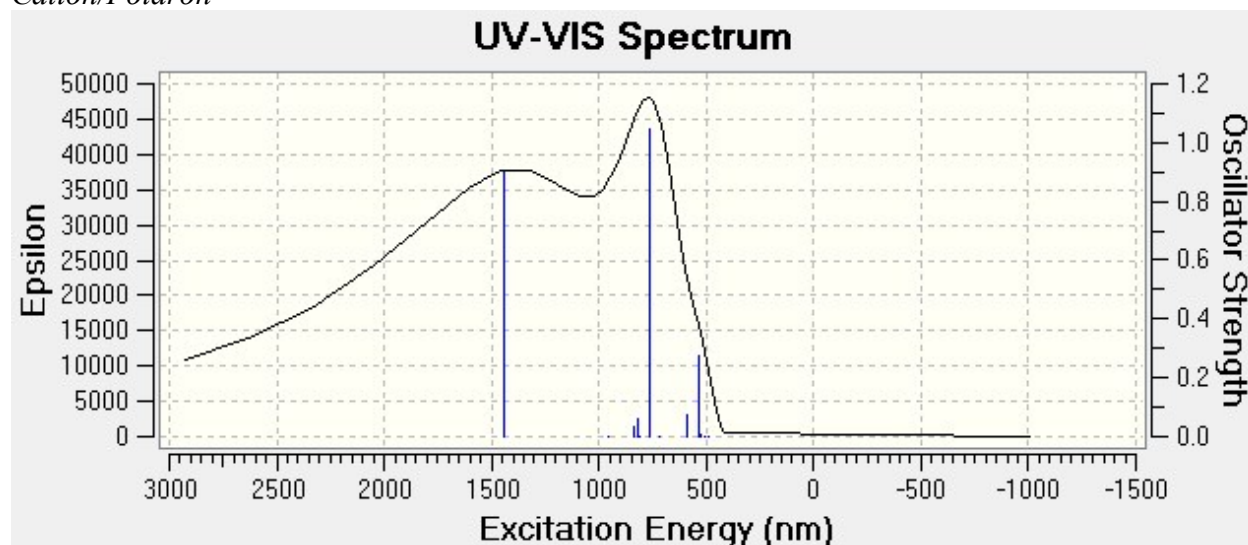
Alpha virt. eigenvalues --	2.45277	2.45317	2.46037	2.46062	2.46394
Alpha virt. eigenvalues --	2.46607	2.46901	2.46901	2.47015	2.47018
Alpha virt. eigenvalues --	2.47987	2.48055	2.48083	2.48307	2.48429
Alpha virt. eigenvalues --	2.48479	2.49071	2.49088	2.49494	2.49655
Alpha virt. eigenvalues --	2.49893	2.50861	2.51293	2.51601	2.51885
Alpha virt. eigenvalues --	2.52534	2.52542	2.53162	2.53743	2.53744
Alpha virt. eigenvalues --	2.54451	2.54493	2.55047	2.55050	2.55902
Alpha virt. eigenvalues --	2.56167	2.56344	2.56407	2.56728	2.56732
Alpha virt. eigenvalues --	2.58064	2.58820	2.59180	2.60143	2.61913
Alpha virt. eigenvalues --	2.62221	2.64942	2.65671	2.67034	2.67227
Alpha virt. eigenvalues --	2.68453	2.68881	2.69775	2.69841	2.72048
Alpha virt. eigenvalues --	2.72463	2.75616	2.75783	2.77839	2.78090
Alpha virt. eigenvalues --	2.79907	2.80407	2.81766	2.81869	2.87334
Alpha virt. eigenvalues --	2.87432	2.89233	2.89239	2.91033	2.91304
Alpha virt. eigenvalues --	2.92345	2.92379	2.93100	2.93184	2.94784
Alpha virt. eigenvalues --	2.95047	2.96910	2.96937	2.97177	2.97249
Alpha virt. eigenvalues --	2.97780	2.97781	2.97982	2.98100	2.98619
Alpha virt. eigenvalues --	2.98637	3.00829	3.00867	3.01338	3.01339
Alpha virt. eigenvalues --	3.01576	3.01720	3.02564	3.02568	3.06354
Alpha virt. eigenvalues --	3.06516	3.06942	3.06942	3.07149	3.07172
Alpha virt. eigenvalues --	3.07490	3.07650	3.07650	3.08468	3.08888
Alpha virt. eigenvalues --	3.08888	3.09325	3.10329	3.10913	3.10957
Alpha virt. eigenvalues --	3.11112	3.11190	3.11721	3.11739	3.22718
Alpha virt. eigenvalues --	3.22801	3.23155	3.23155	3.24737	3.24809
Alpha virt. eigenvalues --	3.25228	3.25228	3.28073	3.28147	3.29461
Alpha virt. eigenvalues --	3.29461	3.31540	3.31698	3.35125	3.35340
Alpha virt. eigenvalues --	3.35747	3.35769	3.36090	3.36091	3.36268
Alpha virt. eigenvalues --	3.36275	3.37130	3.37760	3.39245	3.39614
Alpha virt. eigenvalues --	3.40364	3.40677	3.41754	3.41763	3.47110
Alpha virt. eigenvalues --	3.48324	3.49726	3.49843		

Cyan UV-Vis Spectrum Epsilon/Oscillator Strength – N = 2

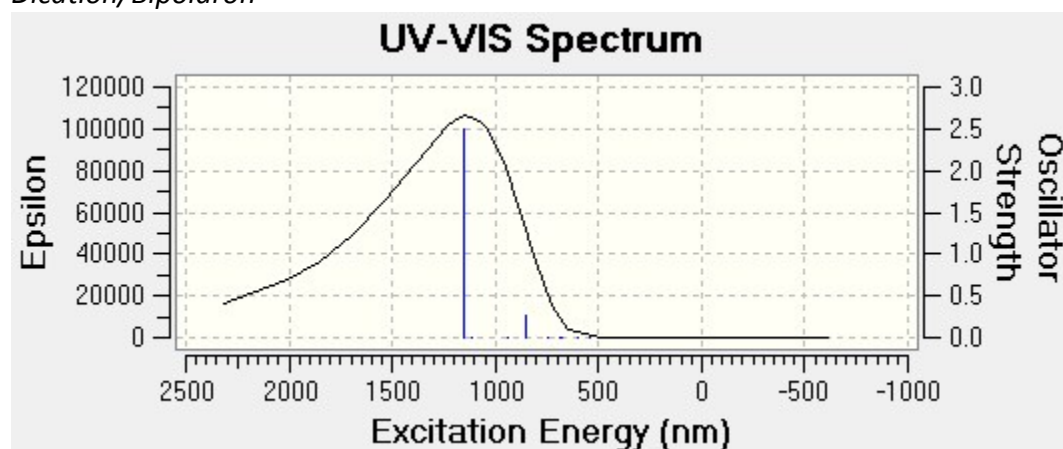
Neutral



Cation/Polaron



Dication/Bipolaron



Cyan Table of Excited States – N = 2

Neutral – 10 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	1.78	695.32	1.5050
2	2.06	600.97	0.0017
3	2.55	487.08	0.0038
4	2.80	442.39	0.0257
5	2.99	414.75	0.1588
6	3.04	407.41	0.0682
7	3.04	407.36	0.0046
8	3.06	405.19	0.8385
9	3.12	397.18	0.0000
10	3.21	386.53	0.0217

Cation/Polaron – 15 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	0.86	1438.06	0.8975
2	1.30	954.69	0.0004
3	1.49	834.36	0.0006
4	1.49	834.20	0.0321
5	1.51	821.38	0.0605
6	1.53	809.66	0.0002
7	1.62	764.72	1.0450
8	1.73	718.04	0.0011
9	2.12	585.16	0.0765
10	2.30	538.71	0.2734
11	2.37	522.73	0.0038
12	2.46	503.32	0.0000
13	2.46	503.30	0.0000
14	2.54	487.84	0.0031
15	2.56	484.27	0.0000

Dication/Bipolaron – 15 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	1.08	1152.71	2.5018
2	1.12	1110.05	0.0007
3	1.12	1109.97	0.0067
4	1.32	942.51	0.0000
5	1.45	855.94	0.2623
6	1.67	742.22	0.0038
7	1.81	684.96	0.0000
8	1.81	684.91	0.0000
9	1.83	678.71	0.0000
10	1.83	678.70	0.0001
11	2.06	602.12	0.0002
12	2.06	601.51	0.0002
13	2.06	601.50	0.0000
14	2.06	601.36	0.0000
15	2.28	544.62	0.0035

Magenta Cartesian Coordinates – N = 2

C 1.57282 -2.79698 0.10219
 C 2.47911 -1.77312 0.07007
 S -0.05498 -2.22132 0.08897
 C 1.84622 -0.48769 0.04042
 O 3.82055 -1.9794 0.09945
 C 0.46584 -0.55167 0.0436
 O 2.494 0.7023 -0.01953
 C 4.5945 -1.09581 -0.70886
 C 3.71445 0.7895 0.71593

H	5.52016	-1.64182	-0.93803
H	4.06556	-0.89981	-1.65362
C	4.93516	0.24163	-0.03495
H	3.85317	1.8588	0.92642
H	3.60611	0.25824	1.67299
C	6.08235	0.10241	0.96975
C	5.42667	1.20644	-1.11824
H	7.00588	-0.19392	0.43263
H	6.28595	1.08642	1.44028
O	5.76026	-0.84875	1.94989
H	5.77158	2.14758	-0.64448
H	6.30498	0.76619	-1.63425
O	4.40232	1.46946	-2.03987
C	6.78112	-0.99031	2.90614
C	4.82328	2.3281	-3.07057
H	6.45107	-1.74515	3.63108
H	7.72818	-1.32678	2.44477
H	6.97564	-0.04129	3.4398
H	3.97	2.47655	-3.74444
H	5.14421	3.31076	-2.67766
H	5.6635	1.89533	-3.64508
C	-0.46584	0.5518	0.04347
C	-1.84622	0.48776	0.04031
S	0.05491	2.22148	0.08854
C	-2.47917	1.77317	0.0697
O	-2.49391	-0.70229	-0.01938
C	-1.57291	2.79707	0.10167
O	-3.82061	1.97943	0.099
C	-3.71437	-0.78942	0.71608
H	-1.78802	3.86174	0.1169
C	-4.59454	1.0956	-0.70906
H	-3.85305	-1.8587	0.92673
H	-3.60603	-0.25802	1.67306
C	-4.93511	-0.24171	-0.03486
H	-5.52025	1.6415	-0.93831
H	-4.06564	0.89943	-1.65381
C	-5.42671	-1.20675	-1.11793
C	-6.08223	-0.10229	0.9699
H	-5.77165	-2.14777	-0.64395
H	-6.30501	-0.76657	-1.63401
O	-4.40241	-1.47004	-2.03955
H	-7.00581	0.19389	0.43278
H	-6.28576	-1.08619	1.44067
O	-5.76007	0.8491	1.94978
C	-4.82347	-2.32886	-3.07007
C	-6.78095	0.99106	2.90595
H	-3.9702	-2.47758	-3.74388
H	-5.14454	-3.31138	-2.67694

H	-5.66362	-1.8961	-3.64468
H	-6.45083	1.74606	3.63069
H	-7.72794	1.32752	2.44444
H	-6.97561	0.04222	3.43987
H	1.78793	-3.86166	0.11766

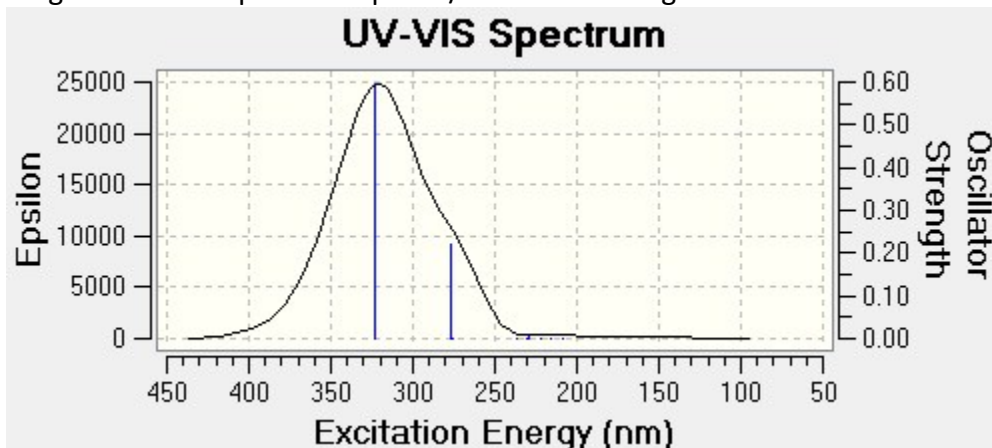
Magenta Energy Levels – N = 2

Alpha occ. eigenvalues --	-89.09314	-89.09314	-19.26336	-19.26335	-19.25721
Alpha occ. eigenvalues --	-19.25721	-19.23584	-19.23584	-19.23549	-19.23549
Alpha occ. eigenvalues --	-10.30317	-10.30317	-10.30272	-10.30272	-10.29663
Alpha occ. eigenvalues --	-10.29663	-10.29467	-10.29467	-10.29251	-10.29251
Alpha occ. eigenvalues --	-10.29233	-10.29233	-10.28182	-10.28165	-10.28165
Alpha occ. eigenvalues --	-10.28147	-10.28134	-10.28134	-10.26352	-10.26352
Alpha occ. eigenvalues --	-10.26147	-10.26147	-8.03637	-8.03637	-5.97522
Alpha occ. eigenvalues --	-5.97521	-5.97153	-5.97152	-5.96747	-5.96747
Alpha occ. eigenvalues --	-1.11552	-1.11499	-1.09172	-1.09151	-1.07750
Alpha occ. eigenvalues --	-1.07749	-1.07575	-1.07575	-0.91991	-0.90011
Alpha occ. eigenvalues --	-0.85739	-0.85721	-0.79785	-0.76812	-0.75802
Alpha occ. eigenvalues --	-0.75635	-0.74498	-0.74485	-0.72254	-0.71396
Alpha occ. eigenvalues --	-0.71296	-0.69015	-0.68181	-0.68009	-0.64499
Alpha occ. eigenvalues --	-0.64482	-0.62404	-0.60909	-0.59813	-0.59542
Alpha occ. eigenvalues --	-0.58024	-0.56674	-0.53937	-0.53081	-0.53079
Alpha occ. eigenvalues --	-0.52816	-0.51976	-0.51827	-0.50476	-0.50230
Alpha occ. eigenvalues --	-0.49829	-0.48654	-0.48629	-0.48508	-0.48039
Alpha occ. eigenvalues --	-0.47626	-0.47250	-0.47006	-0.46705	-0.46185
Alpha occ. eigenvalues --	-0.45878	-0.45609	-0.43995	-0.43899	-0.43314
Alpha occ. eigenvalues --	-0.42940	-0.42591	-0.41622	-0.41061	-0.40987
Alpha occ. eigenvalues --	-0.40315	-0.40047	-0.39980	-0.39465	-0.39419
Alpha occ. eigenvalues --	-0.37741	-0.37576	-0.36905	-0.36841	-0.36215
Alpha occ. eigenvalues --	-0.35890	-0.34469	-0.34460	-0.33811	-0.33548
Alpha occ. eigenvalues --	-0.33096	-0.33066	-0.32254	-0.31931	-0.30544
Alpha occ. eigenvalues --	-0.30337	-0.27783	-0.27770	-0.27000	-0.26989
Alpha occ. eigenvalues --	-0.26885	-0.23074	-0.22875	-0.19902	
Alpha virt. eigenvalues --	-0.03597	0.02722	0.04516	0.04786	0.06123
Alpha virt. eigenvalues --	0.06353	0.06459	0.08140	0.08163	0.08361
Alpha virt. eigenvalues --	0.08948	0.09443	0.10081	0.10103	0.10373
Alpha virt. eigenvalues --	0.10457	0.10948	0.11892	0.11969	0.12245
Alpha virt. eigenvalues --	0.13225	0.13256	0.13459	0.13691	0.14001
Alpha virt. eigenvalues --	0.14093	0.14132	0.14282	0.14285	0.14399
Alpha virt. eigenvalues --	0.14988	0.15031	0.15354	0.15467	0.15881
Alpha virt. eigenvalues --	0.16876	0.17030	0.17258	0.17797	0.18461
Alpha virt. eigenvalues --	0.18592	0.18975	0.20075	0.20611	0.21343
Alpha virt. eigenvalues --	0.21564	0.21853	0.22999	0.23142	0.23857
Alpha virt. eigenvalues --	0.23970	0.24115	0.25527	0.26041	0.26100
Alpha virt. eigenvalues --	0.27546	0.27999	0.28299	0.28553	0.29526
Alpha virt. eigenvalues --	0.29544	0.30073	0.30092	0.32585	0.34293
Alpha virt. eigenvalues --	0.38605	0.38876	0.41816	0.42163	0.43042
Alpha virt. eigenvalues --	0.43210	0.44521	0.44614	0.44717	0.45406

Alpha virt. eigenvalues --	0.45771	0.46136	0.46502	0.46837	0.46840
Alpha virt. eigenvalues --	0.47118	0.47280	0.47502	0.47622	0.47982
Alpha virt. eigenvalues --	0.48049	0.48493	0.48717	0.49026	0.49496
Alpha virt. eigenvalues --	0.49600	0.50164	0.50228	0.50609	0.51223
Alpha virt. eigenvalues --	0.51582	0.51947	0.52259	0.52337	0.53082
Alpha virt. eigenvalues --	0.53738	0.53749	0.54766	0.55443	0.55767
Alpha virt. eigenvalues --	0.56001	0.56107	0.57005	0.57106	0.57962
Alpha virt. eigenvalues --	0.57991	0.60148	0.60332	0.60743	0.60806
Alpha virt. eigenvalues --	0.61484	0.61487	0.62205	0.62212	0.62831
Alpha virt. eigenvalues --	0.62952	0.63310	0.63430	0.63938	0.63965
Alpha virt. eigenvalues --	0.64151	0.64201	0.64875	0.64879	0.65398
Alpha virt. eigenvalues --	0.65561	0.66010	0.66402	0.66432	0.66773
Alpha virt. eigenvalues --	0.66931	0.67068	0.67177	0.67373	0.67886
Alpha virt. eigenvalues --	0.68401	0.68454	0.68566	0.68850	0.69399
Alpha virt. eigenvalues --	0.69603	0.69974	0.70641	0.70818	0.71255
Alpha virt. eigenvalues --	0.71773	0.72203	0.73055	0.73614	0.73659
Alpha virt. eigenvalues --	0.74392	0.74702	0.74959	0.75267	0.75329
Alpha virt. eigenvalues --	0.76223	0.76326	0.76423	0.77140	0.77628
Alpha virt. eigenvalues --	0.77740	0.78681	0.80397	0.81630	0.82410
Alpha virt. eigenvalues --	0.83781	0.84014	0.86395	0.87126	0.88028
Alpha virt. eigenvalues --	0.88123	0.88477	0.88540	0.88799	0.91187
Alpha virt. eigenvalues --	0.91574	0.91858	0.92232	0.92439	0.93407
Alpha virt. eigenvalues --	0.95102	0.97473	0.97762	0.98318	0.99259
Alpha virt. eigenvalues --	0.99596	1.00028	1.01086	1.01446	1.01835
Alpha virt. eigenvalues --	1.02988	1.03186	1.04447	1.04622	1.05911
Alpha virt. eigenvalues --	1.07519	1.07621	1.09246	1.09771	1.12371
Alpha virt. eigenvalues --	1.13284	1.13635	1.14176	1.15073	1.16621
Alpha virt. eigenvalues --	1.16814	1.17405	1.18674	1.19584	1.19791
Alpha virt. eigenvalues --	1.19916	1.20465	1.21736	1.23035	1.23131
Alpha virt. eigenvalues --	1.23921	1.24306	1.24630	1.25973	1.26833
Alpha virt. eigenvalues --	1.27250	1.27694	1.27738	1.29034	1.29543
Alpha virt. eigenvalues --	1.30030	1.31777	1.32214	1.32568	1.33521
Alpha virt. eigenvalues --	1.34389	1.34803	1.35219	1.36811	1.36936
Alpha virt. eigenvalues --	1.38328	1.39511	1.39805	1.40332	1.41169
Alpha virt. eigenvalues --	1.41302	1.41354	1.41522	1.41526	1.42548
Alpha virt. eigenvalues --	1.42714	1.42915	1.43765	1.44035	1.44608
Alpha virt. eigenvalues --	1.45038	1.45266	1.45351	1.45507	1.47345
Alpha virt. eigenvalues --	1.47551	1.48379	1.48584	1.49736	1.50828
Alpha virt. eigenvalues --	1.51590	1.52464	1.52738	1.53595	1.53641
Alpha virt. eigenvalues --	1.55112	1.55119	1.56434	1.56570	1.56617
Alpha virt. eigenvalues --	1.57522	1.57898	1.58356	1.58914	1.59234
Alpha virt. eigenvalues --	1.59243	1.59868	1.60594	1.61720	1.62155
Alpha virt. eigenvalues --	1.62665	1.62800	1.62997	1.63179	1.63263
Alpha virt. eigenvalues --	1.63927	1.64051	1.64106	1.64757	1.65204
Alpha virt. eigenvalues --	1.65425	1.65790	1.66660	1.66916	1.68215
Alpha virt. eigenvalues --	1.68463	1.69022	1.69409	1.70019	1.70772
Alpha virt. eigenvalues --	1.71115	1.71175	1.72098	1.72214	1.72428
Alpha virt. eigenvalues --	1.72646	1.73453	1.74163	1.74678	1.75267

Alpha virt. eigenvalues --	1.75640	1.76903	1.77230	1.77547	1.77893
Alpha virt. eigenvalues --	1.78621	1.79123	1.79446	1.79533	1.79902
Alpha virt. eigenvalues --	1.81298	1.82265	1.83026	1.83242	1.83261
Alpha virt. eigenvalues --	1.83353	1.84508	1.84584	1.85864	1.86264
Alpha virt. eigenvalues --	1.87003	1.87244	1.87369	1.87769	1.88206
Alpha virt. eigenvalues --	1.88351	1.89337	1.89486	1.91367	1.92394
Alpha virt. eigenvalues --	1.93664	1.94100	1.95942	1.97142	1.97358
Alpha virt. eigenvalues --	1.98504	1.98869	1.99113	2.00121	2.00493
Alpha virt. eigenvalues --	2.00554	2.00897	2.01648	2.02474	2.03314
Alpha virt. eigenvalues --	2.03573	2.04681	2.05207	2.07006	2.07029
Alpha virt. eigenvalues --	2.07298	2.08097	2.09341	2.09903	2.10308
Alpha virt. eigenvalues --	2.11013	2.13086	2.13108	2.13249	2.13782
Alpha virt. eigenvalues --	2.14913	2.15091	2.17199	2.17618	2.19138
Alpha virt. eigenvalues --	2.19456	2.20651	2.20726	2.22865	2.22866
Alpha virt. eigenvalues --	2.23841	2.24892	2.26587	2.27429	2.28934
Alpha virt. eigenvalues --	2.30582	2.30898	2.31516	2.33579	2.34248
Alpha virt. eigenvalues --	2.34882	2.35147	2.38592	2.38622	2.39797
Alpha virt. eigenvalues --	2.40367	2.42623	2.42655	2.43056	2.43122
Alpha virt. eigenvalues --	2.43872	2.44114	2.44785	2.44976	2.45800
Alpha virt. eigenvalues --	2.45882	2.46189	2.46618	2.48203	2.48337
Alpha virt. eigenvalues --	2.48980	2.49096	2.49390	2.50099	2.50493
Alpha virt. eigenvalues --	2.50578	2.52313	2.53102	2.54194	2.54374
Alpha virt. eigenvalues --	2.54990	2.56332	2.56462	2.57411	2.58526
Alpha virt. eigenvalues --	2.58897	2.60870	2.61548	2.69298	2.69919
Alpha virt. eigenvalues --	2.80558	2.82417	2.92256	2.92673	2.95004
Alpha virt. eigenvalues --	2.95517	2.98438	2.98746	2.99352	2.99410
Alpha virt. eigenvalues --	3.00125	3.00284	3.03051	3.03114	3.04165
Alpha virt. eigenvalues --	3.04463	3.08429	3.08462	3.09113	3.09116
Alpha virt. eigenvalues --	3.11237	3.11253	3.12124	3.13561	3.13770
Alpha virt. eigenvalues --	3.13816	3.24612	3.24665	3.26746	3.26776
Alpha virt. eigenvalues --	3.32148	3.32175	3.37499	3.37624	3.37765
Alpha virt. eigenvalues --	3.37778	3.41336	3.41839	3.43114	3.44087
Alpha virt. eigenvalues --	3.52001	3.52911			

Magenta UV-Vis Spectrum Epsilon/Oscillator Strength – N = 2



Magenta Table of 10 Lowest Excited States – N = 2

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	3.84	322.62	0.5951
2	4.48	276.57	0.2211
3	4.50	275.31	0.0000
4	5.25	236.36	0.0000
5	5.39	230.08	0.0000
6	5.40	229.56	0.0034
7	5.58	222.17	0.0019
8	5.75	215.47	0.0000
9	5.75	215.36	0.0001
10	5.94	208.81	0.0002

Magenta Cartesian Coordinates – N = 3

```

C      0.81682  2.66579 -0.14651
C     -0.45814  3.202   -0.14729
C     -0.47983  4.63097 -0.24093
C      0.77778  5.16673 -0.29754
S      2.00241  3.94977 -0.2488
O     -1.60238  5.39395 -0.23988
O     -1.55608  2.40699 -0.09576
C     -2.6548   2.90959  0.66435
H     -3.22332  2.02368  0.97927
H     -2.2776   3.41931  1.56321
C     -2.71887  4.84989 -0.941
H     -3.33299  5.71424 -1.22992
H     -2.37233  4.35066 -1.85833
C     -3.5637   3.86547 -0.11951
C     -4.48942  3.11566 -1.08203
H     -5.18696  2.48066 -0.49938
H     -5.11097  3.84363 -1.64361
C     -4.47318  4.58202  0.88278
H     -5.21576  5.194   0.33215
H     -5.04558  3.8317   1.46691
O     -3.73869  2.3298  -1.9693
O     -3.71362  5.3904   1.74176
C     -4.55224  1.63176 -2.87873
H     -3.89056  1.0477  -3.53093
H     -5.24412  0.94203 -2.36024
H     -5.15392  2.31983 -3.50158
C     -4.51199  6.04947  2.69303
H     -3.84487  6.65247  3.322
H     -5.25149  6.71677  2.21256
H     -5.05931  5.33356  3.33438
C      1.18395  1.27496 -0.05738
C      2.45847  0.74209 -0.0135
S     -0.01158 -0.00096  0.03047

```

C	2.47718	-0.67728	0.09255
O	3.55579	1.53246	-0.1026
C	1.21723	-1.24414	0.12595
O	3.5997	-1.43396	0.18596
C	4.69204	1.12659	0.65982
C	4.69005	-1.03231	-0.64476
H	5.27488	2.04293	0.82479
H	4.36261	0.7435	1.63681
C	5.56505	0.07116	-0.03183
H	5.28752	-1.94013	-0.80447
H	4.30403	-0.69348	-1.61746
C	6.4212	0.67405	-1.14967
C	6.54217	-0.48432	1.00848
H	7.1349	1.40189	-0.71375
H	7.02756	-0.12524	-1.62389
O	5.60675	1.299	-2.10588
H	7.25689	-1.17024	0.5109
H	7.1392	0.3464	1.43792
O	5.84275	-1.15772	2.0213
C	6.35382	1.84174	-3.166
C	6.70194	-1.67672	3.00575
H	5.6452	2.30278	-3.86565
H	7.06187	2.61426	-2.8127
H	6.93058	1.06351	-3.69994
H	6.07812	-2.1838	3.75268
H	7.41579	-2.40631	2.58024
H	7.28152	-0.87798	3.50505
C	0.88534	-2.64441	0.20641
C	-0.37508	-3.21341	0.18369
S	2.10219	-3.89715	0.32447
C	-0.36111	-4.64274	0.27262
O	-1.49187	-2.44719	0.1153
C	0.90893	-5.14573	0.3491
O	-1.46368	-5.4341	0.25007
C	-2.5663	-2.97624	-0.66138
H	1.19639	-6.1902	0.42939
C	-2.60407	-4.92226	0.93719
H	-3.15212	-2.10435	-0.98363
H	-2.16325	-3.47492	-1.55518
C	-3.46193	-3.95548	0.10806
H	-3.19985	-5.80347	1.21313
H	-2.28381	-4.41869	1.86172
C	-4.41714	-3.23086	1.06114
C	-4.34223	-4.68962	-0.90749
H	-5.12356	-2.61218	0.47159
H	-5.02686	-3.97549	1.61383
O	-3.69679	-2.42853	1.95884
H	-5.0791	-5.31805	-0.3678

H	-4.92228	-3.95036	-1.49803
O	-3.55455	-5.48047	-1.7575
C	-4.5384	-1.75172	2.85873
C	-4.32625	-6.15288	-2.72138
H	-3.89911	-1.15535	3.52201
H	-5.23799	-1.0756	2.33267
H	-5.13344	-2.45507	3.47079
H	-3.63877	-6.74266	-3.34087
H	-5.0605	-6.83424	-2.25278
H	-4.87693	-5.44634	-3.37021
H	1.03929	6.21807	-0.37669

Magenta Energy Levels – N = 3

Alpha occ. eigenvalues --	-89.09285	-89.09262	-89.09221	-19.26363	-19.26319
Alpha occ. eigenvalues --	-19.26293	-19.26270	-19.25734	-19.25718	-19.23583
Alpha occ. eigenvalues --	-19.23576	-19.23571	-19.23570	-19.23565	-19.23531
Alpha occ. eigenvalues --	-10.30381	-10.30323	-10.30295	-10.30270	-10.30252
Alpha occ. eigenvalues --	-10.30218	-10.29686	-10.29658	-10.29652	-10.29636
Alpha occ. eigenvalues --	-10.29494	-10.29483	-10.29263	-10.29260	-10.29257
Alpha occ. eigenvalues --	-10.29255	-10.29246	-10.29239	-10.28174	-10.28174
Alpha occ. eigenvalues --	-10.28173	-10.28172	-10.28168	-10.28161	-10.28125
Alpha occ. eigenvalues --	-10.28106	-10.28025	-10.27963	-10.26421	-10.26358
Alpha occ. eigenvalues --	-10.26349	-10.26133	-10.26097	-8.03606	-8.03584
Alpha occ. eigenvalues --	-8.03488	-5.97491	-5.97469	-5.97390	-5.97123
Alpha occ. eigenvalues --	-5.97100	-5.97011	-5.96715	-5.96693	-5.96564
Alpha occ. eigenvalues --	-1.11790	-1.11521	-1.11494	-1.09447	-1.09143
Alpha occ. eigenvalues --	-1.09124	-1.07760	-1.07758	-1.07739	-1.07586
Alpha occ. eigenvalues --	-1.07584	-1.07560	-0.92387	-0.91108	-0.89691
Alpha occ. eigenvalues --	-0.85788	-0.85758	-0.85709	-0.81016	-0.77973
Alpha occ. eigenvalues --	-0.76471	-0.76345	-0.75647	-0.75453	-0.74507
Alpha occ. eigenvalues --	-0.74506	-0.74481	-0.72560	-0.71843	-0.71345
Alpha occ. eigenvalues --	-0.71319	-0.71098	-0.68390	-0.68213	-0.68033
Alpha occ. eigenvalues --	-0.67910	-0.64530	-0.64498	-0.64475	-0.63299
Alpha occ. eigenvalues --	-0.61609	-0.60784	-0.59853	-0.59752	-0.59140
Alpha occ. eigenvalues --	-0.58351	-0.56943	-0.56344	-0.54018	-0.53329
Alpha occ. eigenvalues --	-0.53109	-0.53073	-0.53044	-0.52745	-0.52035
Alpha occ. eigenvalues --	-0.51898	-0.51824	-0.50643	-0.50365	-0.49928
Alpha occ. eigenvalues --	-0.49896	-0.49322	-0.48676	-0.48653	-0.48637
Alpha occ. eigenvalues --	-0.48599	-0.48271	-0.47973	-0.47371	-0.47327
Alpha occ. eigenvalues --	-0.47164	-0.46937	-0.46788	-0.46238	-0.45976
Alpha occ. eigenvalues --	-0.45902	-0.45882	-0.44744	-0.44048	-0.43982
Alpha occ. eigenvalues --	-0.43541	-0.43515	-0.43141	-0.42672	-0.42566
Alpha occ. eigenvalues --	-0.42259	-0.41583	-0.41149	-0.41031	-0.41024
Alpha occ. eigenvalues --	-0.40184	-0.40077	-0.40008	-0.39974	-0.39587
Alpha occ. eigenvalues --	-0.39433	-0.39078	-0.37895	-0.37766	-0.37675
Alpha occ. eigenvalues --	-0.37109	-0.36833	-0.36531	-0.36467	-0.35819
Alpha occ. eigenvalues --	-0.35684	-0.34497	-0.34489	-0.34454	-0.33821
Alpha occ. eigenvalues --	-0.33778	-0.33462	-0.33097	-0.33056	-0.33042

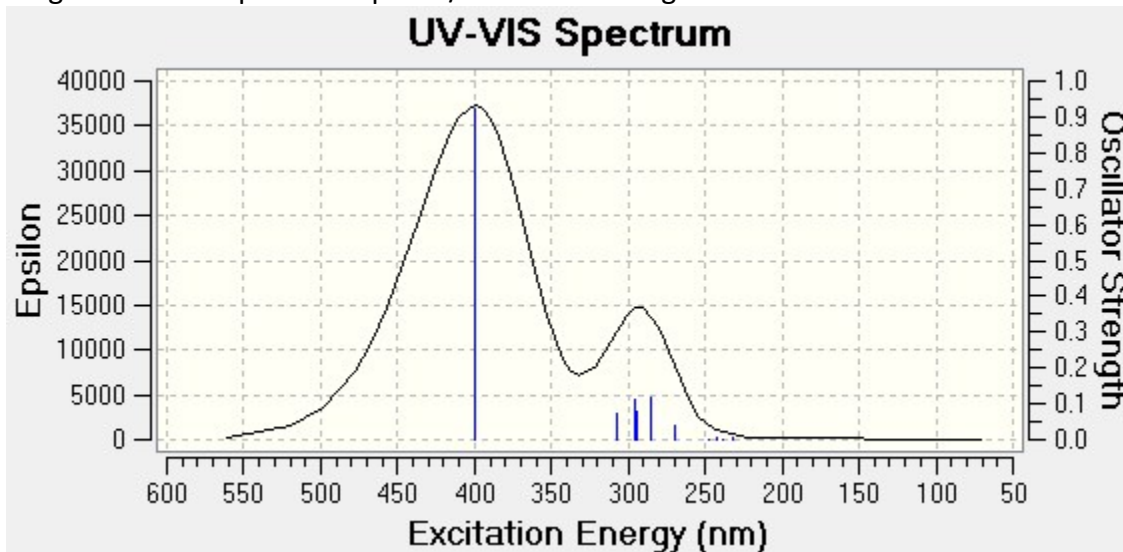
Alpha occ. eigenvalues --	-0.32297	-0.32181	-0.32008	-0.30701	-0.30433
Alpha occ. eigenvalues --	-0.30333	-0.27802	-0.27781	-0.27755	-0.27752
Alpha occ. eigenvalues --	-0.27009	-0.26997	-0.26972	-0.24363	-0.22963
Alpha occ. eigenvalues --	-0.22925	-0.22605	-0.18387		
Alpha virt. eigenvalues --	-0.04955	-0.00268	0.03965	0.04148	0.04578
Alpha virt. eigenvalues --	0.04958	0.05562	0.05692	0.06366	0.06820
Alpha virt. eigenvalues --	0.07550	0.07795	0.08023	0.08189	0.08422
Alpha virt. eigenvalues --	0.08920	0.09339	0.09390	0.09965	0.09988
Alpha virt. eigenvalues --	0.10234	0.10527	0.10787	0.11063	0.11132
Alpha virt. eigenvalues --	0.11646	0.11856	0.12031	0.12111	0.12675
Alpha virt. eigenvalues --	0.13143	0.13238	0.13437	0.13603	0.13751
Alpha virt. eigenvalues --	0.13821	0.14046	0.14089	0.14166	0.14207
Alpha virt. eigenvalues --	0.14290	0.14331	0.14505	0.14871	0.14928
Alpha virt. eigenvalues --	0.15032	0.15085	0.15195	0.15408	0.15619
Alpha virt. eigenvalues --	0.15666	0.16283	0.17024	0.17040	0.17526
Alpha virt. eigenvalues --	0.17554	0.17861	0.18110	0.18293	0.18610
Alpha virt. eigenvalues --	0.18662	0.19373	0.19627	0.20349	0.20570
Alpha virt. eigenvalues --	0.20906	0.21555	0.21712	0.21909	0.22298
Alpha virt. eigenvalues --	0.23009	0.23134	0.23191	0.23776	0.24092
Alpha virt. eigenvalues --	0.24141	0.24388	0.25242	0.25665	0.25955
Alpha virt. eigenvalues --	0.26113	0.26808	0.27499	0.28012	0.28066
Alpha virt. eigenvalues --	0.28345	0.28625	0.28784	0.29596	0.29704
Alpha virt. eigenvalues --	0.29912	0.29917	0.30203	0.32624	0.32706
Alpha virt. eigenvalues --	0.34323	0.36679	0.37656	0.39938	0.41321
Alpha virt. eigenvalues --	0.41565	0.42555	0.42737	0.42852	0.43207
Alpha virt. eigenvalues --	0.43821	0.44421	0.44483	0.44601	0.45002
Alpha virt. eigenvalues --	0.45276	0.45616	0.45799	0.45909	0.46463
Alpha virt. eigenvalues --	0.46470	0.46613	0.46927	0.47121	0.47179
Alpha virt. eigenvalues --	0.47190	0.47275	0.47563	0.47580	0.47676
Alpha virt. eigenvalues --	0.47709	0.47848	0.48272	0.48436	0.48558
Alpha virt. eigenvalues --	0.48837	0.49351	0.49476	0.49699	0.49763
Alpha virt. eigenvalues --	0.49859	0.49986	0.50245	0.50454	0.50528
Alpha virt. eigenvalues --	0.51265	0.51539	0.51859	0.51893	0.52159
Alpha virt. eigenvalues --	0.52450	0.53100	0.53368	0.53529	0.53702
Alpha virt. eigenvalues --	0.53979	0.54767	0.54929	0.55163	0.55475
Alpha virt. eigenvalues --	0.55841	0.56040	0.56055	0.56261	0.56600
Alpha virt. eigenvalues --	0.57302	0.57363	0.57781	0.58093	0.58671
Alpha virt. eigenvalues --	0.59799	0.60457	0.60544	0.60717	0.60912
Alpha virt. eigenvalues --	0.61434	0.61516	0.61633	0.62114	0.62199
Alpha virt. eigenvalues --	0.62220	0.62623	0.62782	0.62954	0.62988
Alpha virt. eigenvalues --	0.63319	0.63416	0.63528	0.63718	0.64043
Alpha virt. eigenvalues --	0.64116	0.64259	0.64492	0.64523	0.64688
Alpha virt. eigenvalues --	0.64876	0.65082	0.65349	0.65591	0.65702
Alpha virt. eigenvalues --	0.65898	0.66183	0.66665	0.66748	0.66939
Alpha virt. eigenvalues --	0.67011	0.67040	0.67105	0.67293	0.67447
Alpha virt. eigenvalues --	0.67548	0.68198	0.68372	0.68414	0.68666
Alpha virt. eigenvalues --	0.68722	0.68886	0.68931	0.69249	0.69502
Alpha virt. eigenvalues --	0.69796	0.69941	0.70154	0.70364	0.71030

Alpha virt. eigenvalues --	0.71088	0.71589	0.71717	0.71866	0.72432
Alpha virt. eigenvalues --	0.73027	0.73387	0.73425	0.73644	0.73719
Alpha virt. eigenvalues --	0.74196	0.74268	0.74938	0.75092	0.75141
Alpha virt. eigenvalues --	0.75552	0.75797	0.76053	0.76271	0.76455
Alpha virt. eigenvalues --	0.76722	0.77043	0.77092	0.77211	0.77612
Alpha virt. eigenvalues --	0.78282	0.78414	0.79890	0.80458	0.81617
Alpha virt. eigenvalues --	0.82035	0.82807	0.83873	0.84182	0.84581
Alpha virt. eigenvalues --	0.85747	0.87367	0.87433	0.87703	0.88035
Alpha virt. eigenvalues --	0.88132	0.88396	0.88650	0.88686	0.89172
Alpha virt. eigenvalues --	0.90164	0.91546	0.91723	0.91933	0.91960
Alpha virt. eigenvalues --	0.92139	0.92255	0.92805	0.93215	0.94004
Alpha virt. eigenvalues --	0.95290	0.95741	0.97593	0.97656	0.97884
Alpha virt. eigenvalues --	0.98699	0.99306	0.99745	0.99980	1.00241
Alpha virt. eigenvalues --	1.00607	1.00667	1.01452	1.02476	1.02663
Alpha virt. eigenvalues --	1.03072	1.03141	1.03773	1.04239	1.04469
Alpha virt. eigenvalues --	1.05582	1.06691	1.06898	1.07807	1.08394
Alpha virt. eigenvalues --	1.09238	1.10466	1.10966	1.11865	1.12637
Alpha virt. eigenvalues --	1.13373	1.13453	1.13459	1.14790	1.15365
Alpha virt. eigenvalues --	1.15811	1.16462	1.16736	1.17186	1.17439
Alpha virt. eigenvalues --	1.18893	1.19054	1.19687	1.19829	1.19861
Alpha virt. eigenvalues --	1.20538	1.20766	1.21265	1.22141	1.22971
Alpha virt. eigenvalues --	1.23115	1.23364	1.23401	1.24355	1.24505
Alpha virt. eigenvalues --	1.25521	1.25594	1.25828	1.26860	1.27170
Alpha virt. eigenvalues --	1.27311	1.27394	1.28026	1.28441	1.29114
Alpha virt. eigenvalues --	1.29850	1.30567	1.30747	1.31616	1.31751
Alpha virt. eigenvalues --	1.32910	1.33087	1.33381	1.34118	1.34492
Alpha virt. eigenvalues --	1.34869	1.35153	1.35226	1.35836	1.36971
Alpha virt. eigenvalues --	1.37536	1.37622	1.38411	1.38850	1.39082
Alpha virt. eigenvalues --	1.39556	1.39767	1.41137	1.41175	1.41219
Alpha virt. eigenvalues --	1.41331	1.41449	1.41469	1.41494	1.41630
Alpha virt. eigenvalues --	1.42300	1.42384	1.42703	1.42972	1.43525
Alpha virt. eigenvalues --	1.43780	1.44350	1.44687	1.44835	1.44869
Alpha virt. eigenvalues --	1.45266	1.45399	1.45498	1.45617	1.45942
Alpha virt. eigenvalues --	1.46795	1.47503	1.47981	1.48192	1.48394
Alpha virt. eigenvalues --	1.48669	1.48774	1.50324	1.50725	1.50946
Alpha virt. eigenvalues --	1.51791	1.52557	1.52621	1.53231	1.53558
Alpha virt. eigenvalues --	1.53875	1.53989	1.54602	1.54678	1.55201
Alpha virt. eigenvalues --	1.56384	1.56639	1.56745	1.56808	1.56868
Alpha virt. eigenvalues --	1.57749	1.58410	1.58563	1.58700	1.58825
Alpha virt. eigenvalues --	1.59111	1.59142	1.59824	1.59920	1.60331
Alpha virt. eigenvalues --	1.60971	1.61367	1.61907	1.62174	1.62468
Alpha virt. eigenvalues --	1.62776	1.62927	1.62972	1.63262	1.63368
Alpha virt. eigenvalues --	1.63434	1.63564	1.63995	1.64175	1.64270
Alpha virt. eigenvalues --	1.64318	1.64520	1.64811	1.65321	1.65550
Alpha virt. eigenvalues --	1.65786	1.65898	1.66596	1.66864	1.67095
Alpha virt. eigenvalues --	1.67898	1.68273	1.68567	1.68758	1.69336
Alpha virt. eigenvalues --	1.69574	1.69843	1.69937	1.70131	1.71623
Alpha virt. eigenvalues --	1.71636	1.71834	1.72035	1.72148	1.72189

Alpha virt. eigenvalues --	1.72256	1.72599	1.72938	1.73839	1.74431
Alpha virt. eigenvalues --	1.74663	1.74860	1.75214	1.75288	1.75822
Alpha virt. eigenvalues --	1.75884	1.76165	1.77229	1.77339	1.77675
Alpha virt. eigenvalues --	1.77855	1.78051	1.79136	1.79209	1.79249
Alpha virt. eigenvalues --	1.79550	1.79719	1.79762	1.80391	1.81368
Alpha virt. eigenvalues --	1.81571	1.82559	1.82617	1.83051	1.83502
Alpha virt. eigenvalues --	1.83751	1.83858	1.84102	1.84573	1.84868
Alpha virt. eigenvalues --	1.84997	1.86120	1.86227	1.86424	1.86831
Alpha virt. eigenvalues --	1.86941	1.87178	1.87293	1.87419	1.87544
Alpha virt. eigenvalues --	1.88580	1.88641	1.89104	1.89393	1.89744
Alpha virt. eigenvalues --	1.91105	1.91290	1.91815	1.93400	1.93883
Alpha virt. eigenvalues --	1.94285	1.95373	1.95694	1.96671	1.96789
Alpha virt. eigenvalues --	1.97758	1.98454	1.98848	1.99067	1.99419
Alpha virt. eigenvalues --	2.00192	2.00415	2.00469	2.00526	2.00701
Alpha virt. eigenvalues --	2.00806	2.01047	2.01533	2.01880	2.02302
Alpha virt. eigenvalues --	2.03475	2.03497	2.04037	2.05157	2.05487
Alpha virt. eigenvalues --	2.06019	2.07044	2.07140	2.07249	2.07905
Alpha virt. eigenvalues --	2.08292	2.09354	2.09387	2.09847	2.10099
Alpha virt. eigenvalues --	2.10764	2.10823	2.13040	2.13138	2.13177
Alpha virt. eigenvalues --	2.13311	2.13883	2.14631	2.14859	2.15115
Alpha virt. eigenvalues --	2.15222	2.16896	2.17494	2.18138	2.19169
Alpha virt. eigenvalues --	2.19358	2.19483	2.20266	2.21235	2.22624
Alpha virt. eigenvalues --	2.22888	2.22915	2.23171	2.24152	2.24422
Alpha virt. eigenvalues --	2.24925	2.26895	2.27521	2.27611	2.28857
Alpha virt. eigenvalues --	2.30137	2.30667	2.30746	2.30963	2.32785
Alpha virt. eigenvalues --	2.33013	2.33781	2.34756	2.34957	2.35050
Alpha virt. eigenvalues --	2.37457	2.37797	2.39196	2.39358	2.39817
Alpha virt. eigenvalues --	2.40657	2.41384	2.41729	2.42390	2.42698
Alpha virt. eigenvalues --	2.42779	2.42930	2.43260	2.43815	2.43950
Alpha virt. eigenvalues --	2.44139	2.44186	2.44658	2.45273	2.45617
Alpha virt. eigenvalues --	2.45779	2.45970	2.46067	2.46351	2.47478
Alpha virt. eigenvalues --	2.48120	2.48128	2.48599	2.49035	2.49201
Alpha virt. eigenvalues --	2.49393	2.49878	2.50069	2.50085	2.50307
Alpha virt. eigenvalues --	2.50478	2.50713	2.52518	2.52612	2.53441
Alpha virt. eigenvalues --	2.54134	2.54301	2.54699	2.54856	2.56199
Alpha virt. eigenvalues --	2.56360	2.56585	2.56907	2.58211	2.58732
Alpha virt. eigenvalues --	2.58863	2.59635	2.61045	2.61683	2.64782
Alpha virt. eigenvalues --	2.69453	2.70027	2.70530	2.79374	2.81969
Alpha virt. eigenvalues --	2.82021	2.92114	2.92397	2.92726	2.94930
Alpha virt. eigenvalues --	2.95433	2.95485	2.98224	2.98628	2.98782
Alpha virt. eigenvalues --	2.99327	2.99375	2.99428	3.00085	3.00152
Alpha virt. eigenvalues --	3.00373	3.03056	3.03128	3.03151	3.04214
Alpha virt. eigenvalues --	3.04592	3.04800	3.08425	3.08440	3.08506
Alpha virt. eigenvalues --	3.09107	3.09151	3.09155	3.11299	3.11318
Alpha virt. eigenvalues --	3.11458	3.12143	3.12821	3.13491	3.13776
Alpha virt. eigenvalues --	3.14156	3.14708	3.24638	3.24651	3.24784
Alpha virt. eigenvalues --	3.26774	3.26805	3.26892	3.32181	3.32198
Alpha virt. eigenvalues --	3.32350	3.37537	3.37559	3.37696	3.37702

Alpha virt. eigenvalues -- 3.37785 3.37931 3.41168 3.41403 3.41759
 Alpha virt. eigenvalues -- 3.43163 3.43773 3.44956 3.51648 3.52427
 Alpha virt. eigenvalues -- 3.53392

Magenta UV-Vis Spectrum Epsilon/Oscillator Strength – N = 3



Magenta Table of 10 Lowest Excited States – N = 3

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	3.10	400.04	0.9197
2	4.03	307.77	0.0732
3	4.20	295.14	0.1095
4	4.20	294.92	0.0784
5	4.35	285.24	0.1151
6	4.61	269.17	0.0377
7	5.02	247.14	0.0003
8	5.12	242.10	0.0075
9	5.20	238.15	0.0010
10	5.35	231.54	0.0054

Magenta Cartesian Coordinates – N = 4

C 0.50252 -0.51424 -0.01409
 C 0.30667 -1.88395 -0.02855
 C 1.51708 -2.63095 -0.04856
 C 2.65262 -1.84206 -0.05284
 S 2.21523 -0.14693 -0.02916
 O 1.59565 -3.98463 -0.08942
 O -0.93855 -2.4195 0.00555
 C -1.13187 -3.60929 -0.75923
 H -2.20589 -3.63818 -0.98844
 H -0.57558 -3.53308 -1.70497
 C 0.62656 -4.68988 0.68729
 H 1.08283 -5.66368 0.91121

H	0.45829	-4.1573	1.63476
C	-0.71695	-4.89275	-0.02744
C	-1.75065	-5.3169	1.02049
H	-2.70487	-5.56739	0.5146
H	-1.40521	-6.24014	1.53004
C	-0.65466	-6.02492	-1.05689
H	-0.45876	-6.98381	-0.53616
H	-1.63971	-6.12667	-1.55755
O	-1.94693	-4.28901	1.95464
O	0.34906	-5.76764	-2.00273
C	-2.8796	-4.64191	2.94564
H	-2.96703	-3.79097	3.63301
H	-3.87429	-4.85561	2.51191
H	-2.55372	-5.53179	3.51598
C	0.43135	-6.77736	-2.97765
H	1.23296	-6.49852	-3.67322
H	0.67199	-7.75889	-2.52867
H	-0.51442	-6.87871	-3.54202
C	-0.50253	0.51425	-0.01407
C	-0.30668	1.88396	-0.0285
S	-2.21524	0.14693	-0.02919
C	-1.5171	2.63096	-0.04843
O	0.93854	2.41952	0.00556
C	-2.65263	1.84206	-0.05269
O	-1.59569	3.98465	-0.08925
C	1.13182	3.60927	-0.75929
C	-0.6265	4.6899	0.68734
H	2.20583	3.63816	-0.98856
H	0.57548	3.53301	-1.705
C	0.71693	4.89276	-0.02754
H	-1.08274	5.66371	0.91129
H	-0.45814	4.15734	1.6348
C	1.75071	5.31699	1.02028
C	0.65453	6.02487	-1.05704
H	2.70488	5.56749	0.51429
H	1.40529	6.24023	1.52983
O	1.94713	4.28914	1.95445
H	0.45865	6.98379	-0.53635
H	1.63953	6.12663	-1.55779
O	-0.34927	5.76752	-2.00278
C	2.8799	4.64209	2.94533
C	-0.43175	6.77724	-2.97768
H	2.96743	3.79118	3.63272
H	3.87454	4.85579	2.51147
H	2.55407	5.532	3.51567
H	-1.23338	6.49833	-3.67319
H	-0.67247	7.75874	-2.52867
H	0.51397	6.87871	-3.54213

C	4.02533	-2.27949	-0.04678
C	5.16081	-1.48958	-0.02468
S	4.47629	-3.97079	-0.03226
C	6.38092	-2.23905	-0.00089
O	5.07741	-0.1357	-0.0562
C	6.16056	-3.58941	0.00137
O	7.62534	-1.7004	0.0511
C	6.02977	0.56409	0.74444
C	7.81026	-0.4966	-0.69045
H	5.56602	1.53369	0.97221
H	6.18501	0.0216	1.68856
C	7.38234	0.77792	0.05144
H	8.88544	-0.45218	-0.91317
H	7.26302	-0.55984	-1.64295
C	7.32939	1.92199	-0.96574
C	8.3998	1.19609	1.11708
H	7.12748	2.87468	-0.43579
H	8.31916	2.03057	-1.45563
O	6.33499	1.67597	-1.9244
H	9.36095	1.45221	0.62735
H	8.04479	2.11538	1.62737
O	8.58482	0.16366	2.04872
C	6.25669	2.70077	-2.88356
C	9.49267	0.5196	3.06148
H	5.46334	2.42906	-3.59138
H	6.00627	3.67373	-2.42111
H	7.20722	2.81669	-3.4371
H	9.57482	-0.3347	3.74533
H	10.49393	0.74683	2.65053
H	9.14518	1.40225	3.63038
C	-4.02535	2.27948	-0.04654
C	-5.16082	1.48955	-0.02448
S	-4.47631	3.97078	-0.03174
C	-6.38095	2.23901	-0.00056
O	-5.07737	0.13569	-0.05614
C	-6.16057	3.58939	0.00187
O	-7.62539	1.70041	0.05132
C	-6.02975	-0.56422	0.74438
H	-6.91011	4.3756	0.00982
C	-7.81029	0.49669	-0.69035
H	-5.566	-1.53387	0.97197
H	-6.18499	-0.02189	1.68859
C	-7.3823	-0.77793	0.05132
H	-8.88548	0.45223	-0.91302
H	-7.26312	0.56007	-1.64288
C	-7.32927	-1.92175	-0.96613
C	-8.39976	-1.19641	1.11685
H	-7.12733	-2.87456	-0.43641

H	-8.31902	-2.03025	-1.45609
O	-6.33483	-1.67543	-1.92467
H	-9.36088	-1.45249	0.62705
H	-8.0447	-2.11579	1.62694
O	-8.58486	-0.1642	2.04872
C	-6.25641	-2.69998	-2.88408
C	-9.49285	-0.52035	3.06127
H	-5.46305	-2.42805	-3.59179
H	-6.00595	-3.67304	-2.42186
H	-7.20691	-2.81584	-3.4377
H	-9.57506	0.3338	3.74532
H	-10.49406	-0.74745	2.65014
H	-9.14547	-1.40313	3.63001
H	6.91009	-4.37567	0.00926

Magenta Energy Levels – N = 4

Alpha occ. eigenvalues -- -89.09253 -89.09253 -89.09176 -89.09176 -19.26343
Alpha occ. eigenvalues -- -19.26343 -19.26338 -19.26338 -19.26256 -19.26256
Alpha occ. eigenvalues -- -19.25718 -19.25718 -19.23565 -19.23565 -19.23564
Alpha occ. eigenvalues -- -19.23564 -19.23560 -19.23560 -19.23559 -19.23559
Alpha occ. eigenvalues -- -10.30368 -10.30368 -10.30322 -10.30321 -10.30271
Alpha occ. eigenvalues -- -10.30270 -10.30210 -10.30210 -10.29668 -10.29668
Alpha occ. eigenvalues -- -10.29665 -10.29665 -10.29602 -10.29602 -10.29470
Alpha occ. eigenvalues -- -10.29470 -10.29267 -10.29267 -10.29259 -10.29259
Alpha occ. eigenvalues -- -10.29240 -10.29240 -10.29239 -10.29239 -10.28165
Alpha occ. eigenvalues -- -10.28165 -10.28154 -10.28154 -10.28153 -10.28153
Alpha occ. eigenvalues -- -10.28151 -10.28151 -10.28128 -10.28128 -10.28005
Alpha occ. eigenvalues -- -10.27987 -10.27986 -10.27968 -10.26428 -10.26428
Alpha occ. eigenvalues -- -10.26337 -10.26336 -10.26084 -10.26084 -8.03575
Alpha occ. eigenvalues -- -8.03575 -8.03443 -8.03443 -5.97460 -5.97460
Alpha occ. eigenvalues -- -5.97346 -5.97346 -5.97092 -5.97091 -5.96968
Alpha occ. eigenvalues -- -5.96968 -5.96684 -5.96684 -5.96518 -5.96518
Alpha occ. eigenvalues -- -1.11810 -1.11765 -1.11482 -1.11482 -1.09453
Alpha occ. eigenvalues -- -1.09425 -1.09123 -1.09122 -1.07758 -1.07757
Alpha occ. eigenvalues -- -1.07745 -1.07745 -1.07581 -1.07580 -1.07571
Alpha occ. eigenvalues -- -1.07571 -0.92543 -0.91732 -0.90558 -0.89516
Alpha occ. eigenvalues -- -0.85801 -0.85795 -0.85715 -0.85687 -0.81614
Alpha occ. eigenvalues -- -0.79212 -0.77281 -0.76562 -0.76174 -0.75999
Alpha occ. eigenvalues -- -0.75492 -0.75405 -0.74514 -0.74505 -0.74489
Alpha occ. eigenvalues -- -0.74488 -0.72648 -0.72277 -0.71741 -0.71327
Alpha occ. eigenvalues -- -0.71303 -0.71251 -0.70467 -0.68243 -0.68223
Alpha occ. eigenvalues -- -0.68049 -0.68041 -0.67622 -0.64525 -0.64505
Alpha occ. eigenvalues -- -0.64495 -0.64469 -0.63770 -0.62223 -0.61192
Alpha occ. eigenvalues -- -0.60785 -0.59864 -0.59805 -0.59630 -0.59030
Alpha occ. eigenvalues -- -0.58334 -0.57306 -0.56486 -0.56267 -0.54036
Alpha occ. eigenvalues -- -0.53588 -0.53212 -0.53111 -0.53071 -0.53060
Alpha occ. eigenvalues -- -0.52885 -0.52698 -0.52078 -0.51940 -0.51850
Alpha occ. eigenvalues -- -0.51820 -0.50715 -0.50528 -0.50264 -0.50017

Alpha occ. eigenvalues --	-0.49847	-0.49743	-0.48700	-0.48693	-0.48650
Alpha occ. eigenvalues --	-0.48641	-0.48629	-0.48582	-0.48112	-0.48102
Alpha occ. eigenvalues --	-0.47707	-0.47367	-0.47303	-0.47221	-0.46986
Alpha occ. eigenvalues --	-0.46960	-0.46797	-0.46520	-0.46062	-0.45914
Alpha occ. eigenvalues --	-0.45893	-0.45885	-0.45523	-0.44587	-0.44088
Alpha occ. eigenvalues --	-0.44032	-0.43836	-0.43592	-0.43427	-0.43232
Alpha occ. eigenvalues --	-0.42826	-0.42812	-0.42749	-0.42140	-0.41785
Alpha occ. eigenvalues --	-0.41353	-0.41208	-0.41084	-0.40999	-0.40979
Alpha occ. eigenvalues --	-0.40171	-0.40118	-0.40031	-0.39991	-0.39978
Alpha occ. eigenvalues --	-0.39640	-0.39498	-0.39404	-0.38903	-0.37988
Alpha occ. eigenvalues --	-0.37790	-0.37726	-0.37557	-0.37205	-0.36962
Alpha occ. eigenvalues --	-0.36740	-0.36545	-0.36429	-0.36043	-0.35727
Alpha occ. eigenvalues --	-0.35585	-0.34484	-0.34475	-0.34460	-0.34448
Alpha occ. eigenvalues --	-0.33877	-0.33770	-0.33596	-0.33457	-0.33124
Alpha occ. eigenvalues --	-0.33092	-0.33067	-0.33052	-0.32336	-0.32244
Alpha occ. eigenvalues --	-0.32233	-0.31902	-0.30746	-0.30741	-0.30507
Alpha occ. eigenvalues --	-0.30135	-0.27909	-0.27782	-0.27780	-0.27766
Alpha occ. eigenvalues --	-0.27751	-0.26992	-0.26991	-0.26983	-0.26983
Alpha occ. eigenvalues --	-0.26037	-0.23621	-0.22947	-0.22889	-0.22732
Alpha occ. eigenvalues --	-0.21461	-0.17549			
Alpha virt. eigenvalues --	-0.05695	-0.02062	0.01510	0.04021	0.04531
Alpha virt. eigenvalues --	0.04610	0.04819	0.05014	0.05148	0.05537
Alpha virt. eigenvalues --	0.05936	0.06809	0.06859	0.06916	0.07559
Alpha virt. eigenvalues --	0.07756	0.08012	0.08088	0.08230	0.08730
Alpha virt. eigenvalues --	0.09083	0.09096	0.09458	0.09494	0.09761
Alpha virt. eigenvalues --	0.09970	0.10081	0.10485	0.10614	0.10657
Alpha virt. eigenvalues --	0.11050	0.11051	0.11217	0.11353	0.11902
Alpha virt. eigenvalues --	0.11969	0.12047	0.12158	0.12647	0.12874
Alpha virt. eigenvalues --	0.13153	0.13240	0.13307	0.13431	0.13523
Alpha virt. eigenvalues --	0.13743	0.13769	0.14095	0.14132	0.14155
Alpha virt. eigenvalues --	0.14164	0.14186	0.14268	0.14377	0.14389
Alpha virt. eigenvalues --	0.14571	0.14690	0.14792	0.14983	0.15009
Alpha virt. eigenvalues --	0.15037	0.15058	0.15114	0.15401	0.15474
Alpha virt. eigenvalues --	0.15511	0.15624	0.15995	0.16875	0.16950
Alpha virt. eigenvalues --	0.16963	0.17451	0.17633	0.17676	0.17708
Alpha virt. eigenvalues --	0.18019	0.18115	0.18387	0.18559	0.18676
Alpha virt. eigenvalues --	0.18840	0.19476	0.19670	0.20161	0.20554
Alpha virt. eigenvalues --	0.20683	0.20846	0.21380	0.21528	0.21624
Alpha virt. eigenvalues --	0.21746	0.22085	0.22782	0.23075	0.23097
Alpha virt. eigenvalues --	0.23116	0.23410	0.23881	0.23888	0.24214
Alpha virt. eigenvalues --	0.24274	0.24556	0.25129	0.25338	0.25812
Alpha virt. eigenvalues --	0.25956	0.26090	0.26381	0.27091	0.27488
Alpha virt. eigenvalues --	0.28028	0.28042	0.28155	0.28489	0.28567
Alpha virt. eigenvalues --	0.28678	0.28970	0.29660	0.29676	0.29905
Alpha virt. eigenvalues --	0.29911	0.30071	0.30303	0.32470	0.32675
Alpha virt. eigenvalues --	0.32722	0.34257	0.35665	0.37100	0.39090
Alpha virt. eigenvalues --	0.39548	0.40919	0.41270	0.41513	0.42498
Alpha virt. eigenvalues --	0.42555	0.42722	0.42871	0.43106	0.43785

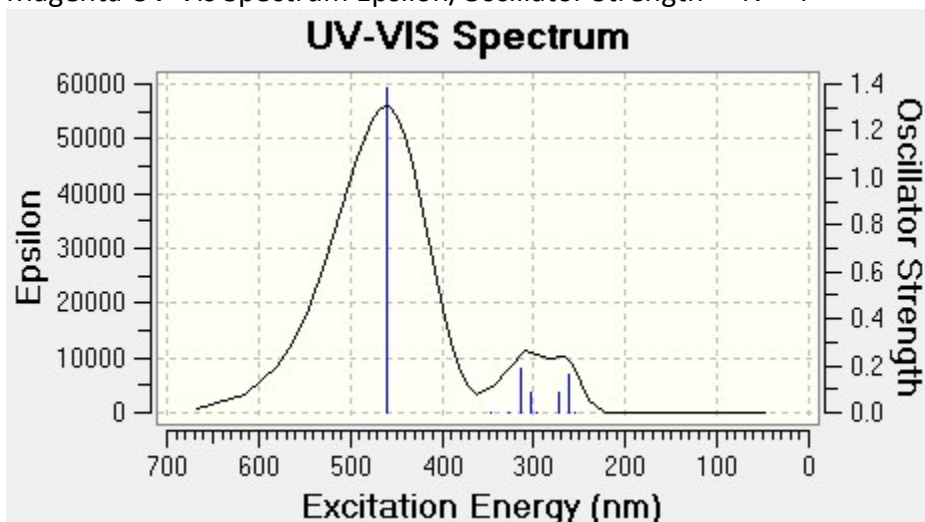
Alpha virt. eigenvalues --	0.43970	0.44327	0.44628	0.44813	0.44823
Alpha virt. eigenvalues --	0.44995	0.45280	0.45564	0.45774	0.45800
Alpha virt. eigenvalues --	0.45966	0.46295	0.46368	0.46582	0.46651
Alpha virt. eigenvalues --	0.46851	0.46857	0.47036	0.47130	0.47141
Alpha virt. eigenvalues --	0.47293	0.47380	0.47473	0.47499	0.47526
Alpha virt. eigenvalues --	0.47667	0.47786	0.47815	0.48136	0.48225
Alpha virt. eigenvalues --	0.48433	0.48554	0.48626	0.49049	0.49156
Alpha virt. eigenvalues --	0.49447	0.49597	0.49682	0.49865	0.49943
Alpha virt. eigenvalues --	0.50021	0.50058	0.50295	0.50312	0.50466
Alpha virt. eigenvalues --	0.50522	0.51346	0.51598	0.51687	0.51876
Alpha virt. eigenvalues --	0.51915	0.52337	0.52512	0.53020	0.53249
Alpha virt. eigenvalues --	0.53408	0.53570	0.53664	0.53941	0.53952
Alpha virt. eigenvalues --	0.54663	0.54816	0.54819	0.55194	0.55210
Alpha virt. eigenvalues --	0.55413	0.55949	0.55998	0.56023	0.56109
Alpha virt. eigenvalues --	0.56247	0.56755	0.57135	0.57206	0.57603
Alpha virt. eigenvalues --	0.57970	0.58091	0.58561	0.58842	0.60048
Alpha virt. eigenvalues --	0.60126	0.60460	0.60526	0.60829	0.60842
Alpha virt. eigenvalues --	0.61390	0.61470	0.61675	0.61732	0.61881
Alpha virt. eigenvalues --	0.62063	0.62200	0.62281	0.62463	0.62706
Alpha virt. eigenvalues --	0.62819	0.62918	0.63054	0.63189	0.63413
Alpha virt. eigenvalues --	0.63428	0.63481	0.63737	0.63777	0.64048
Alpha virt. eigenvalues --	0.64202	0.64235	0.64371	0.64471	0.64515
Alpha virt. eigenvalues --	0.64576	0.64627	0.64944	0.65103	0.65123
Alpha virt. eigenvalues --	0.65457	0.65517	0.65667	0.65802	0.65911
Alpha virt. eigenvalues --	0.66387	0.66600	0.66614	0.66823	0.66962
Alpha virt. eigenvalues --	0.66995	0.67075	0.67113	0.67128	0.67182
Alpha virt. eigenvalues --	0.67354	0.67710	0.67887	0.67968	0.68282
Alpha virt. eigenvalues --	0.68490	0.68506	0.68655	0.68737	0.68799
Alpha virt. eigenvalues --	0.68833	0.68932	0.69307	0.69353	0.69551
Alpha virt. eigenvalues --	0.69604	0.69722	0.70037	0.70228	0.70694
Alpha virt. eigenvalues --	0.70837	0.70920	0.71355	0.71658	0.71681
Alpha virt. eigenvalues --	0.71911	0.72060	0.72395	0.72818	0.73106
Alpha virt. eigenvalues --	0.73155	0.73430	0.73592	0.73685	0.74004
Alpha virt. eigenvalues --	0.74339	0.74564	0.74631	0.74818	0.75040
Alpha virt. eigenvalues --	0.75058	0.75569	0.75706	0.76067	0.76109
Alpha virt. eigenvalues --	0.76164	0.76313	0.76478	0.76625	0.76709
Alpha virt. eigenvalues --	0.76993	0.77096	0.77379	0.77649	0.78071
Alpha virt. eigenvalues --	0.78072	0.78513	0.79720	0.80250	0.80267
Alpha virt. eigenvalues --	0.81621	0.81795	0.82369	0.82866	0.83389
Alpha virt. eigenvalues --	0.84160	0.84318	0.84844	0.86098	0.86650
Alpha virt. eigenvalues --	0.87337	0.87633	0.87869	0.87950	0.88137
Alpha virt. eigenvalues --	0.88322	0.88347	0.88455	0.88624	0.88831
Alpha virt. eigenvalues --	0.89111	0.90225	0.90235	0.91701	0.91780
Alpha virt. eigenvalues --	0.91891	0.91979	0.92159	0.92164	0.92288
Alpha virt. eigenvalues --	0.92321	0.92580	0.92973	0.94041	0.94640
Alpha virt. eigenvalues --	0.95322	0.95383	0.97213	0.97661	0.97757
Alpha virt. eigenvalues --	0.97917	0.97943	0.98762	0.99034	0.99352
Alpha virt. eigenvalues --	0.99692	0.99997	1.00013	1.00521	1.00682

Alpha virt. eigenvalues --	1.01094	1.01763	1.02667	1.02716	1.02808
Alpha virt. eigenvalues --	1.03057	1.03356	1.03532	1.04203	1.04237
Alpha virt. eigenvalues --	1.04452	1.05301	1.05655	1.06494	1.07597
Alpha virt. eigenvalues --	1.07739	1.07791	1.09158	1.09404	1.09971
Alpha virt. eigenvalues --	1.10833	1.11198	1.11522	1.12360	1.13124
Alpha virt. eigenvalues --	1.13127	1.13345	1.13368	1.14756	1.14868
Alpha virt. eigenvalues --	1.15170	1.15665	1.16636	1.16690	1.16989
Alpha virt. eigenvalues --	1.17103	1.17342	1.17908	1.18912	1.19168
Alpha virt. eigenvalues --	1.19400	1.19660	1.19779	1.19894	1.19960
Alpha virt. eigenvalues --	1.20721	1.20731	1.21300	1.21314	1.22438
Alpha virt. eigenvalues --	1.22894	1.22967	1.23225	1.23366	1.23583
Alpha virt. eigenvalues --	1.24426	1.24516	1.24804	1.25758	1.25787
Alpha virt. eigenvalues --	1.25790	1.26238	1.26862	1.26897	1.27319
Alpha virt. eigenvalues --	1.27337	1.27539	1.27968	1.28144	1.28679
Alpha virt. eigenvalues --	1.29315	1.29756	1.30328	1.30509	1.30688
Alpha virt. eigenvalues --	1.31339	1.31855	1.31971	1.32937	1.32956
Alpha virt. eigenvalues --	1.33263	1.33367	1.33822	1.34523	1.34631
Alpha virt. eigenvalues --	1.34985	1.35338	1.35406	1.35949	1.36509
Alpha virt. eigenvalues --	1.37250	1.37594	1.37700	1.38192	1.38460
Alpha virt. eigenvalues --	1.38651	1.39095	1.39382	1.39566	1.39976
Alpha virt. eigenvalues --	1.40630	1.40780	1.41228	1.41233	1.41295
Alpha virt. eigenvalues --	1.41295	1.41480	1.41491	1.41493	1.41545
Alpha virt. eigenvalues --	1.41787	1.41852	1.42391	1.42471	1.42751
Alpha virt. eigenvalues --	1.43025	1.43059	1.43584	1.43619	1.43974
Alpha virt. eigenvalues --	1.44281	1.44696	1.44863	1.45012	1.45064
Alpha virt. eigenvalues --	1.45371	1.45440	1.45456	1.45667	1.46074
Alpha virt. eigenvalues --	1.46304	1.46584	1.47538	1.47715	1.48078
Alpha virt. eigenvalues --	1.48202	1.48505	1.48642	1.48884	1.48971
Alpha virt. eigenvalues --	1.50035	1.50054	1.50596	1.51008	1.51377
Alpha virt. eigenvalues --	1.51833	1.52495	1.52778	1.52886	1.53334
Alpha virt. eigenvalues --	1.53726	1.53785	1.53890	1.54166	1.54379
Alpha virt. eigenvalues --	1.54779	1.54913	1.55382	1.56175	1.56390
Alpha virt. eigenvalues --	1.56554	1.56739	1.56810	1.56974	1.57563
Alpha virt. eigenvalues --	1.57732	1.58450	1.58488	1.58701	1.58816
Alpha virt. eigenvalues --	1.58818	1.58934	1.59276	1.59395	1.59899
Alpha virt. eigenvalues --	1.59944	1.60130	1.60364	1.61242	1.61259
Alpha virt. eigenvalues --	1.61541	1.62083	1.62128	1.62555	1.62821
Alpha virt. eigenvalues --	1.62939	1.63031	1.63113	1.63169	1.63320
Alpha virt. eigenvalues --	1.63443	1.63509	1.63520	1.63824	1.63848
Alpha virt. eigenvalues --	1.64080	1.64166	1.64297	1.64408	1.64581
Alpha virt. eigenvalues --	1.65074	1.65223	1.65398	1.65403	1.65691
Alpha virt. eigenvalues --	1.65709	1.66221	1.66643	1.66860	1.67148
Alpha virt. eigenvalues --	1.67260	1.67574	1.68437	1.68584	1.68865
Alpha virt. eigenvalues --	1.68918	1.68986	1.69341	1.69510	1.69662
Alpha virt. eigenvalues --	1.70108	1.70158	1.70774	1.71033	1.71362
Alpha virt. eigenvalues --	1.71760	1.71983	1.72172	1.72191	1.72230
Alpha virt. eigenvalues --	1.72270	1.72305	1.72346	1.72675	1.73385
Alpha virt. eigenvalues --	1.73724	1.74382	1.74492	1.74897	1.74934

Alpha virt. eigenvalues --	1.75174	1.75305	1.75350	1.75804	1.75928
Alpha virt. eigenvalues --	1.76161	1.76681	1.76904	1.77189	1.77416
Alpha virt. eigenvalues --	1.77887	1.77930	1.78067	1.78179	1.78676
Alpha virt. eigenvalues --	1.79422	1.79477	1.79602	1.79688	1.79869
Alpha virt. eigenvalues --	1.79870	1.80068	1.80746	1.81346	1.81715
Alpha virt. eigenvalues --	1.81779	1.82259	1.82668	1.83030	1.83340
Alpha virt. eigenvalues --	1.83391	1.83920	1.83935	1.84100	1.84398
Alpha virt. eigenvalues --	1.84700	1.84745	1.84896	1.85622	1.85739
Alpha virt. eigenvalues --	1.86253	1.86414	1.86625	1.86918	1.86998
Alpha virt. eigenvalues --	1.87042	1.87145	1.87371	1.87472	1.87525
Alpha virt. eigenvalues --	1.87578	1.88455	1.88725	1.88897	1.89089
Alpha virt. eigenvalues --	1.89425	1.89760	1.90646	1.90902	1.91020
Alpha virt. eigenvalues --	1.91556	1.92715	1.93770	1.94028	1.94461
Alpha virt. eigenvalues --	1.95150	1.95367	1.96460	1.96495	1.96703
Alpha virt. eigenvalues --	1.97226	1.97578	1.98443	1.98486	1.99021
Alpha virt. eigenvalues --	1.99245	1.99669	2.00062	2.00098	2.00401
Alpha virt. eigenvalues --	2.00459	2.00566	2.00750	2.00807	2.00822
Alpha virt. eigenvalues --	2.00974	2.01255	2.01753	2.02004	2.02143
Alpha virt. eigenvalues --	2.03098	2.03399	2.03504	2.04329	2.04366
Alpha virt. eigenvalues --	2.05061	2.05435	2.05867	2.06048	2.07075
Alpha virt. eigenvalues --	2.07196	2.07369	2.07400	2.08092	2.08320
Alpha virt. eigenvalues --	2.08809	2.09264	2.09742	2.09871	2.10037
Alpha virt. eigenvalues --	2.10251	2.10859	2.11008	2.12926	2.13039
Alpha virt. eigenvalues --	2.13157	2.13247	2.13283	2.14207	2.14313
Alpha virt. eigenvalues --	2.14777	2.14917	2.14927	2.15475	2.15743
Alpha virt. eigenvalues --	2.16474	2.17565	2.18186	2.18401	2.19248
Alpha virt. eigenvalues --	2.19422	2.19467	2.19695	2.20581	2.21428
Alpha virt. eigenvalues --	2.21825	2.22308	2.22823	2.22872	2.23131
Alpha virt. eigenvalues --	2.23412	2.24194	2.24391	2.24846	2.25048
Alpha virt. eigenvalues --	2.27044	2.27512	2.27623	2.27820	2.28797
Alpha virt. eigenvalues --	2.30088	2.30671	2.30818	2.30831	2.30927
Alpha virt. eigenvalues --	2.32527	2.32614	2.33517	2.33813	2.34453
Alpha virt. eigenvalues --	2.34721	2.35067	2.35181	2.36158	2.37560
Alpha virt. eigenvalues --	2.38183	2.38866	2.39416	2.39433	2.39634
Alpha virt. eigenvalues --	2.40507	2.41294	2.41972	2.42023	2.42388
Alpha virt. eigenvalues --	2.42561	2.42692	2.42753	2.42863	2.43069
Alpha virt. eigenvalues --	2.43259	2.43817	2.43969	2.44142	2.44189
Alpha virt. eigenvalues --	2.44246	2.44413	2.45063	2.45096	2.45379
Alpha virt. eigenvalues --	2.45795	2.45816	2.45976	2.45976	2.46347
Alpha virt. eigenvalues --	2.46393	2.47067	2.47858	2.48153	2.48230
Alpha virt. eigenvalues --	2.48624	2.49009	2.49213	2.49310	2.49647
Alpha virt. eigenvalues --	2.49856	2.50023	2.50125	2.50140	2.50226
Alpha virt. eigenvalues --	2.50342	2.50657	2.51329	2.52391	2.52649
Alpha virt. eigenvalues --	2.52736	2.53783	2.54213	2.54272	2.54488
Alpha virt. eigenvalues --	2.54554	2.55088	2.56206	2.56219	2.56485
Alpha virt. eigenvalues --	2.56612	2.56685	2.57362	2.58561	2.58704
Alpha virt. eigenvalues --	2.58848	2.59071	2.60652	2.61373	2.61531
Alpha virt. eigenvalues --	2.63846	2.65916	2.69371	2.69884	2.70528

Alpha virt. eigenvalues -- 2.70616 2.79335 2.80664 2.82014 2.82091
Alpha virt. eigenvalues -- 2.92054 2.92095 2.92592 2.92738 2.94915
Alpha virt. eigenvalues -- 2.95329 2.95445 2.95540 2.98230 2.98406
Alpha virt. eigenvalues -- 2.98651 2.98773 2.99345 2.99383 2.99417
Alpha virt. eigenvalues -- 2.99444 3.00073 3.00120 3.00239 3.00450
Alpha virt. eigenvalues -- 3.03055 3.03131 3.03165 3.03183 3.04214
Alpha virt. eigenvalues -- 3.04535 3.04821 3.04956 3.08470 3.08472
Alpha virt. eigenvalues -- 3.08492 3.08525 3.09131 3.09132 3.09170
Alpha virt. eigenvalues -- 3.09178 3.11284 3.11334 3.11464 3.11497
Alpha virt. eigenvalues -- 3.12144 3.12551 3.13088 3.13509 3.13804
Alpha virt. eigenvalues -- 3.14522 3.14533 3.14821 3.24664 3.24681
Alpha virt. eigenvalues -- 3.24729 3.24865 3.26814 3.26814 3.26879
Alpha virt. eigenvalues -- 3.26929 3.32197 3.32200 3.32261 3.32364
Alpha virt. eigenvalues -- 3.37577 3.37585 3.37639 3.37707 3.37708
Alpha virt. eigenvalues -- 3.37764 3.37880 3.37907 3.41176 3.41236
Alpha virt. eigenvalues -- 3.41484 3.41658 3.43045 3.43636 3.44260
Alpha virt. eigenvalues -- 3.45275 3.51556 3.52069 3.52747 3.53721

Magenta UV-Vis Spectrum Epsilon/Oscillator Strength – N = 4



Magenta Table of 10 Lowest Excited States – N = 4

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	2.69	461.18	1.3814
2	3.57	347.27	0.0000
3	3.79	326.75	0.0001
4	3.95	314.00	0.1856
5	4.08	304.16	0.0001
6	4.08	303.75	0.0825
7	4.19	295.84	0.0000
8	4.55	272.32	0.0831
9	4.74	261.80	0.1617
10	4.86	254.90	0.0000

Magenta Cartesian Coordinates – N = 5

C	1.26335	0.43596	0.05694
C	0.70974	-0.83272	0.03406
C	-0.70971	-0.83273	-0.03434
C	-1.26333	0.43595	-0.05718
S	0.	1.64853	-0.0001
O	-1.48673	-1.94391	-0.04623
O	1.48678	-1.94389	0.0459
C	0.98144	-3.05454	0.78799
H	1.8649	-3.64176	1.07368
H	0.49254	-2.69174	1.70414
C	-0.98139	-3.0545	-0.78841
H	-1.86485	-3.6417	-1.07413
H	-0.4925	-2.69163	-1.70454
C	0.00004	-3.93238	-0.00025
C	0.72102	-4.84926	-0.99258
H	1.34283	-5.57713	-0.43327
H	-0.02533	-5.43778	-1.56549
C	-0.72093	-4.84935	0.99202
H	-1.34273	-5.57718	0.43266
H	0.02543	-5.43789	1.56489
O	1.51866	-4.09275	-1.86398
O	-1.51858	-4.0929	1.86347
C	2.19829	-4.89708	-2.7954
H	2.79235	-4.23078	-3.4337
H	2.87669	-5.61377	-2.29602
H	1.49713	-5.47073	-3.42993
C	-2.19821	-4.89731	2.79483
H	-2.79228	-4.23106	3.43317
H	-2.87659	-5.61397	2.2954
H	-1.49704	-5.47098	3.42933
C	2.65666	0.78204	0.12675
C	3.20563	2.04689	0.24425
S	3.92371	-0.42692	0.08943
C	4.62643	2.04719	0.3058
O	2.42797	3.15849	0.26562
C	5.18209	0.78299	0.22972
O	5.40136	3.1489	0.45794
C	2.83494	4.18055	1.17609
C	4.94823	4.33795	-0.19031
H	1.92142	4.74168	1.41603
H	3.21399	3.71866	2.09953
C	3.90033	5.12716	0.606
H	5.84796	4.95171	-0.33266
H	4.53981	4.08462	-1.1796
C	3.29106	6.17526	-0.33017
C	4.52298	5.90052	1.77207
H	2.60729	6.82864	0.24832

H	4.09398	6.82641	-0.73332
O	2.59904	5.54762	-1.37664
H	5.2266	6.65983	1.37532
H	3.72884	6.4526	2.31624
O	5.18814	5.02285	2.6411
C	2.02163	6.47297	-2.26353
C	5.7478	5.69083	3.74434
H	1.50798	5.90129	-3.04687
H	1.28607	7.12224	-1.75304
H	2.785	7.12028	-2.73414
H	6.24045	4.93625	4.3705
H	6.49778	6.44029	3.43012
H	4.9751	6.20647	4.34465
C	-2.65664	0.78201	-0.12697
C	-3.20563	2.04686	-0.24443
S	-3.92368	-0.42697	-0.08979
C	-4.62643	2.04715	-0.30589
O	-2.42798	3.15846	-0.2658
C	-5.18208	0.78296	-0.22979
O	-5.40137	3.14887	-0.45795
C	-2.83501	4.18057	-1.17619
C	-4.94822	4.33788	0.19035
H	-1.9215	4.74173	-1.41615
H	-3.21412	3.71874	-2.09962
C	-3.90036	5.12715	-0.60597
H	-5.84795	4.95162	0.3328
H	-4.53974	4.08449	1.17961
C	-3.29103	6.17518	0.33024
C	-4.52308	5.90059	-1.77194
H	-2.60728	6.82859	-0.24824
H	-4.09392	6.82632	0.73348
O	-2.59896	5.54747	1.37664
H	-5.22668	6.65987	-1.3751
H	-3.72898	6.45271	-2.31611
O	-5.18828	5.02299	-2.64101
C	-2.02149	6.47276	2.26355
C	-5.74799	5.69105	-3.74418
H	-1.5078	5.90102	3.04683
H	-1.28595	7.12206	1.75307
H	-2.78484	7.12004	2.73425
H	-6.24065	4.93652	-4.37038
H	-6.49797	6.44048	-3.42986
H	-4.97532	6.20676	-4.34447
C	-6.58086	0.43854	-0.22802
C	-7.13809	-0.8202	-0.09121
S	-7.84811	1.63939	-0.35631
C	-8.5701	-0.81746	-0.08867
O	-6.36127	-1.92928	0.00263

C	-9.08656	0.44254	-0.2235
O	-9.35318	-1.91407	0.06967
C	-6.80988	-2.91945	0.92776
C	-8.86704	-3.11849	-0.51815
H	-5.90905	-3.47305	1.22676
H	-7.22807	-2.42689	1.81788
C	-7.85107	-3.88319	0.34257
H	-9.75642	-3.74305	-0.68068
H	-8.41684	-2.89855	-1.49777
C	-7.20404	-4.95714	-0.53754
C	-8.51773	-4.6255	1.50438
H	-6.5425	-5.59205	0.08585
H	-7.98984	-5.62206	-0.95209
O	-6.47253	-4.35976	-1.575
H	-9.20787	-5.39403	1.10165
H	-7.74484	-5.16464	2.09049
O	-9.21229	-3.72659	2.32779
C	-5.86372	-5.31012	-2.41285
C	-9.80939	-4.36733	3.42739
H	-5.31976	-4.76128	-3.19208
H	-5.14895	-5.94538	-1.8571
H	-6.60988	-5.96999	-2.89362
H	-10.32219	-3.59778	4.01822
H	-10.54911	-5.1243	3.10671
H	-9.05808	-4.86837	4.06603
C	6.58087	0.43859	0.2281
C	7.13811	-0.82016	0.09139
S	7.84812	1.63943	0.35648
C	8.57011	-0.81744	0.08894
O	6.36129	-1.92925	-0.00247
C	9.08658	0.44256	0.22374
O	9.35318	-1.91407	-0.06931
C	6.80994	-2.91943	-0.92757
H	10.13616	0.72018	0.25976
C	8.86699	-3.11848	0.51849
H	5.90913	-3.47301	-1.22663
H	7.22822	-2.42689	-1.81766
C	7.85106	-3.88319	-0.34228
H	9.75635	-3.74304	0.68109
H	8.41672	-2.89852	1.49808
C	7.20394	-4.95707	0.53782
C	8.51778	-4.62557	-1.50401
H	6.54243	-5.59199	-0.08559
H	7.98968	-5.622	0.95247
O	6.47236	-4.35962	1.57519
H	9.2079	-5.39408	-1.10121
H	7.74491	-5.16474	-2.09013
O	9.21238	-3.72672	-2.32746

C	5.86342	-5.30991	2.41301
C	9.80953	-4.36755	-3.42698
H	5.31942	-4.76102	3.19218
H	5.14868	-5.94516	1.85723
H	6.6095	-5.96981	2.89389
H	10.32237	-3.59805	-4.01785
H	10.54923	-5.1245	-3.10621
H	9.05825	-4.86863	-4.06563
H	-10.13616	0.72011	-0.25948

Magenta Energy Levels – N = 5

Alpha occ. eigenvalues -- -89.09234 -89.09234 -89.09173 -89.09173 -89.09154
 Alpha occ. eigenvalues -- -19.26376 -19.26376 -19.26320 -19.26319 -19.26273
 Alpha occ. eigenvalues -- -19.26273 -19.26214 -19.26214 -19.25721 -19.25721
 Alpha occ. eigenvalues -- -19.23577 -19.23577 -19.23575 -19.23575 -19.23568
 Alpha occ. eigenvalues -- -19.23568 -19.23551 -19.23551 -19.23530 -19.23530
 Alpha occ. eigenvalues -- -10.30383 -10.30383 -10.30359 -10.30315 -10.30279
 Alpha occ. eigenvalues -- -10.30279 -10.30256 -10.30256 -10.30163 -10.30163
 Alpha occ. eigenvalues -- -10.29685 -10.29685 -10.29683 -10.29682 -10.29615
 Alpha occ. eigenvalues -- -10.29615 -10.29571 -10.29571 -10.29465 -10.29465
 Alpha occ. eigenvalues -- -10.29280 -10.29279 -10.29256 -10.29256 -10.29239
 Alpha occ. eigenvalues -- -10.29239 -10.29235 -10.29235 -10.29230 -10.29230
 Alpha occ. eigenvalues -- -10.28169 -10.28169 -10.28167 -10.28167 -10.28166
 Alpha occ. eigenvalues -- -10.28166 -10.28156 -10.28156 -10.28147 -10.28147
 Alpha occ. eigenvalues -- -10.28102 -10.28102 -10.28030 -10.28029 -10.27989
 Alpha occ. eigenvalues -- -10.27988 -10.27954 -10.27953 -10.26428 -10.26411
 Alpha occ. eigenvalues -- -10.26411 -10.26327 -10.26327 -10.26040 -10.26040
 Alpha occ. eigenvalues -- -8.03555 -8.03555 -8.03440 -8.03440 -8.03422
 Alpha occ. eigenvalues -- -5.97441 -5.97441 -5.97343 -5.97343 -5.97326
 Alpha occ. eigenvalues -- -5.97072 -5.97072 -5.96965 -5.96965 -5.96949
 Alpha occ. eigenvalues -- -5.96664 -5.96664 -5.96515 -5.96515 -5.96495
 Alpha occ. eigenvalues -- -1.11811 -1.11769 -1.11747 -1.11454 -1.11454
 Alpha occ. eigenvalues -- -1.09439 -1.09424 -1.09399 -1.09104 -1.09104
 Alpha occ. eigenvalues -- -1.07772 -1.07749 -1.07749 -1.07746 -1.07746
 Alpha occ. eigenvalues -- -1.07594 -1.07571 -1.07571 -1.07567 -1.07567
 Alpha occ. eigenvalues -- -0.92621 -0.92066 -0.91199 -0.90199 -0.89409
 Alpha occ. eigenvalues -- -0.85819 -0.85808 -0.85768 -0.85707 -0.85684
 Alpha occ. eigenvalues -- -0.81952 -0.80085 -0.78184 -0.76964 -0.76549
 Alpha occ. eigenvalues -- -0.76340 -0.75856 -0.75855 -0.75410 -0.75363
 Alpha occ. eigenvalues -- -0.74525 -0.74501 -0.74498 -0.74487 -0.74487
 Alpha occ. eigenvalues -- -0.72690 -0.72486 -0.71985 -0.71727 -0.71310
 Alpha occ. eigenvalues -- -0.71295 -0.71260 -0.71144 -0.69853 -0.68227
 Alpha occ. eigenvalues -- -0.68222 -0.68075 -0.68047 -0.68020 -0.67387
 Alpha occ. eigenvalues -- -0.64540 -0.64532 -0.64486 -0.64484 -0.64456
 Alpha occ. eigenvalues -- -0.64049 -0.62685 -0.61693 -0.60995 -0.60760
 Alpha occ. eigenvalues -- -0.59887 -0.59835 -0.59744 -0.59531 -0.58854
 Alpha occ. eigenvalues -- -0.58390 -0.57469 -0.56805 -0.56303 -0.56237
 Alpha occ. eigenvalues -- -0.54039 -0.53761 -0.53273 -0.53193 -0.53132

Alpha occ. eigenvalues --	-0.53071	-0.53050	-0.52996	-0.52803	-0.52678
Alpha occ. eigenvalues --	-0.52097	-0.51984	-0.51897	-0.51832	-0.51820
Alpha occ. eigenvalues --	-0.50752	-0.50727	-0.50446	-0.50124	-0.49908
Alpha occ. eigenvalues --	-0.49892	-0.49811	-0.49063	-0.48750	-0.48695
Alpha occ. eigenvalues --	-0.48655	-0.48637	-0.48624	-0.48623	-0.48383
Alpha occ. eigenvalues --	-0.48322	-0.48034	-0.47926	-0.47548	-0.47377
Alpha occ. eigenvalues --	-0.47330	-0.47220	-0.47106	-0.46985	-0.46977
Alpha occ. eigenvalues --	-0.46802	-0.46732	-0.46174	-0.45930	-0.45908
Alpha occ. eigenvalues --	-0.45886	-0.45879	-0.45870	-0.44842	-0.44556
Alpha occ. eigenvalues --	-0.44119	-0.44113	-0.43902	-0.43758	-0.43532
Alpha occ. eigenvalues --	-0.43494	-0.43243	-0.42997	-0.42980	-0.42852
Alpha occ. eigenvalues --	-0.42612	-0.42455	-0.41956	-0.41485	-0.41285
Alpha occ. eigenvalues --	-0.41106	-0.41091	-0.41027	-0.40974	-0.40872
Alpha occ. eigenvalues --	-0.40173	-0.40126	-0.40055	-0.40017	-0.39986
Alpha occ. eigenvalues --	-0.39977	-0.39606	-0.39562	-0.39443	-0.39415
Alpha occ. eigenvalues --	-0.38706	-0.38098	-0.37837	-0.37791	-0.37710
Alpha occ. eigenvalues --	-0.37464	-0.37314	-0.37078	-0.36868	-0.36657
Alpha occ. eigenvalues --	-0.36568	-0.36309	-0.36088	-0.35929	-0.35590
Alpha occ. eigenvalues --	-0.35522	-0.34516	-0.34459	-0.34453	-0.34428
Alpha occ. eigenvalues --	-0.34422	-0.33872	-0.33825	-0.33660	-0.33539
Alpha occ. eigenvalues --	-0.33482	-0.33108	-0.33088	-0.33069	-0.33053
Alpha occ. eigenvalues --	-0.33050	-0.32354	-0.32331	-0.32265	-0.32161
Alpha occ. eigenvalues --	-0.31891	-0.30820	-0.30754	-0.30622	-0.30296
Alpha occ. eigenvalues --	-0.30047	-0.28021	-0.27801	-0.27780	-0.27764
Alpha occ. eigenvalues --	-0.27760	-0.27738	-0.27043	-0.27016	-0.26987
Alpha occ. eigenvalues --	-0.26976	-0.26975	-0.26959	-0.24509	-0.23563
Alpha occ. eigenvalues --	-0.22895	-0.22881	-0.22720	-0.22574	-0.20201
Alpha occ. eigenvalues --	-0.17059				
Alpha virt. eigenvalues --	-0.06169	-0.03218	-0.00199	0.02535	0.03932
Alpha virt. eigenvalues --	0.04396	0.04635	0.04686	0.04862	0.04896
Alpha virt. eigenvalues --	0.05029	0.05383	0.05605	0.05932	0.06444
Alpha virt. eigenvalues --	0.06798	0.06858	0.07331	0.07503	0.07821
Alpha virt. eigenvalues --	0.08088	0.08182	0.08310	0.08345	0.08771
Alpha virt. eigenvalues --	0.08892	0.09040	0.09124	0.09226	0.09306
Alpha virt. eigenvalues --	0.09801	0.09846	0.10095	0.10232	0.10647
Alpha virt. eigenvalues --	0.10699	0.10895	0.10987	0.11129	0.11140
Alpha virt. eigenvalues --	0.11398	0.11443	0.11775	0.11935	0.12021
Alpha virt. eigenvalues --	0.12079	0.12175	0.12507	0.12699	0.12720
Alpha virt. eigenvalues --	0.13043	0.13175	0.13284	0.13292	0.13408
Alpha virt. eigenvalues --	0.13549	0.13768	0.13830	0.13927	0.13974
Alpha virt. eigenvalues --	0.14057	0.14087	0.14096	0.14170	0.14233
Alpha virt. eigenvalues --	0.14293	0.14316	0.14391	0.14415	0.14687
Alpha virt. eigenvalues --	0.14703	0.14855	0.14914	0.15004	0.15105
Alpha virt. eigenvalues --	0.15219	0.15232	0.15283	0.15400	0.15426
Alpha virt. eigenvalues --	0.15715	0.15959	0.16023	0.16473	0.16568
Alpha virt. eigenvalues --	0.16990	0.17071	0.17220	0.17438	0.17498
Alpha virt. eigenvalues --	0.17612	0.17658	0.17791	0.17920	0.18050
Alpha virt. eigenvalues --	0.18154	0.18380	0.18523	0.18692	0.18715

Alpha virt. eigenvalues --	0.19039	0.19484	0.19658	0.19850	0.20264
Alpha virt. eigenvalues --	0.20537	0.20708	0.20930	0.21073	0.21407
Alpha virt. eigenvalues --	0.21715	0.21904	0.21969	0.22029	0.22156
Alpha virt. eigenvalues --	0.22915	0.23095	0.23105	0.23164	0.23223
Alpha virt. eigenvalues --	0.23612	0.23768	0.23879	0.24110	0.24358
Alpha virt. eigenvalues --	0.24466	0.24796	0.25148	0.25207	0.25728
Alpha virt. eigenvalues --	0.25885	0.25975	0.26095	0.26286	0.26531
Alpha virt. eigenvalues --	0.27243	0.27578	0.27904	0.27959	0.28075
Alpha virt. eigenvalues --	0.28288	0.28464	0.28528	0.28630	0.28839
Alpha virt. eigenvalues --	0.29217	0.29688	0.29842	0.29843	0.29985
Alpha virt. eigenvalues --	0.30040	0.30181	0.30301	0.32390	0.32627
Alpha virt. eigenvalues --	0.32807	0.32809	0.34197	0.35108	0.36480
Alpha virt. eigenvalues --	0.38075	0.39014	0.39698	0.40843	0.41159
Alpha virt. eigenvalues --	0.41266	0.41771	0.42381	0.42471	0.42591
Alpha virt. eigenvalues --	0.42747	0.42843	0.43017	0.43775	0.43837
Alpha virt. eigenvalues --	0.43874	0.44268	0.44430	0.44693	0.44811
Alpha virt. eigenvalues --	0.45052	0.45088	0.45110	0.45566	0.45658
Alpha virt. eigenvalues --	0.45698	0.45888	0.45905	0.46273	0.46346
Alpha virt. eigenvalues --	0.46587	0.46591	0.46649	0.46670	0.46865
Alpha virt. eigenvalues --	0.46907	0.47056	0.47157	0.47208	0.47290
Alpha virt. eigenvalues --	0.47327	0.47366	0.47421	0.47494	0.47505
Alpha virt. eigenvalues --	0.47648	0.47723	0.47788	0.47954	0.48064
Alpha virt. eigenvalues --	0.48087	0.48261	0.48445	0.48551	0.48610
Alpha virt. eigenvalues --	0.48861	0.49058	0.49210	0.49404	0.49477
Alpha virt. eigenvalues --	0.49483	0.49686	0.49702	0.49934	0.49998
Alpha virt. eigenvalues --	0.50118	0.50172	0.50251	0.50321	0.50342
Alpha virt. eigenvalues --	0.50464	0.50693	0.51355	0.51610	0.51620
Alpha virt. eigenvalues --	0.51736	0.51879	0.52173	0.52302	0.52397
Alpha virt. eigenvalues --	0.53021	0.53119	0.53243	0.53379	0.53579
Alpha virt. eigenvalues --	0.53705	0.53804	0.53922	0.54123	0.54505
Alpha virt. eigenvalues --	0.54713	0.54836	0.55036	0.55100	0.55138
Alpha virt. eigenvalues --	0.55337	0.55488	0.55972	0.55992	0.56028
Alpha virt. eigenvalues --	0.56104	0.56131	0.56252	0.56677	0.56970
Alpha virt. eigenvalues --	0.57299	0.57375	0.57735	0.58007	0.58152
Alpha virt. eigenvalues --	0.58349	0.58653	0.58785	0.59942	0.60279
Alpha virt. eigenvalues --	0.60331	0.60364	0.60715	0.60759	0.60921
Alpha virt. eigenvalues --	0.61009	0.61177	0.61290	0.61555	0.61599
Alpha virt. eigenvalues --	0.61942	0.61956	0.62147	0.62378	0.62386
Alpha virt. eigenvalues --	0.62474	0.62475	0.62711	0.62715	0.63046
Alpha virt. eigenvalues --	0.63103	0.63247	0.63269	0.63275	0.63411
Alpha virt. eigenvalues --	0.63415	0.63597	0.63697	0.63721	0.63942
Alpha virt. eigenvalues --	0.64089	0.64158	0.64351	0.64425	0.64483
Alpha virt. eigenvalues --	0.64665	0.64719	0.64845	0.64959	0.64966
Alpha virt. eigenvalues --	0.65058	0.65120	0.65211	0.65224	0.65440
Alpha virt. eigenvalues --	0.65501	0.65899	0.65950	0.66052	0.66069
Alpha virt. eigenvalues --	0.66442	0.66560	0.66737	0.66772	0.66790
Alpha virt. eigenvalues --	0.66893	0.66934	0.67160	0.67257	0.67264
Alpha virt. eigenvalues --	0.67276	0.67379	0.67586	0.67674	0.67975

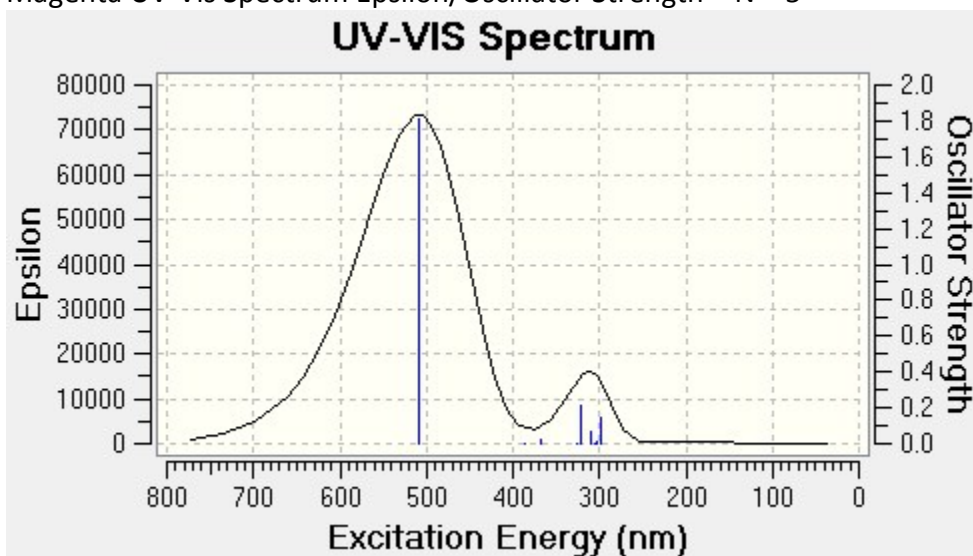
Alpha virt. eigenvalues --	0.68116	0.68446	0.68494	0.68603	0.68616
Alpha virt. eigenvalues --	0.68735	0.68821	0.68859	0.68919	0.68979
Alpha virt. eigenvalues --	0.69125	0.69248	0.69453	0.69501	0.69625
Alpha virt. eigenvalues --	0.69847	0.70008	0.70204	0.70462	0.70525
Alpha virt. eigenvalues --	0.70648	0.70874	0.71051	0.71425	0.71510
Alpha virt. eigenvalues --	0.71610	0.71951	0.72024	0.72218	0.72373
Alpha virt. eigenvalues --	0.72653	0.72717	0.73059	0.73127	0.73318
Alpha virt. eigenvalues --	0.73343	0.73517	0.73901	0.73939	0.74166
Alpha virt. eigenvalues --	0.74560	0.74652	0.74668	0.74922	0.75025
Alpha virt. eigenvalues --	0.75376	0.75461	0.75578	0.75665	0.75682
Alpha virt. eigenvalues --	0.75736	0.75887	0.76197	0.76239	0.76505
Alpha virt. eigenvalues --	0.76605	0.76750	0.77045	0.77111	0.77177
Alpha virt. eigenvalues --	0.77217	0.77738	0.77897	0.77927	0.78211
Alpha virt. eigenvalues --	0.78606	0.78734	0.79599	0.79982	0.80299
Alpha virt. eigenvalues --	0.80390	0.81813	0.81855	0.82067	0.82587
Alpha virt. eigenvalues --	0.82926	0.83333	0.83788	0.84314	0.84627
Alpha virt. eigenvalues --	0.85483	0.86213	0.86257	0.87151	0.87189
Alpha virt. eigenvalues --	0.87602	0.87982	0.88004	0.88263	0.88322
Alpha virt. eigenvalues --	0.88377	0.88450	0.88480	0.88590	0.88750
Alpha virt. eigenvalues --	0.89030	0.89097	0.90384	0.90395	0.90438
Alpha virt. eigenvalues --	0.91657	0.91747	0.91813	0.91970	0.91998
Alpha virt. eigenvalues --	0.92059	0.92282	0.92353	0.92394	0.92455
Alpha virt. eigenvalues --	0.92725	0.92950	0.93901	0.94117	0.95126
Alpha virt. eigenvalues --	0.95306	0.95487	0.96221	0.97394	0.97629
Alpha virt. eigenvalues --	0.97760	0.97796	0.97975	0.98142	0.99037
Alpha virt. eigenvalues --	0.99178	0.99310	0.99652	0.99653	0.99962
Alpha virt. eigenvalues --	1.00008	1.00367	1.00530	1.00996	1.01209
Alpha virt. eigenvalues --	1.01556	1.02652	1.02676	1.02958	1.03139
Alpha virt. eigenvalues --	1.03175	1.03359	1.03383	1.03681	1.03875
Alpha virt. eigenvalues --	1.04109	1.04787	1.05177	1.05300	1.06381
Alpha virt. eigenvalues --	1.06903	1.07510	1.07687	1.07770	1.09060
Alpha virt. eigenvalues --	1.09226	1.09368	1.09703	1.10425	1.10602
Alpha virt. eigenvalues --	1.11463	1.11915	1.12201	1.12392	1.13138
Alpha virt. eigenvalues --	1.13156	1.13241	1.13420	1.14158	1.14713
Alpha virt. eigenvalues --	1.14896	1.15133	1.15594	1.16531	1.16687
Alpha virt. eigenvalues --	1.16831	1.16933	1.17118	1.17146	1.17277
Alpha virt. eigenvalues --	1.18289	1.18948	1.19216	1.19351	1.19563
Alpha virt. eigenvalues --	1.19745	1.19800	1.19879	1.20059	1.20087
Alpha virt. eigenvalues --	1.20758	1.20803	1.20955	1.21305	1.21668
Alpha virt. eigenvalues --	1.22437	1.22649	1.22918	1.23135	1.23402
Alpha virt. eigenvalues --	1.23404	1.23852	1.24128	1.24397	1.24580
Alpha virt. eigenvalues --	1.25522	1.25620	1.25921	1.25948	1.26094
Alpha virt. eigenvalues --	1.26419	1.26769	1.27012	1.27019	1.27308
Alpha virt. eigenvalues --	1.27342	1.27506	1.27906	1.28224	1.28594
Alpha virt. eigenvalues --	1.29307	1.29431	1.29700	1.30426	1.30435
Alpha virt. eigenvalues --	1.30571	1.31134	1.31617	1.31641	1.31647
Alpha virt. eigenvalues --	1.32269	1.32977	1.33234	1.33287	1.33378
Alpha virt. eigenvalues --	1.33414	1.33914	1.34347	1.34679	1.34836

Alpha virt. eigenvalues --	1.35314	1.35350	1.35673	1.36165	1.36278
Alpha virt. eigenvalues --	1.36688	1.37330	1.37486	1.37504	1.37688
Alpha virt. eigenvalues --	1.38241	1.38473	1.38835	1.39126	1.39352
Alpha virt. eigenvalues --	1.39390	1.39558	1.39695	1.40346	1.40542
Alpha virt. eigenvalues --	1.40962	1.41171	1.41246	1.41257	1.41259
Alpha virt. eigenvalues --	1.41296	1.41433	1.41454	1.41495	1.41516
Alpha virt. eigenvalues --	1.41549	1.41668	1.41968	1.42209	1.42305
Alpha virt. eigenvalues --	1.42615	1.42618	1.42771	1.42956	1.43296
Alpha virt. eigenvalues --	1.43677	1.43910	1.44012	1.44331	1.44373
Alpha virt. eigenvalues --	1.44691	1.44699	1.44908	1.45114	1.45323
Alpha virt. eigenvalues --	1.45372	1.45442	1.45532	1.45717	1.45832
Alpha virt. eigenvalues --	1.46245	1.46283	1.46591	1.47423	1.47690
Alpha virt. eigenvalues --	1.47868	1.48043	1.48157	1.48244	1.48336
Alpha virt. eigenvalues --	1.48683	1.48953	1.48976	1.49848	1.50031
Alpha virt. eigenvalues --	1.50349	1.50571	1.50580	1.50902	1.51753
Alpha virt. eigenvalues --	1.51822	1.52644	1.52708	1.52765	1.52905
Alpha virt. eigenvalues --	1.53587	1.53706	1.53829	1.53852	1.53952
Alpha virt. eigenvalues --	1.54257	1.54329	1.54698	1.54912	1.55016
Alpha virt. eigenvalues --	1.55478	1.56154	1.56280	1.56584	1.56640
Alpha virt. eigenvalues --	1.56770	1.56883	1.57035	1.57338	1.57345
Alpha virt. eigenvalues --	1.57873	1.57966	1.58459	1.58616	1.58765
Alpha virt. eigenvalues --	1.58822	1.58897	1.58999	1.59010	1.59236
Alpha virt. eigenvalues --	1.59574	1.59693	1.59999	1.60319	1.60476
Alpha virt. eigenvalues --	1.60656	1.60929	1.61473	1.61529	1.61710
Alpha virt. eigenvalues --	1.62195	1.62403	1.62477	1.62772	1.62864
Alpha virt. eigenvalues --	1.62968	1.63093	1.63141	1.63164	1.63219
Alpha virt. eigenvalues --	1.63436	1.63495	1.63561	1.63657	1.63665
Alpha virt. eigenvalues --	1.63827	1.63898	1.64029	1.64254	1.64301
Alpha virt. eigenvalues --	1.64428	1.64440	1.64722	1.64754	1.65197
Alpha virt. eigenvalues --	1.65236	1.65471	1.65483	1.65758	1.65763
Alpha virt. eigenvalues --	1.65946	1.66030	1.66479	1.66853	1.67155
Alpha virt. eigenvalues --	1.67376	1.67387	1.67886	1.67923	1.68541
Alpha virt. eigenvalues --	1.68607	1.68728	1.69124	1.69182	1.69241
Alpha virt. eigenvalues --	1.69534	1.69571	1.69857	1.70020	1.70265
Alpha virt. eigenvalues --	1.70622	1.70959	1.71186	1.71483	1.71486
Alpha virt. eigenvalues --	1.71890	1.72048	1.72162	1.72194	1.72212
Alpha virt. eigenvalues --	1.72291	1.72321	1.72371	1.72488	1.72618
Alpha virt. eigenvalues --	1.72670	1.73560	1.73590	1.74230	1.74593
Alpha virt. eigenvalues --	1.74757	1.74849	1.75009	1.75130	1.75287
Alpha virt. eigenvalues --	1.75334	1.75478	1.75721	1.75921	1.76124
Alpha virt. eigenvalues --	1.76465	1.76623	1.76952	1.77333	1.77418
Alpha virt. eigenvalues --	1.77629	1.77711	1.78032	1.78043	1.78130
Alpha virt. eigenvalues --	1.78237	1.78757	1.78990	1.79485	1.79586
Alpha virt. eigenvalues --	1.79664	1.79731	1.79832	1.79894	1.80171
Alpha virt. eigenvalues --	1.80290	1.81150	1.81414	1.81661	1.81673
Alpha virt. eigenvalues --	1.81866	1.82465	1.82516	1.82877	1.83182
Alpha virt. eigenvalues --	1.83310	1.83539	1.83888	1.83964	1.84322
Alpha virt. eigenvalues --	1.84352	1.84640	1.84719	1.84844	1.84886

Alpha virt. eigenvalues --	1.84921	1.85944	1.86030	1.86163	1.86296
Alpha virt. eigenvalues --	1.86376	1.86727	1.86809	1.86920	1.86971
Alpha virt. eigenvalues --	1.87036	1.87153	1.87444	1.87484	1.87548
Alpha virt. eigenvalues --	1.87592	1.87716	1.88666	1.88699	1.88966
Alpha virt. eigenvalues --	1.89062	1.89170	1.89650	1.89927	1.90277
Alpha virt. eigenvalues --	1.90519	1.91087	1.91208	1.91711	1.92236
Alpha virt. eigenvalues --	1.93196	1.94065	1.94247	1.94264	1.94735
Alpha virt. eigenvalues --	1.95095	1.95776	1.96163	1.96306	1.96699
Alpha virt. eigenvalues --	1.97023	1.97175	1.97916	1.98251	1.98608
Alpha virt. eigenvalues --	1.98634	1.99109	1.99234	1.99740	1.99822
Alpha virt. eigenvalues --	2.00019	2.00228	2.00326	2.00440	2.00608
Alpha virt. eigenvalues --	2.00631	2.00803	2.00844	2.00988	2.01028
Alpha virt. eigenvalues --	2.01281	2.01488	2.01944	2.02072	2.02149
Alpha virt. eigenvalues --	2.02421	2.03309	2.03492	2.03511	2.04312
Alpha virt. eigenvalues --	2.04422	2.04855	2.05169	2.05219	2.05720
Alpha virt. eigenvalues --	2.05853	2.06085	2.07147	2.07254	2.07268
Alpha virt. eigenvalues --	2.07350	2.07590	2.08134	2.08356	2.08737
Alpha virt. eigenvalues --	2.08962	2.09645	2.09855	2.09933	2.09984
Alpha virt. eigenvalues --	2.10100	2.10372	2.10916	2.10961	2.12730
Alpha virt. eigenvalues --	2.12970	2.13090	2.13183	2.13286	2.13308
Alpha virt. eigenvalues --	2.13722	2.14318	2.14790	2.14846	2.14863
Alpha virt. eigenvalues --	2.15000	2.15269	2.15439	2.15744	2.16861
Alpha virt. eigenvalues --	2.17635	2.18156	2.18317	2.18503	2.19143
Alpha virt. eigenvalues --	2.19339	2.19484	2.19642	2.19758	2.20712
Alpha virt. eigenvalues --	2.21000	2.21720	2.21720	2.22674	2.22874
Alpha virt. eigenvalues --	2.22974	2.23071	2.23188	2.23420	2.24234
Alpha virt. eigenvalues --	2.24266	2.24808	2.24938	2.25034	2.27212
Alpha virt. eigenvalues --	2.27426	2.27675	2.27877	2.27934	2.28859
Alpha virt. eigenvalues --	2.29928	2.30365	2.30523	2.30873	2.30936
Alpha virt. eigenvalues --	2.31050	2.32362	2.32424	2.33504	2.33523
Alpha virt. eigenvalues --	2.33624	2.34303	2.34586	2.34679	2.34900
Alpha virt. eigenvalues --	2.35202	2.35443	2.36927	2.37665	2.38076
Alpha virt. eigenvalues --	2.38891	2.38946	2.39180	2.39262	2.39969
Alpha virt. eigenvalues --	2.40539	2.41127	2.41519	2.41650	2.42143
Alpha virt. eigenvalues --	2.42154	2.42386	2.42423	2.42514	2.42836
Alpha virt. eigenvalues --	2.42936	2.43097	2.43158	2.43465	2.43649
Alpha virt. eigenvalues --	2.44001	2.44086	2.44152	2.44265	2.44370
Alpha virt. eigenvalues --	2.44455	2.44995	2.45114	2.45310	2.45312
Alpha virt. eigenvalues --	2.45669	2.45887	2.45904	2.46014	2.46033
Alpha virt. eigenvalues --	2.46323	2.46398	2.46761	2.47550	2.47784
Alpha virt. eigenvalues --	2.47872	2.48354	2.48432	2.48712	2.49111
Alpha virt. eigenvalues --	2.49180	2.49483	2.49489	2.49683	2.49914
Alpha virt. eigenvalues --	2.50118	2.50172	2.50184	2.50230	2.50236
Alpha virt. eigenvalues --	2.50423	2.50542	2.50633	2.51868	2.52301
Alpha virt. eigenvalues --	2.52607	2.52747	2.53054	2.53937	2.54152
Alpha virt. eigenvalues --	2.54268	2.54375	2.54738	2.54831	2.55018
Alpha virt. eigenvalues --	2.56069	2.56217	2.56342	2.56618	2.56666
Alpha virt. eigenvalues --	2.56771	2.56901	2.57899	2.58439	2.58796

Alpha virt. eigenvalues -- 2.58952 2.59175 2.59536 2.60897 2.61492
Alpha virt. eigenvalues -- 2.61510 2.63396 2.64714 2.66478 2.69599
Alpha virt. eigenvalues -- 2.70055 2.70198 2.70614 2.70892 2.79400
Alpha virt. eigenvalues -- 2.80174 2.81205 2.82015 2.82048 2.92073
Alpha virt. eigenvalues -- 2.92147 2.92330 2.92641 2.92744 2.94873
Alpha virt. eigenvalues -- 2.95334 2.95383 2.95506 2.95536 2.98249
Alpha virt. eigenvalues -- 2.98252 2.98515 2.98659 2.98786 2.99340
Alpha virt. eigenvalues -- 2.99386 2.99391 2.99442 2.99446 3.00070
Alpha virt. eigenvalues -- 3.00107 3.00165 3.00295 3.00498 3.03046
Alpha virt. eigenvalues -- 3.03115 3.03131 3.03184 3.03194 3.04171
Alpha virt. eigenvalues -- 3.04444 3.04758 3.04938 3.05138 3.08464
Alpha virt. eigenvalues -- 3.08498 3.08498 3.08525 3.08547 3.09135
Alpha virt. eigenvalues -- 3.09158 3.09161 3.09192 3.09199 3.11288
Alpha virt. eigenvalues -- 3.11331 3.11405 3.11506 3.11559 3.12169
Alpha virt. eigenvalues -- 3.12303 3.12837 3.13130 3.13343 3.14100
Alpha virt. eigenvalues -- 3.14463 3.14478 3.15103 3.15136 3.24679
Alpha virt. eigenvalues -- 3.24683 3.24728 3.24794 3.24901 3.26830
Alpha virt. eigenvalues -- 3.26840 3.26891 3.26899 3.26991 3.32211
Alpha virt. eigenvalues -- 3.32228 3.32284 3.32303 3.32468 3.37555
Alpha virt. eigenvalues -- 3.37583 3.37656 3.37665 3.37729 3.37803
Alpha virt. eigenvalues -- 3.37820 3.37866 3.37913 3.37963 3.41048
Alpha virt. eigenvalues -- 3.41226 3.41385 3.41400 3.41513 3.43008
Alpha virt. eigenvalues -- 3.43585 3.44099 3.44794 3.45380 3.51522
Alpha virt. eigenvalues -- 3.51834 3.52398 3.53048 3.53941

Magenta UV-Vis Spectrum Epsilon/Oscillator Strength – N = 5



Magenta Table of 10 Lowest Excited States – N = 5

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	2.44	509.06	1.8149
2	3.21	385.95	0.0002
3	3.37	368.43	0.0216

4	3.80	326.08	0.0016
5	3.86	321.31	0.2144
6	4.00	309.78	0.0631
7	4.00	309.75	0.0039
8	4.08	304.05	0.0000
9	4.08	303.80	0.0138
10	4.14	298.88	0.1472

Magenta Cartesian Coordinates – N = 6

C -3.20395 0.41491 0.01455
 C -2.88925 -0.93329 0.00659
 C -1.49195 -1.1908 -0.01655
 C -0.71693 -0.04329 -0.02977
 S -1.74079 1.37881 -0.01026
 O -0.92726 -2.4233 -0.05349
 O -3.85541 -1.88456 0.04679
 C -3.60831 -3.05997 -0.7254
 H -4.59983 -3.47574 -0.951
 H -3.1232 -2.78161 -1.67242
 C -1.57685 -3.43401 0.71804
 H -0.79865 -4.17584 0.94348
 H -1.93158 -3.00178 1.6652
 C -2.75066 -4.10892 -0.0044
 C -3.55634 -4.89522 1.03418
 H -4.35019 -5.47423 0.52062
 H -2.89562 -5.63175 1.53653
 C -2.27676 -5.12825 -1.04434
 H -1.74034 -5.95211 -0.53176
 H -3.15583 -5.58148 -1.5474
 O -4.11861 -4.0215 1.97651
 O -1.44058 -4.51073 -1.98633
 C -4.85801 -4.702 2.95959
 H -5.25364 -3.94921 3.65313
 H -5.70361 -5.2625 2.51911
 H -4.22879 -5.41475 3.5247
 C -0.99548 -5.40897 -2.97188
 H -0.3554 -4.84715 -3.66386
 H -0.40835 -6.23739 -2.53351
 H -1.8392 -5.84596 -3.53795
 C -4.5131 1.00775 0.01351
 C -4.82852 2.35526 -0.00507
 S -5.97553 0.0429 -0.00013
 C -6.22749 2.611 -0.02811
 O -3.86315 3.30751 0.02657
 C -6.99902 1.46336 -0.02918
 O -6.79401 3.84254 -0.07469
 C -4.11245 4.47735 -0.75306
 C -6.14427 4.85973 0.68864

H	-3.12168	4.89288	-0.98233
H	-4.59807	4.19243	-1.69787
C	-4.97042	5.53004	-0.03814
H	-6.92256	5.6031	0.90825
H	-5.78944	4.43505	1.63918
C	-4.16491	6.32229	0.99616
C	-5.4433	6.54334	-1.08435
H	-3.36999	6.89713	0.47961
H	-4.82529	7.06277	1.49311
O	-3.6044	5.45414	1.94471
H	-5.98187	7.36938	-0.57767
H	-4.56342	6.99474	-1.58763
O	-6.27632	5.91991	-2.02533
C	-2.86551	6.14044	2.92418
C	-6.7136	6.81134	-3.02069
H	-2.47124	5.39187	3.62304
H	-2.01898	6.69734	2.48096
H	-3.49479	6.85739	3.48389
H	-7.35317	6.2462	-3.71042
H	-7.29887	7.64607	-2.5922
H	-5.86549	7.2395	-3.58694
C	0.71694	0.0433	-0.02977
C	1.49195	1.19081	-0.01653
S	1.74079	-1.37879	-0.01028
C	2.88925	0.9333	0.00661
O	0.92727	2.42331	-0.05345
C	3.20395	-0.4149	0.01455
O	3.85542	1.88457	0.04683
C	1.57686	3.43401	0.7181
C	3.60832	3.05999	-0.72533
H	0.79865	4.17583	0.94355
H	1.93158	3.00176	1.66526
C	2.75067	4.10893	-0.00432
H	4.59984	3.47576	-0.95093
H	3.12321	2.78165	-1.67236
C	2.27678	5.12828	-1.04423
C	3.55636	4.8952	1.03428
H	1.74037	5.95214	-0.53164
H	3.15585	5.58153	-1.54728
O	1.4406	4.5108	-1.98625
H	4.35021	5.47422	0.52074
H	2.89564	5.63172	1.53665
O	4.11862	4.02145	1.97658
C	0.99551	5.40907	-2.97177
C	4.85802	4.70192	2.95968
H	0.35544	4.84727	-3.66378
H	0.40839	6.23748	-2.53339
H	1.83924	5.84607	-3.53783

H	5.25364	3.94911	3.65321
H	5.70362	5.26243	2.51923
H	4.2288	5.41466	3.52482
C	4.5131	-1.00774	0.01351
C	4.82851	-2.35526	-0.00508
S	5.97553	-0.0429	-0.00012
C	6.22748	-2.611	-0.02811
O	3.86315	-3.3075	0.02655
C	6.99902	-1.46337	-0.02917
O	6.794	-3.84254	-0.0747
C	4.11244	-4.47734	-0.75308
C	6.14426	-4.85974	0.68863
H	3.12167	-4.89287	-0.98235
H	4.59807	-4.19242	-1.69788
C	4.9704	-5.53003	-0.03815
H	6.92254	-5.60311	0.90824
H	5.78943	-4.43505	1.63917
C	4.16488	-6.32227	0.99615
C	5.44328	-6.54335	-1.08436
H	3.36996	-6.89711	0.4796
H	4.82525	-7.06276	1.4931
O	3.60438	-5.45412	1.94469
H	5.98184	-7.36939	-0.57767
H	4.56339	-6.99474	-1.58763
O	6.2763	-5.91993	-2.02534
C	2.86548	-6.1404	2.92416
C	6.71358	-6.81137	-3.02069
H	2.4712	-5.39182	3.62301
H	2.01894	-6.6973	2.48094
H	3.49475	-6.85735	3.48388
H	7.35315	-6.24624	-3.71043
H	7.29884	-7.6461	-2.5922
H	5.86546	-7.23953	-3.58694
C	8.43669	-1.37276	-0.02141
C	9.20857	-0.22478	0.00018
S	9.47044	-2.78551	-0.00121
C	10.61739	-0.48102	0.029
O	8.63913	1.00605	-0.03692
C	10.90167	-1.81936	0.0348
O	11.58162	0.47291	0.08106
C	9.27679	2.01144	0.75067
H	11.88534	-2.28007	0.04578
C	11.32323	1.65271	-0.67692
H	8.4945	2.7498	0.97393
H	9.62179	1.57216	1.69822
C	10.45688	2.69389	0.04645
H	12.3106	2.08145	-0.89814
H	10.84251	1.3833	-1.6293

C	9.99115	3.72203	-0.98876
C	11.24907	3.47398	1.09984
H	9.44852	4.54057	-0.47415
H	10.87416	4.18126	-1.47945
O	9.16462	3.11248	-1.94462
H	12.05142	4.05367	0.60053
H	10.58211	4.20992	1.59487
O	11.79579	2.59735	2.04897
C	8.72759	4.01991	-2.92527
C	12.50827	3.27767	3.05195
H	8.09463	3.46437	-3.62882
H	8.13539	4.84332	-2.48424
H	9.57593	4.46361	-3.47916
H	12.89363	2.5243	3.75064
H	13.35943	3.84658	2.63373
H	11.86121	3.98296	3.60623
C	-8.43669	1.37275	-0.02143
C	-9.20857	0.22477	0.00016
S	-9.47045	2.78549	-0.00123
C	-10.61739	0.48101	0.02897
O	-8.63912	-1.00606	-0.03694
C	-10.90167	1.81934	0.03477
O	-11.58162	-0.47293	0.08101
C	-9.27679	-2.01145	0.75064
H	-11.88534	2.28005	0.04574
C	-11.32321	-1.65273	-0.67696
H	-8.49449	-2.74981	0.9739
H	-9.62179	-1.57217	1.69819
C	-10.45687	-2.69391	0.04641
H	-12.31059	-2.08147	-0.89819
H	-10.84248	-1.38331	-1.62934
C	-9.99113	-3.72204	-0.98879
C	-11.24906	-3.47399	1.0998
H	-9.44851	-4.54058	-0.47417
H	-10.87414	-4.18128	-1.47948
O	-9.1646	-3.1125	-1.94464
H	-12.05142	-4.05369	0.60049
H	-10.58211	-4.20993	1.59484
O	-11.7958	-2.59736	2.04892
C	-8.72756	-4.01993	-2.92529
C	-12.50828	-3.27768	3.05191
H	-8.0946	-3.4644	-3.62884
H	-8.13537	-4.84334	-2.48426
H	-9.57589	-4.46364	-3.47918
H	-12.89365	-2.5243	3.75059
H	-13.35944	-3.84659	2.63368
H	-11.86123	-3.98296	3.60619

Magenta Energy Levels – N = 6

Neutral

Alpha occ. eigenvalues -- -89.09237 -89.09237 -89.09153 -89.09153 -89.09119
Alpha occ. eigenvalues -- -89.09119 -19.26337 -19.26337 -19.26319 -19.26319
Alpha occ. eigenvalues -- -19.26317 -19.26317 -19.26315 -19.26315 -19.26255
Alpha occ. eigenvalues -- -19.26255 -19.25703 -19.25703 -19.23563 -19.23563
Alpha occ. eigenvalues -- -19.23560 -19.23560 -19.23556 -19.23556 -19.23551
Alpha occ. eigenvalues -- -19.23551 -19.23549 -19.23549 -19.23545 -19.23545
Alpha occ. eigenvalues -- -10.30355 -10.30355 -10.30334 -10.30333 -10.30300
Alpha occ. eigenvalues -- -10.30300 -10.30290 -10.30289 -10.30257 -10.30257
Alpha occ. eigenvalues -- -10.30202 -10.30202 -10.29655 -10.29655 -10.29643
Alpha occ. eigenvalues -- -10.29643 -10.29641 -10.29641 -10.29636 -10.29636
Alpha occ. eigenvalues -- -10.29594 -10.29594 -10.29451 -10.29451 -10.29258
Alpha occ. eigenvalues -- -10.29258 -10.29253 -10.29253 -10.29247 -10.29247
Alpha occ. eigenvalues -- -10.29238 -10.29238 -10.29232 -10.29232 -10.29227
Alpha occ. eigenvalues -- -10.29227 -10.28152 -10.28152 -10.28148 -10.28148
Alpha occ. eigenvalues -- -10.28146 -10.28146 -10.28142 -10.28142 -10.28136
Alpha occ. eigenvalues -- -10.28136 -10.28133 -10.28133 -10.28113 -10.28112
Alpha occ. eigenvalues -- -10.27993 -10.27993 -10.27989 -10.27960 -10.27960
Alpha occ. eigenvalues -- -10.27955 -10.27955 -10.27951 -10.26408 -10.26408
Alpha occ. eigenvalues -- -10.26406 -10.26406 -10.26323 -10.26323 -10.26079
Alpha occ. eigenvalues -- -10.26079 -8.03559 -8.03559 -8.03419 -8.03419
Alpha occ. eigenvalues -- -8.03386 -8.03386 -5.97445 -5.97445 -5.97323
Alpha occ. eigenvalues -- -5.97323 -5.97290 -5.97290 -5.97076 -5.97076
Alpha occ. eigenvalues -- -5.96945 -5.96945 -5.96913 -5.96912 -5.96668
Alpha occ. eigenvalues -- -5.96668 -5.96493 -5.96493 -5.96458 -5.96458
Alpha occ. eigenvalues -- -1.11800 -1.11777 -1.11750 -1.11728 -1.11469
Alpha occ. eigenvalues -- -1.11469 -1.09434 -1.09427 -1.09409 -1.09387
Alpha occ. eigenvalues -- -1.09109 -1.09109 -1.07757 -1.07755 -1.07743
Alpha occ. eigenvalues -- -1.07743 -1.07739 -1.07739 -1.07579 -1.07579
Alpha occ. eigenvalues -- -1.07566 -1.07566 -1.07566 -1.07565 -0.92649
Alpha occ. eigenvalues -- -0.92262 -0.91618 -0.90802 -0.89965 -0.89329
Alpha occ. eigenvalues -- -0.85807 -0.85806 -0.85776 -0.85761 -0.85705
Alpha occ. eigenvalues -- -0.85686 -0.82148 -0.80692 -0.79003 -0.77629
Alpha occ. eigenvalues -- -0.76766 -0.76604 -0.76242 -0.76191 -0.75773
Alpha occ. eigenvalues -- -0.75654 -0.75363 -0.75317 -0.74515 -0.74506
Alpha occ. eigenvalues -- -0.74496 -0.74493 -0.74482 -0.74481 -0.72682
Alpha occ. eigenvalues -- -0.72576 -0.72270 -0.71817 -0.71709 -0.71310
Alpha occ. eigenvalues -- -0.71305 -0.71252 -0.71231 -0.70845 -0.69368
Alpha occ. eigenvalues -- -0.68222 -0.68218 -0.68068 -0.68066 -0.68024
Alpha occ. eigenvalues -- -0.68016 -0.67218 -0.64569 -0.64508 -0.64493
Alpha occ. eigenvalues -- -0.64479 -0.64477 -0.64449 -0.64212 -0.63036
Alpha occ. eigenvalues -- -0.62119 -0.61387 -0.60909 -0.60753 -0.59864
Alpha occ. eigenvalues -- -0.59847 -0.59794 -0.59695 -0.59401 -0.58831
Alpha occ. eigenvalues -- -0.58421 -0.57590 -0.56974 -0.56582 -0.56276
Alpha occ. eigenvalues -- -0.56123 -0.54039 -0.53879 -0.53426 -0.53200
Alpha occ. eigenvalues -- -0.53186 -0.53120 -0.53073 -0.53060 -0.53034
Alpha occ. eigenvalues -- -0.52906 -0.52750 -0.52648 -0.52107 -0.52025

Alpha occ. eigenvalues --	-0.51927	-0.51863	-0.51824	-0.51814	-0.50874
Alpha occ. eigenvalues --	-0.50777	-0.50547	-0.50232	-0.50039	-0.49960
Alpha occ. eigenvalues --	-0.49840	-0.49826	-0.49484	-0.48755	-0.48708
Alpha occ. eigenvalues --	-0.48673	-0.48638	-0.48635	-0.48629	-0.48620
Alpha occ. eigenvalues --	-0.48597	-0.48492	-0.48230	-0.48116	-0.48023
Alpha occ. eigenvalues --	-0.47681	-0.47492	-0.47328	-0.47306	-0.47236
Alpha occ. eigenvalues --	-0.47161	-0.47021	-0.46980	-0.46939	-0.46793
Alpha occ. eigenvalues --	-0.46778	-0.46390	-0.46047	-0.45909	-0.45903
Alpha occ. eigenvalues --	-0.45883	-0.45875	-0.45871	-0.45507	-0.44578
Alpha occ. eigenvalues --	-0.44544	-0.44124	-0.44069	-0.43914	-0.43882
Alpha occ. eigenvalues --	-0.43693	-0.43571	-0.43481	-0.43286	-0.43106
Alpha occ. eigenvalues --	-0.42997	-0.42968	-0.42783	-0.42624	-0.42338
Alpha occ. eigenvalues --	-0.42331	-0.41812	-0.41473	-0.41238	-0.41133
Alpha occ. eigenvalues --	-0.41072	-0.41063	-0.40993	-0.40983	-0.40600
Alpha occ. eigenvalues --	-0.40153	-0.40144	-0.40071	-0.40025	-0.39999
Alpha occ. eigenvalues --	-0.39976	-0.39976	-0.39649	-0.39562	-0.39470
Alpha occ. eigenvalues --	-0.39433	-0.39393	-0.38694	-0.38132	-0.37820
Alpha occ. eigenvalues --	-0.37817	-0.37690	-0.37645	-0.37434	-0.37341
Alpha occ. eigenvalues --	-0.37116	-0.36959	-0.36746	-0.36656	-0.36542
Alpha occ. eigenvalues --	-0.36312	-0.36260	-0.35927	-0.35835	-0.35553
Alpha occ. eigenvalues --	-0.35462	-0.34485	-0.34465	-0.34458	-0.34452
Alpha occ. eigenvalues --	-0.34431	-0.34428	-0.33906	-0.33825	-0.33667
Alpha occ. eigenvalues --	-0.33645	-0.33477	-0.33474	-0.33105	-0.33100
Alpha occ. eigenvalues --	-0.33093	-0.33069	-0.33057	-0.33043	-0.32361
Alpha occ. eigenvalues --	-0.32330	-0.32327	-0.32172	-0.32082	-0.31883
Alpha occ. eigenvalues --	-0.31081	-0.30758	-0.30702	-0.30514	-0.30164
Alpha occ. eigenvalues --	-0.30130	-0.27942	-0.27782	-0.27777	-0.27766
Alpha occ. eigenvalues --	-0.27765	-0.27752	-0.27741	-0.27501	-0.26985
Alpha occ. eigenvalues --	-0.26984	-0.26975	-0.26974	-0.26970	-0.26969
Alpha occ. eigenvalues --	-0.25630	-0.23782	-0.23490	-0.22927	-0.22911
Alpha occ. eigenvalues --	-0.22733	-0.22710	-0.21918	-0.19304	-0.16670
Alpha virt. eigenvalues --	-0.06445	-0.04050	-0.01441	0.01021	0.03229
Alpha virt. eigenvalues --	0.03900	0.04298	0.04621	0.04699	0.04801
Alpha virt. eigenvalues --	0.04989	0.05101	0.05354	0.05401	0.05596
Alpha virt. eigenvalues --	0.06046	0.06126	0.06157	0.06859	0.06952
Alpha virt. eigenvalues --	0.07145	0.07573	0.07719	0.07781	0.07939
Alpha virt. eigenvalues --	0.08042	0.08145	0.08225	0.08727	0.08779
Alpha virt. eigenvalues --	0.08881	0.09037	0.09236	0.09345	0.09363
Alpha virt. eigenvalues --	0.09529	0.09826	0.09874	0.10080	0.10219
Alpha virt. eigenvalues --	0.10428	0.10556	0.10625	0.10679	0.10862
Alpha virt. eigenvalues --	0.10913	0.11069	0.11183	0.11290	0.11491
Alpha virt. eigenvalues --	0.11758	0.11944	0.11973	0.11993	0.12073
Alpha virt. eigenvalues --	0.12220	0.12393	0.12583	0.12961	0.13137
Alpha virt. eigenvalues --	0.13179	0.13210	0.13234	0.13359	0.13407
Alpha virt. eigenvalues --	0.13439	0.13488	0.13687	0.13801	0.13978
Alpha virt. eigenvalues --	0.14070	0.14128	0.14153	0.14196	0.14197
Alpha virt. eigenvalues --	0.14224	0.14268	0.14321	0.14357	0.14397
Alpha virt. eigenvalues --	0.14410	0.14437	0.14614	0.14671	0.14823

Alpha virt. eigenvalues --	0.14881	0.14987	0.14995	0.15022	0.15039
Alpha virt. eigenvalues --	0.15063	0.15074	0.15092	0.15196	0.15338
Alpha virt. eigenvalues --	0.15376	0.15510	0.15636	0.15821	0.15828
Alpha virt. eigenvalues --	0.16065	0.16788	0.16922	0.16954	0.17287
Alpha virt. eigenvalues --	0.17328	0.17441	0.17537	0.17599	0.17718
Alpha virt. eigenvalues --	0.17776	0.17961	0.17970	0.18164	0.18239
Alpha virt. eigenvalues --	0.18390	0.18522	0.18624	0.18731	0.18801
Alpha virt. eigenvalues --	0.19281	0.19455	0.19563	0.19944	0.20146
Alpha virt. eigenvalues --	0.20564	0.20678	0.20807	0.20812	0.21002
Alpha virt. eigenvalues --	0.21409	0.21521	0.21563	0.21670	0.21750
Alpha virt. eigenvalues --	0.21956	0.22182	0.22526	0.22992	0.23073
Alpha virt. eigenvalues --	0.23093	0.23159	0.23168	0.23305	0.23796
Alpha virt. eigenvalues --	0.23893	0.23905	0.24110	0.24121	0.24327
Alpha virt. eigenvalues --	0.24456	0.24771	0.25057	0.25105	0.25426
Alpha virt. eigenvalues --	0.25754	0.25767	0.25940	0.26052	0.26303
Alpha virt. eigenvalues --	0.26309	0.26847	0.27295	0.27548	0.27975
Alpha virt. eigenvalues --	0.28010	0.28181	0.28234	0.28358	0.28502
Alpha virt. eigenvalues --	0.28560	0.28693	0.28802	0.28848	0.29299
Alpha virt. eigenvalues --	0.29635	0.29722	0.29889	0.29893	0.29989
Alpha virt. eigenvalues --	0.30043	0.30245	0.30392	0.32293	0.32498
Alpha virt. eigenvalues --	0.32654	0.32793	0.32815	0.34188	0.34804
Alpha virt. eigenvalues --	0.35944	0.37309	0.38394	0.39340	0.39675
Alpha virt. eigenvalues --	0.40685	0.40969	0.41046	0.41505	0.41635
Alpha virt. eigenvalues --	0.42344	0.42554	0.42580	0.42682	0.42740
Alpha virt. eigenvalues --	0.42933	0.43149	0.43594	0.43935	0.44048
Alpha virt. eigenvalues --	0.44061	0.44253	0.44447	0.44566	0.44725
Alpha virt. eigenvalues --	0.44848	0.45033	0.45083	0.45269	0.45395
Alpha virt. eigenvalues --	0.45660	0.45706	0.45886	0.45923	0.45947
Alpha virt. eigenvalues --	0.46205	0.46328	0.46491	0.46542	0.46569
Alpha virt. eigenvalues --	0.46638	0.46772	0.46842	0.46875	0.47003
Alpha virt. eigenvalues --	0.47065	0.47078	0.47116	0.47136	0.47298
Alpha virt. eigenvalues --	0.47342	0.47366	0.47419	0.47520	0.47549
Alpha virt. eigenvalues --	0.47601	0.47649	0.47705	0.47780	0.47847
Alpha virt. eigenvalues --	0.47918	0.48057	0.48110	0.48170	0.48355
Alpha virt. eigenvalues --	0.48521	0.48568	0.48649	0.48922	0.49101
Alpha virt. eigenvalues --	0.49142	0.49243	0.49449	0.49558	0.49667
Alpha virt. eigenvalues --	0.49756	0.49809	0.49943	0.50032	0.50085
Alpha virt. eigenvalues --	0.50214	0.50248	0.50254	0.50275	0.50320
Alpha virt. eigenvalues --	0.50427	0.50565	0.50660	0.51405	0.51521
Alpha virt. eigenvalues --	0.51660	0.51786	0.51810	0.52203	0.52238
Alpha virt. eigenvalues --	0.52372	0.52492	0.53045	0.53052	0.53251
Alpha virt. eigenvalues --	0.53378	0.53415	0.53540	0.53567	0.53722
Alpha virt. eigenvalues --	0.53775	0.54092	0.54115	0.54366	0.54732
Alpha virt. eigenvalues --	0.54801	0.54897	0.54995	0.55087	0.55182
Alpha virt. eigenvalues --	0.55247	0.55307	0.55476	0.55938	0.56023
Alpha virt. eigenvalues --	0.56027	0.56078	0.56141	0.56152	0.56288
Alpha virt. eigenvalues --	0.56820	0.56890	0.57152	0.57270	0.57462
Alpha virt. eigenvalues --	0.57811	0.58025	0.58121	0.58341	0.58623

Alpha virt. eigenvalues --	0.58899	0.58923	0.60036	0.60076	0.60305
Alpha virt. eigenvalues --	0.60370	0.60658	0.60707	0.60901	0.60977
Alpha virt. eigenvalues --	0.61183	0.61243	0.61315	0.61477	0.61732
Alpha virt. eigenvalues --	0.61733	0.62038	0.62075	0.62112	0.62112
Alpha virt. eigenvalues --	0.62203	0.62282	0.62325	0.62453	0.62556
Alpha virt. eigenvalues --	0.62871	0.62898	0.63012	0.63053	0.63138
Alpha virt. eigenvalues --	0.63202	0.63268	0.63400	0.63400	0.63627
Alpha virt. eigenvalues --	0.63669	0.63706	0.63730	0.63811	0.63986
Alpha virt. eigenvalues --	0.64026	0.64086	0.64287	0.64403	0.64433
Alpha virt. eigenvalues --	0.64458	0.64540	0.64555	0.64562	0.64642
Alpha virt. eigenvalues --	0.64761	0.64901	0.64999	0.65069	0.65228
Alpha virt. eigenvalues --	0.65351	0.65559	0.65577	0.65692	0.65716
Alpha virt. eigenvalues --	0.65807	0.65944	0.66073	0.66335	0.66426
Alpha virt. eigenvalues --	0.66656	0.66760	0.66785	0.66881	0.66904
Alpha virt. eigenvalues --	0.66930	0.67023	0.67090	0.67124	0.67153
Alpha virt. eigenvalues --	0.67206	0.67234	0.67380	0.67588	0.67646
Alpha virt. eigenvalues --	0.67730	0.67919	0.68231	0.68268	0.68455
Alpha virt. eigenvalues --	0.68464	0.68483	0.68583	0.68678	0.68723
Alpha virt. eigenvalues --	0.68725	0.68800	0.68854	0.68874	0.68935
Alpha virt. eigenvalues --	0.69164	0.69285	0.69406	0.69514	0.69534
Alpha virt. eigenvalues --	0.69635	0.69730	0.69862	0.69993	0.70381
Alpha virt. eigenvalues --	0.70397	0.70793	0.70889	0.70939	0.70956
Alpha virt. eigenvalues --	0.71190	0.71521	0.71580	0.71677	0.71718
Alpha virt. eigenvalues --	0.72002	0.72129	0.72186	0.72250	0.72531
Alpha virt. eigenvalues --	0.72992	0.73027	0.73073	0.73183	0.73242
Alpha virt. eigenvalues --	0.73394	0.73780	0.73904	0.73926	0.73990
Alpha virt. eigenvalues --	0.74386	0.74519	0.74602	0.74648	0.74886
Alpha virt. eigenvalues --	0.74975	0.75046	0.75329	0.75487	0.75609
Alpha virt. eigenvalues --	0.75626	0.75791	0.75909	0.76001	0.76316
Alpha virt. eigenvalues --	0.76382	0.76403	0.76417	0.76469	0.76562
Alpha virt. eigenvalues --	0.76654	0.76857	0.76885	0.77132	0.77140
Alpha virt. eigenvalues --	0.77489	0.77637	0.77839	0.77908	0.77929
Alpha virt. eigenvalues --	0.78235	0.78590	0.79398	0.79854	0.80284
Alpha virt. eigenvalues --	0.80288	0.80289	0.81665	0.81687	0.81991
Alpha virt. eigenvalues --	0.82318	0.82814	0.82971	0.83412	0.83531
Alpha virt. eigenvalues --	0.84105	0.84253	0.84587	0.85793	0.85978
Alpha virt. eigenvalues --	0.86383	0.86490	0.87358	0.87415	0.87571
Alpha virt. eigenvalues --	0.87956	0.88009	0.88138	0.88218	0.88247
Alpha virt. eigenvalues --	0.88358	0.88405	0.88471	0.88562	0.88633
Alpha virt. eigenvalues --	0.88745	0.88754	0.89192	0.89955	0.90334
Alpha virt. eigenvalues --	0.90417	0.90980	0.91456	0.91784	0.91788
Alpha virt. eigenvalues --	0.91866	0.91967	0.91982	0.92013	0.92199
Alpha virt. eigenvalues --	0.92312	0.92442	0.92444	0.92620	0.92704
Alpha virt. eigenvalues --	0.93137	0.93340	0.94178	0.94282	0.95266
Alpha virt. eigenvalues --	0.95315	0.95502	0.95551	0.97219	0.97464
Alpha virt. eigenvalues --	0.97696	0.97810	0.97843	0.97877	0.97990
Alpha virt. eigenvalues --	0.98002	0.99010	0.99242	0.99291	0.99411
Alpha virt. eigenvalues --	0.99687	0.99854	0.99980	1.00085	1.00440

Alpha virt. eigenvalues --	1.00482	1.00972	1.01079	1.01442	1.01693
Alpha virt. eigenvalues --	1.02561	1.02646	1.02861	1.02882	1.02982
Alpha virt. eigenvalues --	1.03246	1.03328	1.03519	1.03571	1.03842
Alpha virt. eigenvalues --	1.03857	1.04290	1.04901	1.04941	1.05203
Alpha virt. eigenvalues --	1.06026	1.06477	1.07013	1.07464	1.07610
Alpha virt. eigenvalues --	1.07929	1.08204	1.09134	1.09165	1.09537
Alpha virt. eigenvalues --	1.09560	1.10209	1.10517	1.10824	1.11246
Alpha virt. eigenvalues --	1.11828	1.11999	1.12685	1.12738	1.13110
Alpha virt. eigenvalues --	1.13232	1.13374	1.13398	1.14164	1.14765
Alpha virt. eigenvalues --	1.14949	1.15014	1.15177	1.15234	1.16573
Alpha virt. eigenvalues --	1.16575	1.16816	1.16830	1.16952	1.17143
Alpha virt. eigenvalues --	1.17203	1.17221	1.17557	1.18110	1.19073
Alpha virt. eigenvalues --	1.19082	1.19469	1.19632	1.19680	1.19751
Alpha virt. eigenvalues --	1.19874	1.19915	1.19938	1.20041	1.20330
Alpha virt. eigenvalues --	1.20730	1.20881	1.21020	1.21157	1.21594
Alpha virt. eigenvalues --	1.21705	1.22598	1.22655	1.23051	1.23071
Alpha virt. eigenvalues --	1.23249	1.23359	1.23585	1.23806	1.23919
Alpha virt. eigenvalues --	1.24444	1.24661	1.25300	1.25534	1.25709
Alpha virt. eigenvalues --	1.25769	1.26044	1.26087	1.26199	1.26379
Alpha virt. eigenvalues --	1.26774	1.26954	1.27151	1.27231	1.27348
Alpha virt. eigenvalues --	1.27436	1.27457	1.27809	1.27878	1.28178
Alpha virt. eigenvalues --	1.28367	1.29450	1.29497	1.29587	1.30291
Alpha virt. eigenvalues --	1.30343	1.30388	1.30569	1.30810	1.31279
Alpha virt. eigenvalues --	1.31530	1.31753	1.31906	1.32536	1.32894
Alpha virt. eigenvalues --	1.32983	1.33025	1.33148	1.33295	1.33386
Alpha virt. eigenvalues --	1.34220	1.34286	1.34547	1.34798	1.34829
Alpha virt. eigenvalues --	1.35320	1.35416	1.35825	1.35912	1.36150
Alpha virt. eigenvalues --	1.36309	1.36781	1.37513	1.37574	1.37738
Alpha virt. eigenvalues --	1.37860	1.38185	1.38276	1.38452	1.38777
Alpha virt. eigenvalues --	1.39207	1.39213	1.39388	1.39514	1.39681
Alpha virt. eigenvalues --	1.39864	1.40428	1.40683	1.40768	1.40983
Alpha virt. eigenvalues --	1.41218	1.41222	1.41272	1.41284	1.41338
Alpha virt. eigenvalues --	1.41342	1.41449	1.41496	1.41501	1.41506
Alpha virt. eigenvalues --	1.41526	1.41559	1.41738	1.41820	1.42103
Alpha virt. eigenvalues --	1.42258	1.42271	1.42714	1.42750	1.42824
Alpha virt. eigenvalues --	1.43026	1.43054	1.43265	1.43670	1.43853
Alpha virt. eigenvalues --	1.44009	1.44104	1.44507	1.44521	1.44609
Alpha virt. eigenvalues --	1.44736	1.44954	1.45020	1.45139	1.45335
Alpha virt. eigenvalues --	1.45392	1.45412	1.45520	1.45587	1.45812
Alpha virt. eigenvalues --	1.45929	1.46399	1.46438	1.46578	1.47525
Alpha virt. eigenvalues --	1.47715	1.47868	1.47934	1.48076	1.48205
Alpha virt. eigenvalues --	1.48497	1.48552	1.48603	1.48760	1.49153
Alpha virt. eigenvalues --	1.49170	1.49782	1.49901	1.50272	1.50403
Alpha virt. eigenvalues --	1.50438	1.50733	1.50900	1.51465	1.51598
Alpha virt. eigenvalues --	1.51952	1.52506	1.52614	1.52777	1.52884
Alpha virt. eigenvalues --	1.53416	1.53536	1.53739	1.53756	1.53869
Alpha virt. eigenvalues --	1.54034	1.54241	1.54427	1.54500	1.54518
Alpha virt. eigenvalues --	1.54713	1.54945	1.55230	1.55525	1.56162

Alpha virt. eigenvalues --	1.56306	1.56459	1.56526	1.56696	1.56709
Alpha virt. eigenvalues --	1.56822	1.56999	1.57140	1.57175	1.57548
Alpha virt. eigenvalues --	1.57845	1.58003	1.58454	1.58545	1.58688
Alpha virt. eigenvalues --	1.58762	1.58862	1.58896	1.58942	1.58954
Alpha virt. eigenvalues --	1.59237	1.59263	1.59482	1.59821	1.60013
Alpha virt. eigenvalues --	1.60083	1.60218	1.60421	1.60519	1.61344
Alpha virt. eigenvalues --	1.61526	1.61762	1.61787	1.61851	1.62072
Alpha virt. eigenvalues --	1.62451	1.62544	1.62605	1.62857	1.62924
Alpha virt. eigenvalues --	1.63028	1.63043	1.63119	1.63198	1.63224
Alpha virt. eigenvalues --	1.63314	1.63433	1.63489	1.63527	1.63538
Alpha virt. eigenvalues --	1.63599	1.63697	1.63937	1.63970	1.64017
Alpha virt. eigenvalues --	1.64171	1.64189	1.64287	1.64391	1.64504
Alpha virt. eigenvalues --	1.64674	1.64674	1.64771	1.65254	1.65360
Alpha virt. eigenvalues --	1.65441	1.65506	1.65640	1.65676	1.65898
Alpha virt. eigenvalues --	1.65959	1.66254	1.66431	1.66822	1.67046
Alpha virt. eigenvalues --	1.67221	1.67351	1.67692	1.67945	1.68013
Alpha virt. eigenvalues --	1.68274	1.68452	1.68588	1.68706	1.68986
Alpha virt. eigenvalues --	1.69141	1.69292	1.69483	1.69563	1.69693
Alpha virt. eigenvalues --	1.69849	1.70147	1.70165	1.70267	1.70354
Alpha virt. eigenvalues --	1.70918	1.71084	1.71239	1.71693	1.71699
Alpha virt. eigenvalues --	1.71886	1.71911	1.72143	1.72202	1.72227
Alpha virt. eigenvalues --	1.72255	1.72273	1.72281	1.72428	1.72530
Alpha virt. eigenvalues --	1.72547	1.72622	1.72804	1.73581	1.73807
Alpha virt. eigenvalues --	1.74309	1.74328	1.74714	1.74907	1.74938
Alpha virt. eigenvalues --	1.74977	1.75138	1.75261	1.75285	1.75369
Alpha virt. eigenvalues --	1.75410	1.75834	1.75858	1.75994	1.76369
Alpha virt. eigenvalues --	1.76541	1.76799	1.76929	1.77234	1.77290
Alpha virt. eigenvalues --	1.77435	1.77701	1.77896	1.77931	1.78103
Alpha virt. eigenvalues --	1.78155	1.78348	1.78350	1.79039	1.79104
Alpha virt. eigenvalues --	1.79464	1.79572	1.79581	1.79673	1.79731
Alpha virt. eigenvalues --	1.79875	1.79965	1.80048	1.80216	1.80385
Alpha virt. eigenvalues --	1.81226	1.81488	1.81518	1.81874	1.81935
Alpha virt. eigenvalues --	1.82087	1.82421	1.82452	1.82889	1.83088
Alpha virt. eigenvalues --	1.83448	1.83538	1.83687	1.83723	1.84065
Alpha virt. eigenvalues --	1.84068	1.84280	1.84432	1.84621	1.84690
Alpha virt. eigenvalues --	1.84856	1.84893	1.84912	1.85057	1.85886
Alpha virt. eigenvalues --	1.85994	1.86322	1.86431	1.86581	1.86626
Alpha virt. eigenvalues --	1.86881	1.86889	1.87001	1.87028	1.87104
Alpha virt. eigenvalues --	1.87285	1.87299	1.87404	1.87449	1.87514
Alpha virt. eigenvalues --	1.87589	1.87657	1.88015	1.88464	1.88570
Alpha virt. eigenvalues --	1.88666	1.88962	1.89062	1.89173	1.89491
Alpha virt. eigenvalues --	1.89623	1.90154	1.90539	1.90726	1.91175
Alpha virt. eigenvalues --	1.91331	1.91411	1.91917	1.92644	1.93430
Alpha virt. eigenvalues --	1.94078	1.94199	1.94305	1.94985	1.95027
Alpha virt. eigenvalues --	1.95333	1.95641	1.96336	1.96429	1.96667
Alpha virt. eigenvalues --	1.96760	1.97328	1.97458	1.98113	1.98124
Alpha virt. eigenvalues --	1.98571	1.98830	1.98991	1.99164	1.99273
Alpha virt. eigenvalues --	1.99787	1.99938	1.99995	2.00332	2.00354

Alpha virt. eigenvalues --	2.00402	2.00428	2.00554	2.00686	2.00755
Alpha virt. eigenvalues --	2.00775	2.00814	2.00923	2.01050	2.01087
Alpha virt. eigenvalues --	2.01244	2.01404	2.01956	2.02054	2.02092
Alpha virt. eigenvalues --	2.02159	2.03091	2.03343	2.03508	2.03553
Alpha virt. eigenvalues --	2.04264	2.04450	2.04759	2.05088	2.05248
Alpha virt. eigenvalues --	2.05382	2.05558	2.05857	2.05989	2.06214
Alpha virt. eigenvalues --	2.07146	2.07191	2.07327	2.07410	2.07536
Alpha virt. eigenvalues --	2.07682	2.08264	2.08317	2.08668	2.08937
Alpha virt. eigenvalues --	2.09430	2.09504	2.09834	2.09989	2.10014
Alpha virt. eigenvalues --	2.10070	2.10079	2.10521	2.10923	2.10942
Alpha virt. eigenvalues --	2.12757	2.13010	2.13134	2.13189	2.13195
Alpha virt. eigenvalues --	2.13261	2.13366	2.13570	2.14444	2.14523
Alpha virt. eigenvalues --	2.14787	2.14859	2.14939	2.14951	2.14995
Alpha virt. eigenvalues --	2.15398	2.15736	2.16044	2.17209	2.17627
Alpha virt. eigenvalues --	2.18106	2.18349	2.18448	2.18486	2.19229
Alpha virt. eigenvalues --	2.19337	2.19423	2.19651	2.19651	2.19793
Alpha virt. eigenvalues --	2.20870	2.21043	2.21482	2.21759	2.22336
Alpha virt. eigenvalues --	2.22373	2.22807	2.22817	2.23016	2.23146
Alpha virt. eigenvalues --	2.23270	2.23620	2.24269	2.24341	2.24776
Alpha virt. eigenvalues --	2.24955	2.25116	2.25138	2.27179	2.27316
Alpha virt. eigenvalues --	2.27532	2.27679	2.27911	2.28022	2.28858
Alpha virt. eigenvalues --	2.29657	2.30661	2.30752	2.30850	2.30906
Alpha virt. eigenvalues --	2.30927	2.30980	2.32046	2.32376	2.33141
Alpha virt. eigenvalues --	2.33200	2.33726	2.33806	2.33851	2.34443
Alpha virt. eigenvalues --	2.34653	2.34950	2.35105	2.35132	2.35385
Alpha virt. eigenvalues --	2.36138	2.37324	2.37906	2.38462	2.38806
Alpha virt. eigenvalues --	2.39041	2.39234	2.39353	2.39575	2.40270
Alpha virt. eigenvalues --	2.40443	2.41088	2.41314	2.41613	2.41877
Alpha virt. eigenvalues --	2.42220	2.42404	2.42438	2.42560	2.42615
Alpha virt. eigenvalues --	2.42625	2.42803	2.42839	2.42886	2.43059
Alpha virt. eigenvalues --	2.43171	2.43301	2.43696	2.43924	2.43933
Alpha virt. eigenvalues --	2.44164	2.44168	2.44210	2.44278	2.44286
Alpha virt. eigenvalues --	2.44558	2.44882	2.45193	2.45243	2.45291
Alpha virt. eigenvalues --	2.45426	2.45790	2.45797	2.45912	2.45929
Alpha virt. eigenvalues --	2.45986	2.46097	2.46279	2.46339	2.47105
Alpha virt. eigenvalues --	2.47177	2.47740	2.47905	2.48002	2.48224
Alpha virt. eigenvalues --	2.48495	2.48634	2.49023	2.49045	2.49168
Alpha virt. eigenvalues --	2.49353	2.49518	2.49726	2.49867	2.50023
Alpha virt. eigenvalues --	2.50059	2.50121	2.50136	2.50213	2.50255
Alpha virt. eigenvalues --	2.50341	2.50391	2.50573	2.50972	2.52109
Alpha virt. eigenvalues --	2.52282	2.52481	2.52681	2.52762	2.53162
Alpha virt. eigenvalues --	2.54032	2.54252	2.54312	2.54367	2.54402
Alpha virt. eigenvalues --	2.54718	2.54757	2.54951	2.56158	2.56210
Alpha virt. eigenvalues --	2.56275	2.56402	2.56568	2.56682	2.56699
Alpha virt. eigenvalues --	2.56931	2.57505	2.58473	2.58613	2.58717
Alpha virt. eigenvalues --	2.58848	2.59007	2.59125	2.59986	2.61158
Alpha virt. eigenvalues --	2.61387	2.61832	2.63526	2.64333	2.65338
Alpha virt. eigenvalues --	2.66762	2.69347	2.69825	2.70094	2.70278

Alpha virt. eigenvalues --	2.70902	2.70985	2.79481	2.79900	2.80816
Alpha virt. eigenvalues --	2.81357	2.82006	2.82054	2.91983	2.91996
Alpha virt. eigenvalues --	2.92211	2.92299	2.92649	2.92782	2.94913
Alpha virt. eigenvalues --	2.95223	2.95348	2.95414	2.95502	2.95513
Alpha virt. eigenvalues --	2.98240	2.98297	2.98379	2.98583	2.98708
Alpha virt. eigenvalues --	2.98838	2.99352	2.99382	2.99405	2.99422
Alpha virt. eigenvalues --	2.99458	2.99469	3.00075	3.00090	3.00137
Alpha virt. eigenvalues --	3.00221	3.00357	3.00560	3.03049	3.03099
Alpha virt. eigenvalues --	3.03155	3.03158	3.03213	3.03214	3.04241
Alpha virt. eigenvalues --	3.04423	3.04724	3.04905	3.05039	3.05074
Alpha virt. eigenvalues --	3.08498	3.08500	3.08534	3.08535	3.08551
Alpha virt. eigenvalues --	3.08580	3.09151	3.09153	3.09177	3.09184
Alpha virt. eigenvalues --	3.09214	3.09228	3.11254	3.11317	3.11381
Alpha virt. eigenvalues --	3.11415	3.11524	3.11554	3.12134	3.12285
Alpha virt. eigenvalues --	3.12657	3.13092	3.13460	3.13685	3.13919
Alpha virt. eigenvalues --	3.14395	3.14617	3.14786	3.14806	3.15092
Alpha virt. eigenvalues --	3.24688	3.24691	3.24759	3.24764	3.24848
Alpha virt. eigenvalues --	3.24950	3.26829	3.26829	3.26924	3.26934
Alpha virt. eigenvalues --	3.26947	3.27005	3.32202	3.32207	3.32265
Alpha virt. eigenvalues --	3.32267	3.32315	3.32420	3.37583	3.37595
Alpha virt. eigenvalues --	3.37630	3.37658	3.37710	3.37711	3.37740
Alpha virt. eigenvalues --	3.37793	3.37856	3.37865	3.37928	3.37946
Alpha virt. eigenvalues --	3.41171	3.41260	3.41345	3.41505	3.41514
Alpha virt. eigenvalues --	3.41569	3.42665	3.43279	3.43723	3.44363
Alpha virt. eigenvalues --	3.45037	3.45517	3.51548	3.51690	3.52109
Alpha virt. eigenvalues --	3.52625	3.53275	3.54122		

Cation/Polaron

Alpha occ. eigenvalues --	-89.11930	-89.11930	-89.11509	-89.11509	-89.10947
Alpha occ. eigenvalues --	-89.10947	-19.29020	-19.29020	-19.28757	-19.28757
Alpha occ. eigenvalues --	-19.28735	-19.28735	-19.28144	-19.28144	-19.28070
Alpha occ. eigenvalues --	-19.28070	-19.26918	-19.26918	-19.24530	-19.24530
Alpha occ. eigenvalues --	-19.24511	-19.24511	-19.24436	-19.24436	-19.24362
Alpha occ. eigenvalues --	-19.24362	-19.24278	-19.24278	-19.24209	-19.24209
Alpha occ. eigenvalues --	-10.33990	-10.33989	-10.33625	-10.33625	-10.33578
Alpha occ. eigenvalues --	-10.33578	-10.32805	-10.32805	-10.32571	-10.32571
Alpha occ. eigenvalues --	-10.32117	-10.32117	-10.31992	-10.31954	-10.31882
Alpha occ. eigenvalues --	-10.31882	-10.31363	-10.31363	-10.31291	-10.31291
Alpha occ. eigenvalues --	-10.31203	-10.31203	-10.31105	-10.31105	-10.31041
Alpha occ. eigenvalues --	-10.31041	-10.30920	-10.30920	-10.30726	-10.30725
Alpha occ. eigenvalues --	-10.30374	-10.30374	-10.30280	-10.30280	-10.30276
Alpha occ. eigenvalues --	-10.30276	-10.30159	-10.30159	-10.30141	-10.30140
Alpha occ. eigenvalues --	-10.30126	-10.30126	-10.29963	-10.29963	-10.29937
Alpha occ. eigenvalues --	-10.29937	-10.28952	-10.28952	-10.28934	-10.28934
Alpha occ. eigenvalues --	-10.28896	-10.28896	-10.28797	-10.28797	-10.28793
Alpha occ. eigenvalues --	-10.28793	-10.28705	-10.28705	-10.28241	-10.28241
Alpha occ. eigenvalues --	-10.27775	-10.27775	-10.27581	-10.27581	-10.27224
Alpha occ. eigenvalues --	-10.27224	-8.06229	-8.06229	-8.05795	-8.05795

Alpha	occ. eigenvalues	--	-8.05274	-8.05274	-6.00141	-6.00141	-5.99754
Alpha	occ. eigenvalues	--	-5.99754	-5.99703	-5.99703	-5.99317	-5.99317
Alpha	occ. eigenvalues	--	-5.99261	-5.99261	-5.99160	-5.99160	-5.98844
Alpha	occ. eigenvalues	--	-5.98844	-5.98785	-5.98785	-5.98378	-5.98378
Alpha	occ. eigenvalues	--	-1.14311	-1.14254	-1.13881	-1.13880	-1.13040
Alpha	occ. eigenvalues	--	-1.13040	-1.11912	-1.11885	-1.11460	-1.11460
Alpha	occ. eigenvalues	--	-1.10508	-1.10508	-1.08735	-1.08734	-1.08615
Alpha	occ. eigenvalues	--	-1.08615	-1.08542	-1.08542	-1.08446	-1.08446
Alpha	occ. eigenvalues	--	-1.08411	-1.08411	-1.08251	-1.08250	-0.95894
Alpha	occ. eigenvalues	--	-0.95064	-0.94247	-0.93434	-0.92260	-0.91965
Alpha	occ. eigenvalues	--	-0.87305	-0.87262	-0.87068	-0.87050	-0.86681
Alpha	occ. eigenvalues	--	-0.86669	-0.85302	-0.83414	-0.81585	-0.80060
Alpha	occ. eigenvalues	--	-0.79013	-0.78934	-0.78393	-0.78144	-0.77718
Alpha	occ. eigenvalues	--	-0.77635	-0.77239	-0.77188	-0.75481	-0.75454
Alpha	occ. eigenvalues	--	-0.75340	-0.75338	-0.75170	-0.75170	-0.74655
Alpha	occ. eigenvalues	--	-0.74388	-0.73992	-0.73484	-0.73356	-0.72836
Alpha	occ. eigenvalues	--	-0.72715	-0.72530	-0.72378	-0.72367	-0.71421
Alpha	occ. eigenvalues	--	-0.69701	-0.69363	-0.69273	-0.69165	-0.69135
Alpha	occ. eigenvalues	--	-0.68917	-0.68885	-0.66940	-0.65724	-0.65426
Alpha	occ. eigenvalues	--	-0.65304	-0.65301	-0.65254	-0.65128	-0.65097
Alpha	occ. eigenvalues	--	-0.64463	-0.63710	-0.62899	-0.62845	-0.61710
Alpha	occ. eigenvalues	--	-0.61541	-0.61291	-0.61030	-0.60904	-0.60458
Alpha	occ. eigenvalues	--	-0.60140	-0.59437	-0.58755	-0.58732	-0.58246
Alpha	occ. eigenvalues	--	-0.58056	-0.55897	-0.55499	-0.55028	-0.54789
Alpha	occ. eigenvalues	--	-0.54759	-0.54680	-0.54506	-0.54489	-0.54262
Alpha	occ. eigenvalues	--	-0.54250	-0.54035	-0.54032	-0.53698	-0.53354
Alpha	occ. eigenvalues	--	-0.53042	-0.53011	-0.52882	-0.52680	-0.52677
Alpha	occ. eigenvalues	--	-0.52311	-0.52034	-0.51825	-0.51657	-0.51521
Alpha	occ. eigenvalues	--	-0.51465	-0.51064	-0.50911	-0.50203	-0.49957
Alpha	occ. eigenvalues	--	-0.49951	-0.49738	-0.49660	-0.49656	-0.49541
Alpha	occ. eigenvalues	--	-0.49540	-0.49348	-0.49346	-0.49268	-0.49242
Alpha	occ. eigenvalues	--	-0.49148	-0.49046	-0.48655	-0.48634	-0.48592
Alpha	occ. eigenvalues	--	-0.48319	-0.48269	-0.48126	-0.48109	-0.47897
Alpha	occ. eigenvalues	--	-0.47762	-0.47598	-0.47593	-0.47396	-0.47336
Alpha	occ. eigenvalues	--	-0.47203	-0.47144	-0.46963	-0.46808	-0.46191
Alpha	occ. eigenvalues	--	-0.46180	-0.46079	-0.45921	-0.45905	-0.45656
Alpha	occ. eigenvalues	--	-0.45554	-0.45202	-0.45166	-0.44997	-0.44890
Alpha	occ. eigenvalues	--	-0.44844	-0.44607	-0.44295	-0.44148	-0.43976
Alpha	occ. eigenvalues	--	-0.43880	-0.43427	-0.43019	-0.42741	-0.42733
Alpha	occ. eigenvalues	--	-0.42648	-0.42452	-0.42324	-0.42056	-0.42056
Alpha	occ. eigenvalues	--	-0.41776	-0.41232	-0.41108	-0.41087	-0.41008
Alpha	occ. eigenvalues	--	-0.40915	-0.40907	-0.40845	-0.40770	-0.40695
Alpha	occ. eigenvalues	--	-0.40694	-0.40503	-0.40497	-0.40084	-0.39574
Alpha	occ. eigenvalues	--	-0.39512	-0.39388	-0.39137	-0.39096	-0.39058
Alpha	occ. eigenvalues	--	-0.38637	-0.38597	-0.38326	-0.38168	-0.38115
Alpha	occ. eigenvalues	--	-0.38028	-0.37801	-0.37461	-0.37434	-0.37108
Alpha	occ. eigenvalues	--	-0.37071	-0.35742	-0.35715	-0.35578	-0.35572
Alpha	occ. eigenvalues	--	-0.35497	-0.35410	-0.35284	-0.35266	-0.35167

Alpha occ. eigenvalues --	-0.34972	-0.34914	-0.34595	-0.34469	-0.34445
Alpha occ. eigenvalues --	-0.34336	-0.34210	-0.34184	-0.34159	-0.34148
Alpha occ. eigenvalues --	-0.33938	-0.33911	-0.33842	-0.33778	-0.33337
Alpha occ. eigenvalues --	-0.33049	-0.32566	-0.32349	-0.32281	-0.31909
Alpha occ. eigenvalues --	-0.31769	-0.30245	-0.29726	-0.28801	-0.28791
Alpha occ. eigenvalues --	-0.28662	-0.28661	-0.28484	-0.28483	-0.28115
Alpha occ. eigenvalues --	-0.27916	-0.27915	-0.27797	-0.27797	-0.27649
Alpha occ. eigenvalues --	-0.27649	-0.26172	-0.26023	-0.25337	-0.25117
Alpha occ. eigenvalues --	-0.24496	-0.24461	-0.24460	-0.21916	-0.19958
Alpha virt. eigenvalues --	-0.09395	-0.06592	-0.03993	-0.01534	0.00746
Alpha virt. eigenvalues --	0.01583	0.01732	0.02176	0.02637	0.02720
Alpha virt. eigenvalues --	0.03006	0.03209	0.03694	0.03846	0.04060
Alpha virt. eigenvalues --	0.04324	0.04817	0.05038	0.05299	0.05596
Alpha virt. eigenvalues --	0.06017	0.06024	0.06371	0.06705	0.06857
Alpha virt. eigenvalues --	0.07151	0.07181	0.07281	0.07326	0.07358
Alpha virt. eigenvalues --	0.07402	0.07719	0.07888	0.07932	0.08216
Alpha virt. eigenvalues --	0.08374	0.08589	0.08594	0.08850	0.08962
Alpha virt. eigenvalues --	0.09151	0.09189	0.09396	0.09562	0.09588
Alpha virt. eigenvalues --	0.09648	0.09742	0.09823	0.10160	0.10293
Alpha virt. eigenvalues --	0.10344	0.10784	0.10954	0.11021	0.11089
Alpha virt. eigenvalues --	0.11181	0.11238	0.11356	0.11808	0.11928
Alpha virt. eigenvalues --	0.12095	0.12177	0.12215	0.12381	0.12410
Alpha virt. eigenvalues --	0.12477	0.12608	0.12663	0.12764	0.12942
Alpha virt. eigenvalues --	0.13051	0.13160	0.13166	0.13321	0.13322
Alpha virt. eigenvalues --	0.13419	0.13438	0.13469	0.13522	0.13574
Alpha virt. eigenvalues --	0.13595	0.13633	0.13775	0.13797	0.13855
Alpha virt. eigenvalues --	0.13973	0.14122	0.14165	0.14209	0.14211
Alpha virt. eigenvalues --	0.14309	0.14311	0.14389	0.14390	0.14513
Alpha virt. eigenvalues --	0.14578	0.14631	0.14810	0.14911	0.14958
Alpha virt. eigenvalues --	0.15140	0.15608	0.15993	0.16032	0.16154
Alpha virt. eigenvalues --	0.16211	0.16276	0.16436	0.16504	0.16555
Alpha virt. eigenvalues --	0.16681	0.16685	0.16827	0.17023	0.17135
Alpha virt. eigenvalues --	0.17225	0.17336	0.17451	0.17520	0.17671
Alpha virt. eigenvalues --	0.17950	0.17967	0.18201	0.18434	0.18786
Alpha virt. eigenvalues --	0.19662	0.19797	0.19828	0.19883	0.20061
Alpha virt. eigenvalues --	0.20279	0.20625	0.20634	0.20852	0.20880
Alpha virt. eigenvalues --	0.20994	0.21128	0.21276	0.21778	0.21918
Alpha virt. eigenvalues --	0.21936	0.22016	0.22226	0.22266	0.22380
Alpha virt. eigenvalues --	0.22771	0.22803	0.22867	0.22924	0.23127
Alpha virt. eigenvalues --	0.23144	0.23290	0.23432	0.23480	0.23752
Alpha virt. eigenvalues --	0.24201	0.24563	0.24756	0.24788	0.24999
Alpha virt. eigenvalues --	0.25079	0.25513	0.25779	0.26312	0.26370
Alpha virt. eigenvalues --	0.26394	0.26523	0.26695	0.26793	0.27077
Alpha virt. eigenvalues --	0.27235	0.27482	0.27625	0.27707	0.27906
Alpha virt. eigenvalues --	0.28362	0.28419	0.28733	0.28801	0.29003
Alpha virt. eigenvalues --	0.29132	0.29318	0.29356	0.29984	0.30410
Alpha virt. eigenvalues --	0.30412	0.30872	0.30898	0.32065	0.32898
Alpha virt. eigenvalues --	0.33910	0.35188	0.36181	0.37274	0.37286

Alpha virt. eigenvalues --	0.38841	0.38956	0.39190	0.39720	0.39875
Alpha virt. eigenvalues --	0.40792	0.40943	0.40965	0.41166	0.41350
Alpha virt. eigenvalues --	0.41467	0.41769	0.41970	0.41978	0.42234
Alpha virt. eigenvalues --	0.42385	0.42572	0.42835	0.42897	0.43356
Alpha virt. eigenvalues --	0.43386	0.43549	0.43604	0.43795	0.43894
Alpha virt. eigenvalues --	0.44234	0.44258	0.44349	0.44423	0.44512
Alpha virt. eigenvalues --	0.44814	0.44832	0.44995	0.45080	0.45307
Alpha virt. eigenvalues --	0.45371	0.45395	0.45511	0.45600	0.45633
Alpha virt. eigenvalues --	0.45673	0.45695	0.45776	0.45807	0.45851
Alpha virt. eigenvalues --	0.45890	0.45933	0.46014	0.46110	0.46156
Alpha virt. eigenvalues --	0.46313	0.46352	0.46458	0.46539	0.46672
Alpha virt. eigenvalues --	0.46721	0.46758	0.46850	0.46992	0.47082
Alpha virt. eigenvalues --	0.47231	0.47238	0.47267	0.47425	0.47637
Alpha virt. eigenvalues --	0.47699	0.47792	0.47846	0.47960	0.48127
Alpha virt. eigenvalues --	0.48150	0.48292	0.48359	0.48438	0.48521
Alpha virt. eigenvalues --	0.48746	0.48839	0.48873	0.48894	0.49014
Alpha virt. eigenvalues --	0.49059	0.49096	0.49278	0.49412	0.50057
Alpha virt. eigenvalues --	0.50191	0.50208	0.50322	0.50499	0.50580
Alpha virt. eigenvalues --	0.50713	0.51148	0.51206	0.51230	0.51344
Alpha virt. eigenvalues --	0.51375	0.51554	0.51973	0.52050	0.52205
Alpha virt. eigenvalues --	0.52207	0.52472	0.52510	0.52586	0.52802
Alpha virt. eigenvalues --	0.53027	0.53208	0.53241	0.53526	0.53601
Alpha virt. eigenvalues --	0.53767	0.53960	0.54254	0.54621	0.54761
Alpha virt. eigenvalues --	0.54807	0.54814	0.54897	0.55056	0.55109
Alpha virt. eigenvalues --	0.55111	0.55155	0.55459	0.55805	0.56134
Alpha virt. eigenvalues --	0.56237	0.56687	0.56727	0.56861	0.57190
Alpha virt. eigenvalues --	0.57347	0.57444	0.58513	0.58682	0.59106
Alpha virt. eigenvalues --	0.59166	0.59319	0.59490	0.59522	0.59687
Alpha virt. eigenvalues --	0.59944	0.60023	0.60129	0.60168	0.60441
Alpha virt. eigenvalues --	0.60508	0.60684	0.60902	0.60915	0.61087
Alpha virt. eigenvalues --	0.61137	0.61228	0.61268	0.61312	0.61432
Alpha virt. eigenvalues --	0.61448	0.61755	0.61761	0.61902	0.62003
Alpha virt. eigenvalues --	0.62053	0.62196	0.62248	0.62302	0.62387
Alpha virt. eigenvalues --	0.62633	0.62668	0.62685	0.62704	0.62943
Alpha virt. eigenvalues --	0.62976	0.63035	0.63332	0.63343	0.63362
Alpha virt. eigenvalues --	0.63448	0.63513	0.63667	0.63669	0.63756
Alpha virt. eigenvalues --	0.63770	0.63817	0.63927	0.64074	0.64123
Alpha virt. eigenvalues --	0.64194	0.64256	0.64279	0.64330	0.64519
Alpha virt. eigenvalues --	0.64824	0.64851	0.64957	0.65091	0.65304
Alpha virt. eigenvalues --	0.65489	0.65507	0.65669	0.65728	0.65755
Alpha virt. eigenvalues --	0.65773	0.65814	0.65951	0.66057	0.66072
Alpha virt. eigenvalues --	0.66118	0.66180	0.66291	0.66421	0.66515
Alpha virt. eigenvalues --	0.66531	0.66734	0.66996	0.67072	0.67076
Alpha virt. eigenvalues --	0.67241	0.67270	0.67344	0.67405	0.67482
Alpha virt. eigenvalues --	0.67648	0.67811	0.67838	0.67854	0.67904
Alpha virt. eigenvalues --	0.68068	0.68147	0.68159	0.68241	0.68308
Alpha virt. eigenvalues --	0.68431	0.68490	0.68542	0.68656	0.68957
Alpha virt. eigenvalues --	0.68968	0.69298	0.69399	0.69495	0.69533

Alpha virt. eigenvalues --	0.69908	0.70103	0.70263	0.70339	0.70355
Alpha virt. eigenvalues --	0.70612	0.70634	0.71046	0.71092	0.71124
Alpha virt. eigenvalues --	0.71533	0.71680	0.71691	0.71751	0.72053
Alpha virt. eigenvalues --	0.72076	0.72680	0.72682	0.72795	0.72889
Alpha virt. eigenvalues --	0.73164	0.73268	0.73466	0.73557	0.73811
Alpha virt. eigenvalues --	0.73819	0.73889	0.73979	0.74115	0.74245
Alpha virt. eigenvalues --	0.74489	0.74552	0.74683	0.74807	0.74925
Alpha virt. eigenvalues --	0.75134	0.75350	0.75400	0.75483	0.75594
Alpha virt. eigenvalues --	0.75652	0.75668	0.75722	0.75812	0.75896
Alpha virt. eigenvalues --	0.76114	0.76237	0.76483	0.76580	0.76709
Alpha virt. eigenvalues --	0.77141	0.77523	0.77934	0.78089	0.78406
Alpha virt. eigenvalues --	0.78664	0.78735	0.80289	0.80503	0.80519
Alpha virt. eigenvalues --	0.81083	0.81102	0.81206	0.81560	0.81726
Alpha virt. eigenvalues --	0.82448	0.82538	0.82700	0.83789	0.83976
Alpha virt. eigenvalues --	0.84456	0.84765	0.85607	0.85816	0.85998
Alpha virt. eigenvalues --	0.86317	0.86644	0.86715	0.86897	0.86917
Alpha virt. eigenvalues --	0.87001	0.87067	0.87116	0.87256	0.87315
Alpha virt. eigenvalues --	0.87489	0.87794	0.87808	0.88429	0.88602
Alpha virt. eigenvalues --	0.88618	0.89307	0.89337	0.90607	0.90636
Alpha virt. eigenvalues --	0.90795	0.90855	0.90956	0.90979	0.91041
Alpha virt. eigenvalues --	0.91245	0.91371	0.91443	0.91501	0.91542
Alpha virt. eigenvalues --	0.91631	0.91663	0.92828	0.92896	0.93510
Alpha virt. eigenvalues --	0.93701	0.93894	0.94119	0.95194	0.95379
Alpha virt. eigenvalues --	0.95883	0.96094	0.96341	0.96514	0.96757
Alpha virt. eigenvalues --	0.96808	0.97607	0.97671	0.97768	0.98076
Alpha virt. eigenvalues --	0.98313	0.98377	0.98776	0.98895	0.98978
Alpha virt. eigenvalues --	0.99217	0.99594	0.99702	0.99915	0.99972
Alpha virt. eigenvalues --	1.00365	1.00781	1.01158	1.01246	1.01346
Alpha virt. eigenvalues --	1.01703	1.01840	1.01928	1.02055	1.02088
Alpha virt. eigenvalues --	1.02351	1.02506	1.02996	1.03264	1.03300
Alpha virt. eigenvalues --	1.03881	1.04374	1.04929	1.05307	1.05494
Alpha virt. eigenvalues --	1.06118	1.06279	1.07097	1.07144	1.07332
Alpha virt. eigenvalues --	1.07532	1.08210	1.08728	1.09179	1.09359
Alpha virt. eigenvalues --	1.09947	1.10006	1.10647	1.10743	1.11237
Alpha virt. eigenvalues --	1.11456	1.12067	1.12223	1.12245	1.12579
Alpha virt. eigenvalues --	1.12890	1.12972	1.13334	1.13421	1.14650
Alpha virt. eigenvalues --	1.15058	1.15532	1.15635	1.15748	1.15797
Alpha virt. eigenvalues --	1.15884	1.15986	1.16227	1.16756	1.17785
Alpha virt. eigenvalues --	1.17849	1.18172	1.18247	1.18414	1.18625
Alpha virt. eigenvalues --	1.18645	1.18743	1.18853	1.19097	1.19128
Alpha virt. eigenvalues --	1.19394	1.19451	1.19619	1.19672	1.19947
Alpha virt. eigenvalues --	1.19953	1.21414	1.21487	1.21704	1.21776
Alpha virt. eigenvalues --	1.21839	1.21969	1.22253	1.22531	1.22672
Alpha virt. eigenvalues --	1.23327	1.23435	1.23867	1.24027	1.24319
Alpha virt. eigenvalues --	1.24451	1.24605	1.24631	1.24737	1.24941
Alpha virt. eigenvalues --	1.25264	1.25465	1.25733	1.25925	1.25946
Alpha virt. eigenvalues --	1.26327	1.26331	1.26481	1.26555	1.26853
Alpha virt. eigenvalues --	1.26915	1.27295	1.28071	1.28177	1.28562

Alpha virt. eigenvalues --	1.28690	1.28760	1.28994	1.29016	1.29527
Alpha virt. eigenvalues --	1.29759	1.30256	1.30761	1.30846	1.31210
Alpha virt. eigenvalues --	1.31477	1.31505	1.31670	1.31817	1.31885
Alpha virt. eigenvalues --	1.32293	1.32364	1.32798	1.33380	1.33549
Alpha virt. eigenvalues --	1.33983	1.34183	1.34287	1.34309	1.34698
Alpha virt. eigenvalues --	1.34736	1.35398	1.36143	1.36217	1.36384
Alpha virt. eigenvalues --	1.36468	1.36671	1.36709	1.36932	1.37255
Alpha virt. eigenvalues --	1.37570	1.37738	1.37835	1.37884	1.37976
Alpha virt. eigenvalues --	1.38204	1.38655	1.38881	1.39090	1.39484
Alpha virt. eigenvalues --	1.40204	1.40234	1.40337	1.40492	1.40498
Alpha virt. eigenvalues --	1.40518	1.40569	1.40660	1.40709	1.40779
Alpha virt. eigenvalues --	1.40855	1.40877	1.40894	1.40907	1.40919
Alpha virt. eigenvalues --	1.40952	1.41107	1.41282	1.41410	1.41631
Alpha virt. eigenvalues --	1.41659	1.41786	1.42039	1.42392	1.42398
Alpha virt. eigenvalues --	1.42534	1.42758	1.42918	1.43083	1.43344
Alpha virt. eigenvalues --	1.43406	1.43588	1.43614	1.43931	1.44037
Alpha virt. eigenvalues --	1.44127	1.44127	1.44323	1.44356	1.44491
Alpha virt. eigenvalues --	1.44688	1.44979	1.45064	1.45142	1.46281
Alpha virt. eigenvalues --	1.46457	1.46568	1.46618	1.46845	1.46920
Alpha virt. eigenvalues --	1.47029	1.47066	1.47184	1.47390	1.47418
Alpha virt. eigenvalues --	1.47451	1.48078	1.48461	1.48781	1.48827
Alpha virt. eigenvalues --	1.48967	1.49322	1.49461	1.49998	1.50168
Alpha virt. eigenvalues --	1.50379	1.51075	1.51286	1.51402	1.51492
Alpha virt. eigenvalues --	1.51899	1.51995	1.52270	1.52347	1.52714
Alpha virt. eigenvalues --	1.52736	1.52816	1.52871	1.52941	1.53160
Alpha virt. eigenvalues --	1.53285	1.53485	1.53879	1.54097	1.54702
Alpha virt. eigenvalues --	1.54766	1.55037	1.55157	1.55552	1.55755
Alpha virt. eigenvalues --	1.55932	1.55953	1.56066	1.56148	1.56174
Alpha virt. eigenvalues --	1.56637	1.56795	1.57111	1.57323	1.57451
Alpha virt. eigenvalues --	1.57550	1.57696	1.57754	1.57810	1.57909
Alpha virt. eigenvalues --	1.57947	1.58061	1.58256	1.58713	1.58721
Alpha virt. eigenvalues --	1.58837	1.58929	1.59079	1.59085	1.59793
Alpha virt. eigenvalues --	1.59834	1.60373	1.60450	1.60733	1.61082
Alpha virt. eigenvalues --	1.61152	1.61294	1.61471	1.61823	1.61929
Alpha virt. eigenvalues --	1.62002	1.62018	1.62146	1.62233	1.62311
Alpha virt. eigenvalues --	1.62337	1.62420	1.62442	1.62551	1.62609
Alpha virt. eigenvalues --	1.62661	1.62698	1.62713	1.62876	1.62896
Alpha virt. eigenvalues --	1.63186	1.63187	1.63231	1.63310	1.63470
Alpha virt. eigenvalues --	1.63566	1.63662	1.63699	1.63968	1.64205
Alpha virt. eigenvalues --	1.64228	1.64415	1.64535	1.64689	1.64701
Alpha virt. eigenvalues --	1.64871	1.64915	1.64982	1.65458	1.65634
Alpha virt. eigenvalues --	1.66056	1.66168	1.66269	1.66448	1.66693
Alpha virt. eigenvalues --	1.66719	1.67062	1.67460	1.67605	1.67778
Alpha virt. eigenvalues --	1.67872	1.67995	1.68123	1.68329	1.68499
Alpha virt. eigenvalues --	1.68525	1.68581	1.68735	1.68919	1.69027
Alpha virt. eigenvalues --	1.69477	1.69702	1.69819	1.70334	1.70398
Alpha virt. eigenvalues --	1.70544	1.70694	1.71052	1.71157	1.71179
Alpha virt. eigenvalues --	1.71331	1.71362	1.71397	1.71421	1.71444

Alpha virt. eigenvalues --	1.71486	1.71522	1.71524	1.72216	1.72336
Alpha virt. eigenvalues --	1.72879	1.72996	1.73235	1.73373	1.73396
Alpha virt. eigenvalues --	1.73552	1.73592	1.73774	1.73792	1.74040
Alpha virt. eigenvalues --	1.74220	1.74654	1.74793	1.74834	1.74944
Alpha virt. eigenvalues --	1.75337	1.75391	1.75609	1.75951	1.76159
Alpha virt. eigenvalues --	1.76309	1.76354	1.76664	1.76716	1.76768
Alpha virt. eigenvalues --	1.76849	1.76902	1.76973	1.77720	1.77826
Alpha virt. eigenvalues --	1.78126	1.78368	1.78390	1.78571	1.78583
Alpha virt. eigenvalues --	1.78605	1.78706	1.78895	1.78975	1.79199
Alpha virt. eigenvalues --	1.79892	1.80067	1.80158	1.80226	1.80288
Alpha virt. eigenvalues --	1.80645	1.81078	1.81227	1.81721	1.81772
Alpha virt. eigenvalues --	1.82223	1.82258	1.82412	1.82499	1.82643
Alpha virt. eigenvalues --	1.82788	1.82798	1.83021	1.83217	1.83544
Alpha virt. eigenvalues --	1.83738	1.83791	1.83810	1.83838	1.84223
Alpha virt. eigenvalues --	1.84594	1.84907	1.84956	1.84967	1.85201
Alpha virt. eigenvalues --	1.85325	1.85438	1.85472	1.85559	1.85682
Alpha virt. eigenvalues --	1.86006	1.86074	1.86227	1.86251	1.86454
Alpha virt. eigenvalues --	1.86502	1.86658	1.86686	1.87057	1.87302
Alpha virt. eigenvalues --	1.87373	1.87589	1.87751	1.87790	1.88159
Alpha virt. eigenvalues --	1.88159	1.88403	1.88943	1.89163	1.89514
Alpha virt. eigenvalues --	1.89659	1.89685	1.90200	1.91038	1.91991
Alpha virt. eigenvalues --	1.92363	1.92611	1.92732	1.92932	1.92977
Alpha virt. eigenvalues --	1.93563	1.93922	1.94465	1.94713	1.94870
Alpha virt. eigenvalues --	1.94900	1.95546	1.95606	1.96559	1.96697
Alpha virt. eigenvalues --	1.97127	1.97333	1.97486	1.97750	1.97776
Alpha virt. eigenvalues --	1.98179	1.98531	1.98567	1.98879	1.98935
Alpha virt. eigenvalues --	1.99322	1.99330	1.99373	1.99434	1.99621
Alpha virt. eigenvalues --	1.99628	1.99759	1.99791	1.99859	1.99952
Alpha virt. eigenvalues --	2.00009	2.00035	2.00390	2.00503	2.00739
Alpha virt. eigenvalues --	2.00845	2.01715	2.02272	2.02555	2.02698
Alpha virt. eigenvalues --	2.03099	2.03174	2.03282	2.03332	2.03900
Alpha virt. eigenvalues --	2.03977	2.04304	2.04657	2.04771	2.05093
Alpha virt. eigenvalues --	2.06093	2.06144	2.06389	2.06402	2.06521
Alpha virt. eigenvalues --	2.06535	2.07133	2.07168	2.07512	2.07782
Alpha virt. eigenvalues --	2.08163	2.08192	2.08731	2.08837	2.08903
Alpha virt. eigenvalues --	2.08924	2.09015	2.09275	2.09608	2.09627
Alpha virt. eigenvalues --	2.10832	2.11701	2.12207	2.12243	2.12337
Alpha virt. eigenvalues --	2.12376	2.12518	2.12534	2.12806	2.13157
Alpha virt. eigenvalues --	2.13241	2.13794	2.13855	2.13955	2.14124
Alpha virt. eigenvalues --	2.14243	2.14333	2.14482	2.15850	2.16277
Alpha virt. eigenvalues --	2.16581	2.16865	2.17058	2.17317	2.17928
Alpha virt. eigenvalues --	2.17961	2.18208	2.18394	2.18395	2.18532
Alpha virt. eigenvalues --	2.19219	2.19461	2.19790	2.19849	2.20276
Alpha virt. eigenvalues --	2.20369	2.21564	2.21571	2.21989	2.21996
Alpha virt. eigenvalues --	2.22223	2.22364	2.22929	2.23001	2.23216
Alpha virt. eigenvalues --	2.23431	2.23622	2.23682	2.25950	2.26169
Alpha virt. eigenvalues --	2.26513	2.26587	2.26733	2.26914	2.27451
Alpha virt. eigenvalues --	2.28155	2.29506	2.29747	2.29844	2.29938

Alpha virt. eigenvalues --	2.29964	2.29980	2.30457	2.31001	2.31657
Alpha virt. eigenvalues --	2.31717	2.31987	2.32358	2.32530	2.33139
Alpha virt. eigenvalues --	2.33326	2.33749	2.33979	2.34030	2.34223
Alpha virt. eigenvalues --	2.34706	2.35897	2.36557	2.36943	2.36972
Alpha virt. eigenvalues --	2.37244	2.37918	2.38250	2.38384	2.38586
Alpha virt. eigenvalues --	2.39081	2.39782	2.40007	2.40215	2.40460
Alpha virt. eigenvalues --	2.40621	2.41080	2.41394	2.41450	2.41796
Alpha virt. eigenvalues --	2.41897	2.41941	2.42021	2.42081	2.42193
Alpha virt. eigenvalues --	2.42346	2.42374	2.42451	2.42538	2.42974
Alpha virt. eigenvalues --	2.43215	2.43329	2.43359	2.43436	2.43477
Alpha virt. eigenvalues --	2.43494	2.43676	2.44066	2.44122	2.44268
Alpha virt. eigenvalues --	2.44384	2.44897	2.44961	2.45089	2.45101
Alpha virt. eigenvalues --	2.45196	2.45287	2.45362	2.45408	2.46050
Alpha virt. eigenvalues --	2.46077	2.46512	2.46620	2.46866	2.47278
Alpha virt. eigenvalues --	2.47348	2.47385	2.47711	2.47864	2.47947
Alpha virt. eigenvalues --	2.48281	2.48508	2.48529	2.48557	2.48879
Alpha virt. eigenvalues --	2.48945	2.49105	2.49189	2.49234	2.49300
Alpha virt. eigenvalues --	2.49303	2.49392	2.49659	2.49769	2.50428
Alpha virt. eigenvalues --	2.50933	2.51216	2.51420	2.51489	2.51791
Alpha virt. eigenvalues --	2.52342	2.52791	2.53136	2.53271	2.53337
Alpha virt. eigenvalues --	2.53451	2.53541	2.53724	2.54967	2.55206
Alpha virt. eigenvalues --	2.55373	2.55500	2.55681	2.55739	2.55857
Alpha virt. eigenvalues --	2.55917	2.56137	2.57352	2.57413	2.57701
Alpha virt. eigenvalues --	2.57703	2.57748	2.58018	2.58508	2.59816
Alpha virt. eigenvalues --	2.60204	2.60247	2.61169	2.62322	2.63374
Alpha virt. eigenvalues --	2.64598	2.68035	2.68612	2.68758	2.69125
Alpha virt. eigenvalues --	2.69463	2.69586	2.76962	2.77569	2.78306
Alpha virt. eigenvalues --	2.78747	2.80273	2.80305	2.89651	2.89727
Alpha virt. eigenvalues --	2.90087	2.90261	2.91150	2.91212	2.93029
Alpha virt. eigenvalues --	2.93224	2.93497	2.93514	2.94073	2.94086
Alpha virt. eigenvalues --	2.96185	2.96371	2.96689	2.96916	2.97466
Alpha virt. eigenvalues --	2.97500	2.98287	2.98363	2.98475	2.98480
Alpha virt. eigenvalues --	2.98642	2.98647	2.98995	2.99062	2.99190
Alpha virt. eigenvalues --	2.99252	2.99430	2.99449	3.01982	3.02042
Alpha virt. eigenvalues --	3.02151	3.02186	3.02324	3.02330	3.02406
Alpha virt. eigenvalues --	3.02858	3.02970	3.03088	3.03228	3.03249
Alpha virt. eigenvalues --	3.07516	3.07564	3.07658	3.07673	3.07800
Alpha virt. eigenvalues --	3.07801	3.08204	3.08211	3.08320	3.08324
Alpha virt. eigenvalues --	3.08461	3.08461	3.09167	3.09694	3.09966
Alpha virt. eigenvalues --	3.09997	3.10304	3.10311	3.10765	3.10931
Alpha virt. eigenvalues --	3.11077	3.11331	3.11661	3.12287	3.12380
Alpha virt. eigenvalues --	3.12476	3.12639	3.12641	3.12879	3.12999
Alpha virt. eigenvalues --	3.23769	3.23822	3.23909	3.23946	3.24021
Alpha virt. eigenvalues --	3.24037	3.25885	3.25921	3.26007	3.26028
Alpha virt. eigenvalues --	3.26108	3.26113	3.29990	3.30060	3.30360
Alpha virt. eigenvalues --	3.30391	3.30840	3.30841	3.36446	3.36478
Alpha virt. eigenvalues --	3.36585	3.36672	3.36737	3.36771	3.36827
Alpha virt. eigenvalues --	3.36842	3.36944	3.36972	3.37015	3.37024

Alpha virt. eigenvalues -- 3.39157 3.39181 3.39346 3.39581 3.39737
 Alpha virt. eigenvalues -- 3.39864 3.40826 3.41670 3.42117 3.42453
 Alpha virt. eigenvalues -- 3.42963 3.43160 3.49078 3.49516 3.50135
 Alpha virt. eigenvalues -- 3.50781 3.51457 3.51865
 Beta occ. eigenvalues -- -89.11947 -89.11947 -89.11519 -89.11519 -89.10948
 Beta occ. eigenvalues -- -89.10948 -19.28975 -19.28975 -19.28717 -19.28717
 Beta occ. eigenvalues -- -19.28703 -19.28703 -19.28150 -19.28150 -19.28030
 Beta occ. eigenvalues -- -19.28030 -19.26926 -19.26926 -19.24529 -19.24529
 Beta occ. eigenvalues -- -19.24511 -19.24511 -19.24435 -19.24435 -19.24362
 Beta occ. eigenvalues -- -19.24362 -19.24277 -19.24277 -19.24209 -19.24209
 Beta occ. eigenvalues -- -10.33904 -10.33903 -10.33622 -10.33622 -10.33447
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 Beta occ. eigenvalues -- -10.31930 -10.31930 -10.31896 -10.31896 -10.31859
 Beta occ. eigenvalues -- -10.31820 -10.31290 -10.31290 -10.31203 -10.31203
 Beta occ. eigenvalues -- -10.31148 -10.31148 -10.31102 -10.31102 -10.31026
 Beta occ. eigenvalues -- -10.31026 -10.30921 -10.30921 -10.30723 -10.30723
 Beta occ. eigenvalues -- -10.30375 -10.30375 -10.30281 -10.30281 -10.30276
 Beta occ. eigenvalues -- -10.30276 -10.30185 -10.30185 -10.30159 -10.30159
 Beta occ. eigenvalues -- -10.30127 -10.30126 -10.29963 -10.29963 -10.29937
 Beta occ. eigenvalues -- -10.29937 -10.28951 -10.28951 -10.28934 -10.28933
 Beta occ. eigenvalues -- -10.28896 -10.28896 -10.28797 -10.28797 -10.28793
 Beta occ. eigenvalues -- -10.28793 -10.28705 -10.28705 -10.28112 -10.28112
 Beta occ. eigenvalues -- -10.27773 -10.27773 -10.27579 -10.27579 -10.27223
 Beta occ. eigenvalues -- -10.27223 -8.06247 -8.06247 -8.05805 -8.05805
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 Beta occ. eigenvalues -- -5.99772 -5.99715 -5.99715 -5.99329 -5.99329
 Beta occ. eigenvalues -- -5.99302 -5.99302 -5.99162 -5.99162 -5.98867
 Beta occ. eigenvalues -- -5.98867 -5.98788 -5.98788 -5.98377 -5.98377
 Beta occ. eigenvalues -- -1.14237 -1.14183 -1.13812 -1.13811 -1.12980
 Beta occ. eigenvalues -- -1.12980 -1.11843 -1.11816 -1.11418 -1.11418
 Beta occ. eigenvalues -- -1.10493 -1.10493 -1.08733 -1.08732 -1.08614
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 Beta occ. eigenvalues -- -1.08411 -1.08411 -1.08250 -1.08250 -0.95617
 Beta occ. eigenvalues -- -0.94837 -0.94050 -0.93226 -0.92129 -0.91801
 Beta occ. eigenvalues -- -0.87287 -0.87249 -0.87055 -0.87039 -0.86671
 Beta occ. eigenvalues -- -0.86662 -0.84972 -0.83157 -0.81365 -0.79872
 Beta occ. eigenvalues -- -0.78983 -0.78883 -0.78356 -0.78011 -0.77607
 Beta occ. eigenvalues -- -0.77557 -0.77211 -0.77156 -0.75477 -0.75452
 Beta occ. eigenvalues -- -0.75339 -0.75336 -0.75169 -0.75169 -0.74609
 Beta occ. eigenvalues -- -0.74339 -0.73947 -0.73436 -0.73344 -0.72821
 Beta occ. eigenvalues -- -0.72699 -0.72482 -0.72358 -0.72349 -0.71350
 Beta occ. eigenvalues -- -0.69445 -0.69347 -0.69264 -0.69160 -0.69116
 Beta occ. eigenvalues -- -0.68912 -0.68861 -0.66786 -0.65631 -0.65420
 Beta occ. eigenvalues -- -0.65296 -0.65296 -0.65224 -0.65125 -0.65073
 Beta occ. eigenvalues -- -0.64341 -0.63599 -0.62818 -0.62769 -0.61679
 Beta occ. eigenvalues -- -0.61512 -0.61258 -0.61010 -0.60874 -0.60426
 Beta occ. eigenvalues -- -0.60088 -0.59385 -0.58705 -0.58607 -0.58191
 Beta occ. eigenvalues -- -0.57978 -0.55854 -0.55454 -0.54980 -0.54717

Beta occ. eigenvalues --	-0.54703	-0.54621	-0.54446	-0.54424	-0.54242
Beta occ. eigenvalues --	-0.54231	-0.54000	-0.53996	-0.53658	-0.53313
Beta occ. eigenvalues --	-0.52988	-0.52978	-0.52867	-0.52671	-0.52669
Beta occ. eigenvalues --	-0.52293	-0.52004	-0.51762	-0.51605	-0.51466
Beta occ. eigenvalues --	-0.51389	-0.51018	-0.50858	-0.50155	-0.49929
Beta occ. eigenvalues --	-0.49867	-0.49699	-0.49650	-0.49644	-0.49537
Beta occ. eigenvalues --	-0.49533	-0.49343	-0.49343	-0.49208	-0.49192
Beta occ. eigenvalues --	-0.49049	-0.48938	-0.48572	-0.48546	-0.48523
Beta occ. eigenvalues --	-0.48269	-0.48226	-0.48078	-0.48076	-0.47878
Beta occ. eigenvalues --	-0.47745	-0.47578	-0.47567	-0.47368	-0.47317
Beta occ. eigenvalues --	-0.47183	-0.47119	-0.46946	-0.46788	-0.46115
Beta occ. eigenvalues --	-0.46093	-0.45961	-0.45859	-0.45832	-0.45525
Beta occ. eigenvalues --	-0.45480	-0.45151	-0.45057	-0.44889	-0.44761
Beta occ. eigenvalues --	-0.44755	-0.44457	-0.44122	-0.44103	-0.43936
Beta occ. eigenvalues --	-0.43697	-0.43240	-0.42867	-0.42625	-0.42620
Beta occ. eigenvalues --	-0.42551	-0.42374	-0.42268	-0.42003	-0.42002
Beta occ. eigenvalues --	-0.41726	-0.41217	-0.41013	-0.41003	-0.41000
Beta occ. eigenvalues --	-0.40912	-0.40904	-0.40785	-0.40698	-0.40691
Beta occ. eigenvalues --	-0.40674	-0.40469	-0.40459	-0.40054	-0.39438
Beta occ. eigenvalues --	-0.39359	-0.39327	-0.39093	-0.39017	-0.38926
Beta occ. eigenvalues --	-0.38550	-0.38531	-0.38270	-0.38113	-0.37925
Beta occ. eigenvalues --	-0.37918	-0.37739	-0.37417	-0.37408	-0.37083
Beta occ. eigenvalues --	-0.37050	-0.35714	-0.35688	-0.35556	-0.35544
Beta occ. eigenvalues --	-0.35472	-0.35379	-0.35254	-0.35254	-0.35146
Beta occ. eigenvalues --	-0.34940	-0.34643	-0.34578	-0.34391	-0.34374
Beta occ. eigenvalues --	-0.34241	-0.34189	-0.34118	-0.34108	-0.34046
Beta occ. eigenvalues --	-0.33910	-0.33893	-0.33780	-0.33616	-0.33272
Beta occ. eigenvalues --	-0.32818	-0.32458	-0.32252	-0.32034	-0.31781
Beta occ. eigenvalues --	-0.31677	-0.29937	-0.29245	-0.28796	-0.28787
Beta occ. eigenvalues --	-0.28657	-0.28655	-0.28478	-0.28477	-0.27915
Beta occ. eigenvalues --	-0.27915	-0.27797	-0.27797	-0.27649	-0.27648
Beta occ. eigenvalues --	-0.27412	-0.25871	-0.25858	-0.25022	-0.24750
Beta occ. eigenvalues --	-0.24292	-0.24291	-0.23494	-0.20579	
Beta virt. eigenvalues --	-0.15677	-0.08560	-0.05925	-0.03332	-0.00893
Beta virt. eigenvalues --	0.01338	0.01602	0.01880	0.02299	0.02709
Beta virt. eigenvalues --	0.03018	0.03267	0.03377	0.03760	0.03929
Beta virt. eigenvalues --	0.04128	0.04361	0.04898	0.05067	0.05641
Beta virt. eigenvalues --	0.05656	0.06114	0.06199	0.06621	0.06731
Beta virt. eigenvalues --	0.06962	0.07155	0.07198	0.07351	0.07379
Beta virt. eigenvalues --	0.07425	0.07440	0.07745	0.07928	0.08193
Beta virt. eigenvalues --	0.08332	0.08489	0.08640	0.08938	0.09041
Beta virt. eigenvalues --	0.09093	0.09378	0.09466	0.09472	0.09589
Beta virt. eigenvalues --	0.09635	0.09693	0.09787	0.09833	0.10232
Beta virt. eigenvalues --	0.10323	0.10377	0.10817	0.10983	0.11036
Beta virt. eigenvalues --	0.11108	0.11226	0.11252	0.11378	0.11826
Beta virt. eigenvalues --	0.11970	0.12116	0.12187	0.12233	0.12389
Beta virt. eigenvalues --	0.12423	0.12500	0.12622	0.12680	0.12788
Beta virt. eigenvalues --	0.12955	0.13071	0.13171	0.13181	0.13329

Beta virt. eigenvalues --	0.13333	0.13428	0.13443	0.13478	0.13527
Beta virt. eigenvalues --	0.13577	0.13603	0.13641	0.13785	0.13803
Beta virt. eigenvalues --	0.13875	0.13984	0.14132	0.14184	0.14218
Beta virt. eigenvalues --	0.14219	0.14317	0.14318	0.14394	0.14395
Beta virt. eigenvalues --	0.14516	0.14583	0.14635	0.14818	0.14925
Beta virt. eigenvalues --	0.14965	0.15153	0.15625	0.16005	0.16062
Beta virt. eigenvalues --	0.16162	0.16222	0.16294	0.16460	0.16512
Beta virt. eigenvalues --	0.16563	0.16696	0.16708	0.16850	0.17032
Beta virt. eigenvalues --	0.17157	0.17236	0.17369	0.17469	0.17534
Beta virt. eigenvalues --	0.17702	0.17996	0.18021	0.18257	0.18477
Beta virt. eigenvalues --	0.18849	0.19682	0.19803	0.19835	0.19888
Beta virt. eigenvalues --	0.20072	0.20302	0.20634	0.20649	0.20864
Beta virt. eigenvalues --	0.20886	0.21044	0.21136	0.21286	0.21803
Beta virt. eigenvalues --	0.21936	0.21950	0.22030	0.22236	0.22377
Beta virt. eigenvalues --	0.22393	0.22786	0.22838	0.22939	0.22945
Beta virt. eigenvalues --	0.23141	0.23182	0.23317	0.23446	0.23506
Beta virt. eigenvalues --	0.23839	0.24269	0.24574	0.24805	0.24820
Beta virt. eigenvalues --	0.25032	0.25104	0.25549	0.25820	0.26328
Beta virt. eigenvalues --	0.26434	0.26438	0.26602	0.26737	0.26830
Beta virt. eigenvalues --	0.27115	0.27270	0.27489	0.27632	0.27720
Beta virt. eigenvalues --	0.27923	0.28384	0.28454	0.28754	0.28822
Beta virt. eigenvalues --	0.29019	0.29148	0.29328	0.29370	0.30052
Beta virt. eigenvalues --	0.30498	0.30514	0.30964	0.30986	0.32137
Beta virt. eigenvalues --	0.32958	0.33981	0.35281	0.36305	0.37396
Beta virt. eigenvalues --	0.37423	0.38925	0.39045	0.39291	0.39772
Beta virt. eigenvalues --	0.39937	0.40828	0.40989	0.41018	0.41216
Beta virt. eigenvalues --	0.41383	0.41506	0.41789	0.42008	0.42043
Beta virt. eigenvalues --	0.42296	0.42439	0.42631	0.42899	0.42943
Beta virt. eigenvalues --	0.43392	0.43446	0.43603	0.43668	0.43837
Beta virt. eigenvalues --	0.43966	0.44296	0.44343	0.44413	0.44495
Beta virt. eigenvalues --	0.44619	0.44846	0.44894	0.45095	0.45138
Beta virt. eigenvalues --	0.45416	0.45423	0.45434	0.45546	0.45620
Beta virt. eigenvalues --	0.45663	0.45749	0.45768	0.45831	0.45839
Beta virt. eigenvalues --	0.45913	0.45940	0.45994	0.46066	0.46166
Beta virt. eigenvalues --	0.46264	0.46361	0.46405	0.46518	0.46598
Beta virt. eigenvalues --	0.46719	0.46759	0.46785	0.46859	0.47019
Beta virt. eigenvalues --	0.47102	0.47283	0.47297	0.47337	0.47467
Beta virt. eigenvalues --	0.47694	0.47755	0.47829	0.47965	0.48002
Beta virt. eigenvalues --	0.48202	0.48225	0.48333	0.48397	0.48512
Beta virt. eigenvalues --	0.48595	0.48830	0.48905	0.48943	0.48950
Beta virt. eigenvalues --	0.49054	0.49112	0.49195	0.49318	0.49554
Beta virt. eigenvalues --	0.50214	0.50310	0.50425	0.50466	0.50684
Beta virt. eigenvalues --	0.50690	0.50829	0.51225	0.51275	0.51382
Beta virt. eigenvalues --	0.51456	0.51466	0.51650	0.52033	0.52081
Beta virt. eigenvalues --	0.52260	0.52272	0.52534	0.52567	0.52617
Beta virt. eigenvalues --	0.52901	0.53130	0.53275	0.53321	0.53574
Beta virt. eigenvalues --	0.53651	0.53800	0.54011	0.54280	0.54714
Beta virt. eigenvalues --	0.54817	0.54835	0.54867	0.54921	0.55121

Beta virt. eigenvalues --	0.55128	0.55144	0.55205	0.55548	0.55894
Beta virt. eigenvalues --	0.56189	0.56296	0.56764	0.56801	0.56902
Beta virt. eigenvalues --	0.57232	0.57408	0.57487	0.58634	0.58788
Beta virt. eigenvalues --	0.59188	0.59198	0.59376	0.59546	0.59602
Beta virt. eigenvalues --	0.59706	0.59996	0.60044	0.60154	0.60217
Beta virt. eigenvalues --	0.60500	0.60529	0.60754	0.60935	0.60942
Beta virt. eigenvalues --	0.61111	0.61168	0.61264	0.61282	0.61339
Beta virt. eigenvalues --	0.61459	0.61510	0.61795	0.61797	0.61945
Beta virt. eigenvalues --	0.62030	0.62076	0.62221	0.62276	0.62330
Beta virt. eigenvalues --	0.62422	0.62646	0.62696	0.62702	0.62724
Beta virt. eigenvalues --	0.62954	0.62993	0.63083	0.63357	0.63368
Beta virt. eigenvalues --	0.63401	0.63483	0.63523	0.63676	0.63687
Beta virt. eigenvalues --	0.63770	0.63796	0.63839	0.63937	0.64151
Beta virt. eigenvalues --	0.64166	0.64224	0.64273	0.64347	0.64363
Beta virt. eigenvalues --	0.64548	0.64847	0.64889	0.64994	0.65099
Beta virt. eigenvalues --	0.65322	0.65520	0.65551	0.65699	0.65769
Beta virt. eigenvalues --	0.65769	0.65788	0.65832	0.66002	0.66091
Beta virt. eigenvalues --	0.66096	0.66131	0.66197	0.66300	0.66446
Beta virt. eigenvalues --	0.66535	0.66551	0.66758	0.67016	0.67094
Beta virt. eigenvalues --	0.67105	0.67260	0.67292	0.67368	0.67420
Beta virt. eigenvalues --	0.67532	0.67670	0.67829	0.67858	0.67864
Beta virt. eigenvalues --	0.67913	0.68084	0.68186	0.68188	0.68283
Beta virt. eigenvalues --	0.68338	0.68461	0.68525	0.68564	0.68674
Beta virt. eigenvalues --	0.68982	0.69009	0.69333	0.69443	0.69552
Beta virt. eigenvalues --	0.69571	0.69934	0.70191	0.70335	0.70402
Beta virt. eigenvalues --	0.70421	0.70673	0.70675	0.71064	0.71112
Beta virt. eigenvalues --	0.71171	0.71587	0.71739	0.71759	0.71784
Beta virt. eigenvalues --	0.72073	0.72108	0.72708	0.72711	0.72812
Beta virt. eigenvalues --	0.72914	0.73189	0.73289	0.73491	0.73578
Beta virt. eigenvalues --	0.73821	0.73845	0.73907	0.74014	0.74143
Beta virt. eigenvalues --	0.74295	0.74506	0.74576	0.74714	0.74854
Beta virt. eigenvalues --	0.74948	0.75160	0.75367	0.75415	0.75501
Beta virt. eigenvalues --	0.75610	0.75669	0.75707	0.75751	0.75843
Beta virt. eigenvalues --	0.75919	0.76148	0.76281	0.76527	0.76614
Beta virt. eigenvalues --	0.76730	0.77164	0.77540	0.77994	0.78165
Beta virt. eigenvalues --	0.78521	0.78752	0.78814	0.80349	0.80544
Beta virt. eigenvalues --	0.80566	0.81119	0.81217	0.81341	0.81603
Beta virt. eigenvalues --	0.81756	0.82538	0.82648	0.82747	0.83919
Beta virt. eigenvalues --	0.84039	0.84528	0.84859	0.85670	0.85885
Beta virt. eigenvalues --	0.86031	0.86353	0.86681	0.86812	0.86937
Beta virt. eigenvalues --	0.87004	0.87035	0.87089	0.87153	0.87288
Beta virt. eigenvalues --	0.87341	0.87499	0.87802	0.87836	0.88505
Beta virt. eigenvalues --	0.88661	0.88693	0.89406	0.89518	0.90645
Beta virt. eigenvalues --	0.90672	0.90865	0.90882	0.90983	0.91046
Beta virt. eigenvalues --	0.91102	0.91273	0.91429	0.91458	0.91516
Beta virt. eigenvalues --	0.91561	0.91659	0.91806	0.92917	0.92957
Beta virt. eigenvalues --	0.93628	0.93817	0.93979	0.94209	0.95386
Beta virt. eigenvalues --	0.95517	0.95998	0.96163	0.96394	0.96565

Beta virt. eigenvalues --	0.96795	0.96845	0.97639	0.97807	0.97839
Beta virt. eigenvalues --	0.98220	0.98337	0.98409	0.98810	0.98929
Beta virt. eigenvalues --	0.99028	0.99256	0.99633	0.99714	0.99998
Beta virt. eigenvalues --	1.00060	1.00479	1.00857	1.01235	1.01308
Beta virt. eigenvalues --	1.01429	1.01760	1.01884	1.02008	1.02079
Beta virt. eigenvalues --	1.02125	1.02398	1.02572	1.03069	1.03337
Beta virt. eigenvalues --	1.03357	1.03978	1.04456	1.05041	1.05408
Beta virt. eigenvalues --	1.05581	1.06189	1.06367	1.07180	1.07219
Beta virt. eigenvalues --	1.07409	1.07621	1.08333	1.08780	1.09247
Beta virt. eigenvalues --	1.09447	1.10050	1.10119	1.10786	1.10829
Beta virt. eigenvalues --	1.11332	1.11544	1.12211	1.12277	1.12298
Beta virt. eigenvalues --	1.12757	1.13043	1.13123	1.13432	1.13489
Beta virt. eigenvalues --	1.14744	1.15094	1.15554	1.15669	1.15791
Beta virt. eigenvalues --	1.15824	1.15902	1.16014	1.16243	1.16791
Beta virt. eigenvalues --	1.17824	1.17887	1.18219	1.18314	1.18471
Beta virt. eigenvalues --	1.18649	1.18664	1.18752	1.18864	1.19107
Beta virt. eigenvalues --	1.19140	1.19425	1.19485	1.19651	1.19709
Beta virt. eigenvalues --	1.19987	1.19987	1.21453	1.21507	1.21735
Beta virt. eigenvalues --	1.21816	1.21874	1.22003	1.22289	1.22574
Beta virt. eigenvalues --	1.22700	1.23350	1.23460	1.23892	1.24063
Beta virt. eigenvalues --	1.24360	1.24467	1.24653	1.24656	1.24764
Beta virt. eigenvalues --	1.24960	1.25305	1.25556	1.25797	1.25977
Beta virt. eigenvalues --	1.26052	1.26355	1.26356	1.26504	1.26598
Beta virt. eigenvalues --	1.26907	1.26939	1.27514	1.28108	1.28220
Beta virt. eigenvalues --	1.28649	1.28765	1.28787	1.29068	1.29099
Beta virt. eigenvalues --	1.29663	1.29797	1.30369	1.30807	1.30924
Beta virt. eigenvalues --	1.31264	1.31549	1.31581	1.31736	1.31852
Beta virt. eigenvalues --	1.31937	1.32402	1.32526	1.32903	1.33428
Beta virt. eigenvalues --	1.33592	1.34024	1.34218	1.34361	1.34388
Beta virt. eigenvalues --	1.34762	1.34808	1.35451	1.36185	1.36273
Beta virt. eigenvalues --	1.36414	1.36514	1.36727	1.36760	1.36991
Beta virt. eigenvalues --	1.37316	1.37644	1.37808	1.37885	1.37934
Beta virt. eigenvalues --	1.38050	1.38260	1.38744	1.38970	1.39157
Beta virt. eigenvalues --	1.39537	1.40253	1.40273	1.40360	1.40511
Beta virt. eigenvalues --	1.40515	1.40552	1.40578	1.40673	1.40713
Beta virt. eigenvalues --	1.40783	1.40857	1.40888	1.40909	1.40933
Beta virt. eigenvalues --	1.40950	1.40978	1.41134	1.41342	1.41459
Beta virt. eigenvalues --	1.41663	1.41685	1.41830	1.42073	1.42418
Beta virt. eigenvalues --	1.42439	1.42577	1.42806	1.42959	1.43151
Beta virt. eigenvalues --	1.43374	1.43471	1.43613	1.43648	1.43970
Beta virt. eigenvalues --	1.44057	1.44154	1.44167	1.44352	1.44382
Beta virt. eigenvalues --	1.44530	1.44717	1.45013	1.45098	1.45176
Beta virt. eigenvalues --	1.46360	1.46469	1.46625	1.46645	1.46866
Beta virt. eigenvalues --	1.46941	1.47094	1.47108	1.47272	1.47408
Beta virt. eigenvalues --	1.47473	1.47546	1.48148	1.48503	1.48838
Beta virt. eigenvalues --	1.48879	1.49018	1.49348	1.49492	1.50027
Beta virt. eigenvalues --	1.50201	1.50436	1.51097	1.51310	1.51433
Beta virt. eigenvalues --	1.51519	1.51950	1.52025	1.52304	1.52379

Beta virt. eigenvalues --	1.52741	1.52773	1.52847	1.52912	1.53005
Beta virt. eigenvalues --	1.53201	1.53328	1.53521	1.53913	1.54130
Beta virt. eigenvalues --	1.54760	1.54796	1.55088	1.55198	1.55574
Beta virt. eigenvalues --	1.55774	1.55943	1.55971	1.56097	1.56177
Beta virt. eigenvalues --	1.56187	1.56656	1.56820	1.57135	1.57354
Beta virt. eigenvalues --	1.57475	1.57577	1.57720	1.57765	1.57840
Beta virt. eigenvalues --	1.57935	1.57960	1.58092	1.58295	1.58741
Beta virt. eigenvalues --	1.58767	1.58863	1.58950	1.59132	1.59157
Beta virt. eigenvalues --	1.59846	1.59879	1.60437	1.60485	1.60748
Beta virt. eigenvalues --	1.61108	1.61216	1.61322	1.61505	1.61839
Beta virt. eigenvalues --	1.61945	1.62036	1.62041	1.62176	1.62268
Beta virt. eigenvalues --	1.62320	1.62362	1.62434	1.62456	1.62560
Beta virt. eigenvalues --	1.62617	1.62671	1.62741	1.62765	1.62920
Beta virt. eigenvalues --	1.62934	1.63199	1.63215	1.63240	1.63324
Beta virt. eigenvalues --	1.63491	1.63581	1.63680	1.63709	1.64003
Beta virt. eigenvalues --	1.64242	1.64319	1.64440	1.64549	1.64699
Beta virt. eigenvalues --	1.64718	1.64898	1.64927	1.65006	1.65510
Beta virt. eigenvalues --	1.65668	1.66085	1.66196	1.66329	1.66532
Beta virt. eigenvalues --	1.66712	1.66773	1.67111	1.67478	1.67629
Beta virt. eigenvalues --	1.67826	1.67899	1.68072	1.68138	1.68360
Beta virt. eigenvalues --	1.68532	1.68551	1.68600	1.68772	1.68940
Beta virt. eigenvalues --	1.69038	1.69527	1.69743	1.69844	1.70376
Beta virt. eigenvalues --	1.70449	1.70587	1.70732	1.71080	1.71176
Beta virt. eigenvalues --	1.71210	1.71335	1.71367	1.71424	1.71454
Beta virt. eigenvalues --	1.71460	1.71495	1.71525	1.71527	1.72308
Beta virt. eigenvalues --	1.72360	1.72920	1.73025	1.73296	1.73421
Beta virt. eigenvalues --	1.73434	1.73598	1.73635	1.73804	1.73830
Beta virt. eigenvalues --	1.74071	1.74249	1.74694	1.74815	1.74855
Beta virt. eigenvalues --	1.74985	1.75379	1.75412	1.75642	1.75984
Beta virt. eigenvalues --	1.76174	1.76361	1.76370	1.76694	1.76756
Beta virt. eigenvalues --	1.76811	1.76891	1.76936	1.77019	1.77762
Beta virt. eigenvalues --	1.77860	1.78173	1.78407	1.78416	1.78585
Beta virt. eigenvalues --	1.78604	1.78629	1.78725	1.78928	1.78998
Beta virt. eigenvalues --	1.79225	1.79918	1.80107	1.80234	1.80260
Beta virt. eigenvalues --	1.80345	1.80715	1.81113	1.81254	1.81775
Beta virt. eigenvalues --	1.81805	1.82277	1.82318	1.82444	1.82536
Beta virt. eigenvalues --	1.82735	1.82841	1.82865	1.83074	1.83277
Beta virt. eigenvalues --	1.83558	1.83777	1.83809	1.83833	1.83852
Beta virt. eigenvalues --	1.84285	1.84640	1.84959	1.85022	1.85069
Beta virt. eigenvalues --	1.85231	1.85360	1.85480	1.85515	1.85596
Beta virt. eigenvalues --	1.85731	1.86035	1.86127	1.86238	1.86265
Beta virt. eigenvalues --	1.86465	1.86527	1.86672	1.86713	1.87141
Beta virt. eigenvalues --	1.87366	1.87439	1.87652	1.87780	1.87823
Beta virt. eigenvalues --	1.88190	1.88204	1.88487	1.89005	1.89216
Beta virt. eigenvalues --	1.89618	1.89718	1.89788	1.90287	1.91096
Beta virt. eigenvalues --	1.92030	1.92473	1.92674	1.92836	1.93064
Beta virt. eigenvalues --	1.93145	1.93689	1.94048	1.94644	1.94805
Beta virt. eigenvalues --	1.95005	1.95023	1.95648	1.95734	1.96617

Beta virt. eigenvalues --	1.96767	1.97197	1.97367	1.97536	1.97842
Beta virt. eigenvalues --	1.97873	1.98284	1.98666	1.98689	1.98993
Beta virt. eigenvalues --	1.99033	1.99359	1.99378	1.99426	1.99475
Beta virt. eigenvalues --	1.99651	1.99662	1.99773	1.99807	1.99885
Beta virt. eigenvalues --	1.99963	2.00036	2.00078	2.00437	2.00560
Beta virt. eigenvalues --	2.00862	2.00966	2.01777	2.02287	2.02572
Beta virt. eigenvalues --	2.02707	2.03120	2.03205	2.03314	2.03386
Beta virt. eigenvalues --	2.03935	2.04010	2.04331	2.04679	2.04804
Beta virt. eigenvalues --	2.05123	2.06121	2.06172	2.06411	2.06428
Beta virt. eigenvalues --	2.06545	2.06550	2.07159	2.07203	2.07532
Beta virt. eigenvalues --	2.07821	2.08201	2.08219	2.08752	2.08858
Beta virt. eigenvalues --	2.08920	2.08940	2.09034	2.09297	2.09632
Beta virt. eigenvalues --	2.09652	2.10948	2.11774	2.12227	2.12257
Beta virt. eigenvalues --	2.12353	2.12381	2.12523	2.12543	2.12882
Beta virt. eigenvalues --	2.13242	2.13301	2.13853	2.13866	2.13974
Beta virt. eigenvalues --	2.14133	2.14259	2.14366	2.14531	2.15874
Beta virt. eigenvalues --	2.16305	2.16641	2.16894	2.17086	2.17336
Beta virt. eigenvalues --	2.17964	2.17996	2.18231	2.18422	2.18423
Beta virt. eigenvalues --	2.18557	2.19284	2.19496	2.19825	2.19903
Beta virt. eigenvalues --	2.20344	2.20459	2.21576	2.21582	2.22000
Beta virt. eigenvalues --	2.22004	2.22232	2.22381	2.22954	2.23015
Beta virt. eigenvalues --	2.23246	2.23465	2.23648	2.23708	2.25995
Beta virt. eigenvalues --	2.26207	2.26524	2.26594	2.26740	2.26921
Beta virt. eigenvalues --	2.27473	2.28222	2.29571	2.29761	2.29857
Beta virt. eigenvalues --	2.29947	2.29981	2.29991	2.30503	2.31027
Beta virt. eigenvalues --	2.31717	2.31760	2.32033	2.32390	2.32555
Beta virt. eigenvalues --	2.33170	2.33351	2.33765	2.33990	2.34040
Beta virt. eigenvalues --	2.34231	2.34754	2.35964	2.36594	2.37005
Beta virt. eigenvalues --	2.37035	2.37286	2.37952	2.38276	2.38424
Beta virt. eigenvalues --	2.38651	2.39105	2.39802	2.40050	2.40249
Beta virt. eigenvalues --	2.40486	2.40657	2.41140	2.41427	2.41488
Beta virt. eigenvalues --	2.41802	2.41903	2.41952	2.42024	2.42084
Beta virt. eigenvalues --	2.42204	2.42367	2.42421	2.42461	2.42583
Beta virt. eigenvalues --	2.42997	2.43240	2.43340	2.43366	2.43439
Beta virt. eigenvalues --	2.43482	2.43497	2.43706	2.44109	2.44155
Beta virt. eigenvalues --	2.44293	2.44400	2.44912	2.44967	2.45093
Beta virt. eigenvalues --	2.45103	2.45199	2.45297	2.45370	2.45419
Beta virt. eigenvalues --	2.46076	2.46090	2.46557	2.46649	2.46888
Beta virt. eigenvalues --	2.47287	2.47360	2.47397	2.47733	2.47874
Beta virt. eigenvalues --	2.47959	2.48294	2.48520	2.48537	2.48574
Beta virt. eigenvalues --	2.48886	2.48955	2.49112	2.49196	2.49240
Beta virt. eigenvalues --	2.49306	2.49306	2.49397	2.49664	2.49780
Beta virt. eigenvalues --	2.50483	2.50974	2.51250	2.51450	2.51511
Beta virt. eigenvalues --	2.51831	2.52385	2.52817	2.53153	2.53284
Beta virt. eigenvalues --	2.53360	2.53477	2.53552	2.53728	2.55003
Beta virt. eigenvalues --	2.55229	2.55378	2.55506	2.55684	2.55754
Beta virt. eigenvalues --	2.55867	2.55919	2.56176	2.57389	2.57430
Beta virt. eigenvalues --	2.57712	2.57716	2.57763	2.58036	2.58564

Beta virt. eigenvalues --	2.59850	2.60234	2.60334	2.61267	2.62392
Beta virt. eigenvalues --	2.63435	2.64660	2.68051	2.68630	2.68776
Beta virt. eigenvalues --	2.69139	2.69481	2.69603	2.77058	2.77636
Beta virt. eigenvalues --	2.78374	2.78826	2.80311	2.80344	2.89734
Beta virt. eigenvalues --	2.89802	2.90153	2.90319	2.91195	2.91256
Beta virt. eigenvalues --	2.93085	2.93298	2.93558	2.93568	2.94117
Beta virt. eigenvalues --	2.94129	2.96261	2.96432	2.96742	2.96972
Beta virt. eigenvalues --	2.97499	2.97535	2.98297	2.98372	2.98482
Beta virt. eigenvalues --	2.98488	2.98647	2.98651	2.99002	2.99070
Beta virt. eigenvalues --	2.99198	2.99263	2.99438	2.99459	3.01990
Beta virt. eigenvalues --	3.02055	3.02160	3.02194	3.02333	3.02333
Beta virt. eigenvalues --	3.02461	3.02922	3.03027	3.03145	3.03270
Beta virt. eigenvalues --	3.03294	3.07522	3.07568	3.07661	3.07676
Beta virt. eigenvalues --	3.07801	3.07803	3.08206	3.08212	3.08321
Beta virt. eigenvalues --	3.08325	3.08461	3.08462	3.09240	3.09757
Beta virt. eigenvalues --	3.10017	3.10029	3.10334	3.10340	3.10791
Beta virt. eigenvalues --	3.10957	3.11108	3.11371	3.11730	3.12304
Beta virt. eigenvalues --	3.12410	3.12555	3.12707	3.12707	3.12926
Beta virt. eigenvalues --	3.13064	3.23772	3.23824	3.23911	3.23948
Beta virt. eigenvalues --	3.24023	3.24039	3.25889	3.25924	3.26010
Beta virt. eigenvalues --	3.26030	3.26110	3.26115	3.30044	3.30112
Beta virt. eigenvalues --	3.30401	3.30433	3.30868	3.30869	3.36453
Beta virt. eigenvalues --	3.36486	3.36591	3.36677	3.36740	3.36775
Beta virt. eigenvalues --	3.36830	3.36846	3.36946	3.36974	3.37019
Beta virt. eigenvalues --	3.37027	3.39183	3.39196	3.39366	3.39599
Beta virt. eigenvalues --	3.39750	3.39884	3.40845	3.41687	3.42130
Beta virt. eigenvalues --	3.42472	3.42986	3.43189	3.49127	3.49557
Beta virt. eigenvalues --	3.50172	3.50816	3.51488	3.51911	

Dication/Bipolaron

Alpha occ. eigenvalues --	-89.14440	-89.14440	-89.13920	-89.13920	-89.12921
Alpha occ. eigenvalues --	-89.12921	-19.31316	-19.31315	-19.31052	-19.31052
Alpha occ. eigenvalues --	-19.30975	-19.30975	-19.30136	-19.30136	-19.30122
Alpha occ. eigenvalues --	-19.30122	-19.28347	-19.28347	-19.25443	-19.25443
Alpha occ. eigenvalues --	-19.25411	-19.25411	-19.25309	-19.25309	-19.25186
Alpha occ. eigenvalues --	-19.25186	-19.25042	-19.25042	-19.24897	-19.24896
Alpha occ. eigenvalues --	-10.36955	-10.36955	-10.36575	-10.36575	-10.36511
Alpha occ. eigenvalues --	-10.36511	-10.35529	-10.35529	-10.35505	-10.35505
Alpha occ. eigenvalues --	-10.35347	-10.35308	-10.35115	-10.35115	-10.34690
Alpha occ. eigenvalues --	-10.34690	-10.34217	-10.34217	-10.33867	-10.33867
Alpha occ. eigenvalues --	-10.32758	-10.32758	-10.32646	-10.32646	-10.32619
Alpha occ. eigenvalues --	-10.32619	-10.32529	-10.32529	-10.32235	-10.32235
Alpha occ. eigenvalues --	-10.31967	-10.31967	-10.31402	-10.31402	-10.31242
Alpha occ. eigenvalues --	-10.31242	-10.31232	-10.31232	-10.31067	-10.31067
Alpha occ. eigenvalues --	-10.31016	-10.31015	-10.30743	-10.30743	-10.30709
Alpha occ. eigenvalues --	-10.30709	-10.30689	-10.30689	-10.29726	-10.29726
Alpha occ. eigenvalues --	-10.29689	-10.29689	-10.29644	-10.29644	-10.29476
Alpha occ. eigenvalues --	-10.29476	-10.29467	-10.29467	-10.29280	-10.29280

Alpha occ. eigenvalues -- -10.29032 -10.29032 -10.28762 -10.28762 -10.28212
 Alpha occ. eigenvalues -- -10.28212 -8.08761 -8.08761 -8.08225 -8.08225
 Alpha occ. eigenvalues -- -8.07256 -8.07256 -6.02682 -6.02682 -6.02286
 Alpha occ. eigenvalues -- -6.02286 -6.02140 -6.02140 -6.01781 -6.01781
 Alpha occ. eigenvalues -- -6.01747 -6.01747 -6.01261 -6.01261 -6.01145
 Alpha occ. eigenvalues -- -6.01145 -6.00763 -6.00763 -6.00352 -6.00352
 Alpha occ. eigenvalues -- -1.16493 -1.16430 -1.15966 -1.15966 -1.14818
 Alpha occ. eigenvalues -- -1.14818 -1.14072 -1.14044 -1.13482 -1.13481
 Alpha occ. eigenvalues -- -1.12061 -1.12061 -1.09650 -1.09648 -1.09482
 Alpha occ. eigenvalues -- -1.09482 -1.09444 -1.09444 -1.09247 -1.09247
 Alpha occ. eigenvalues -- -1.09199 -1.09199 -1.08958 -1.08958 -0.98630
 Alpha occ. eigenvalues -- -0.97719 -0.96794 -0.95949 -0.94525 -0.94309
 Alpha occ. eigenvalues -- -0.88685 -0.88624 -0.88395 -0.88323 -0.88002
 Alpha occ. eigenvalues -- -0.87730 -0.87640 -0.85929 -0.83990 -0.82341
 Alpha occ. eigenvalues -- -0.81296 -0.81191 -0.80569 -0.80122 -0.79716
 Alpha occ. eigenvalues -- -0.79705 -0.79059 -0.79010 -0.76649 -0.76448
 Alpha occ. eigenvalues -- -0.76263 -0.76240 -0.76172 -0.76025 -0.75914
 Alpha occ. eigenvalues -- -0.75896 -0.75668 -0.75125 -0.74911 -0.74318
 Alpha occ. eigenvalues -- -0.74137 -0.74011 -0.73608 -0.73541 -0.73293
 Alpha occ. eigenvalues -- -0.71655 -0.70436 -0.70313 -0.70165 -0.70134
 Alpha occ. eigenvalues -- -0.69814 -0.69771 -0.69198 -0.67901 -0.66875
 Alpha occ. eigenvalues -- -0.66257 -0.66229 -0.66186 -0.66045 -0.65861
 Alpha occ. eigenvalues -- -0.65821 -0.65815 -0.64934 -0.64895 -0.63409
 Alpha occ. eigenvalues -- -0.63219 -0.62966 -0.62493 -0.62358 -0.62019
 Alpha occ. eigenvalues -- -0.61818 -0.61220 -0.60780 -0.60495 -0.59962
 Alpha occ. eigenvalues -- -0.59863 -0.57737 -0.57224 -0.56652 -0.56378
 Alpha occ. eigenvalues -- -0.56311 -0.56226 -0.55949 -0.55916 -0.55779
 Alpha occ. eigenvalues -- -0.55742 -0.55457 -0.55270 -0.55133 -0.55066
 Alpha occ. eigenvalues -- -0.54816 -0.54386 -0.53990 -0.53752 -0.53730
 Alpha occ. eigenvalues -- -0.53661 -0.53506 -0.53356 -0.53329 -0.52911
 Alpha occ. eigenvalues -- -0.52885 -0.52553 -0.52373 -0.51651 -0.51454
 Alpha occ. eigenvalues -- -0.51171 -0.50997 -0.50680 -0.50641 -0.50620
 Alpha occ. eigenvalues -- -0.50540 -0.50473 -0.50401 -0.50353 -0.50305
 Alpha occ. eigenvalues -- -0.50110 -0.50103 -0.50028 -0.49884 -0.49851
 Alpha occ. eigenvalues -- -0.49511 -0.49450 -0.49276 -0.49239 -0.48959
 Alpha occ. eigenvalues -- -0.48878 -0.48799 -0.48702 -0.48659 -0.48641
 Alpha occ. eigenvalues -- -0.48271 -0.48271 -0.48242 -0.47952 -0.47933
 Alpha occ. eigenvalues -- -0.47705 -0.47628 -0.47590 -0.47466 -0.47297
 Alpha occ. eigenvalues -- -0.47202 -0.47099 -0.46720 -0.46450 -0.46438
 Alpha occ. eigenvalues -- -0.46335 -0.46017 -0.45764 -0.45734 -0.45525
 Alpha occ. eigenvalues -- -0.45180 -0.44753 -0.44732 -0.44284 -0.44070
 Alpha occ. eigenvalues -- -0.44050 -0.43917 -0.43687 -0.43654 -0.43189
 Alpha occ. eigenvalues -- -0.43177 -0.42751 -0.42445 -0.42330 -0.42105
 Alpha occ. eigenvalues -- -0.42041 -0.42004 -0.41893 -0.41826 -0.41604
 Alpha occ. eigenvalues -- -0.41592 -0.41513 -0.41446 -0.41413 -0.41175
 Alpha occ. eigenvalues -- -0.41109 -0.41019 -0.40893 -0.40649 -0.40464
 Alpha occ. eigenvalues -- -0.40295 -0.40163 -0.40001 -0.39859 -0.39557
 Alpha occ. eigenvalues -- -0.39351 -0.39163 -0.38938 -0.38905 -0.38346

Alpha occ. eigenvalues --	-0.38340	-0.37120	-0.37010	-0.36912	-0.36847
Alpha occ. eigenvalues --	-0.36762	-0.36658	-0.36574	-0.36484	-0.36306
Alpha occ. eigenvalues --	-0.36201	-0.36088	-0.35930	-0.35858	-0.35716
Alpha occ. eigenvalues --	-0.35695	-0.35459	-0.35444	-0.35338	-0.35326
Alpha occ. eigenvalues --	-0.35134	-0.35126	-0.34890	-0.34786	-0.34669
Alpha occ. eigenvalues --	-0.34472	-0.34049	-0.33923	-0.33804	-0.33258
Alpha occ. eigenvalues --	-0.33163	-0.32015	-0.31405	-0.29910	-0.29787
Alpha occ. eigenvalues --	-0.29734	-0.29584	-0.29572	-0.29252	-0.29251
Alpha occ. eigenvalues --	-0.28795	-0.28794	-0.28618	-0.28618	-0.28352
Alpha occ. eigenvalues --	-0.28352	-0.28120	-0.28095	-0.27330	-0.27036
Alpha occ. eigenvalues --	-0.26098	-0.26057	-0.25983	-0.23099	
Alpha virt. eigenvalues --	-0.18989	-0.11450	-0.08563	-0.05925	-0.03468
Alpha virt. eigenvalues --	-0.01186	-0.00793	-0.00617	-0.00109	0.00462
Alpha virt. eigenvalues --	0.00742	0.00879	0.01157	0.01619	0.02081
Alpha virt. eigenvalues --	0.02569	0.03381	0.03539	0.03881	0.04005
Alpha virt. eigenvalues --	0.04124	0.04646	0.04747	0.04925	0.05227
Alpha virt. eigenvalues --	0.05441	0.05953	0.06206	0.06282	0.06337
Alpha virt. eigenvalues --	0.06342	0.06422	0.06522	0.06544	0.06625
Alpha virt. eigenvalues --	0.06745	0.06914	0.07161	0.07317	0.07659
Alpha virt. eigenvalues --	0.07741	0.08158	0.08229	0.08362	0.08670
Alpha virt. eigenvalues --	0.08683	0.08742	0.08851	0.08877	0.08932
Alpha virt. eigenvalues --	0.09409	0.09447	0.09605	0.09942	0.10064
Alpha virt. eigenvalues --	0.10118	0.10251	0.10311	0.10379	0.10635
Alpha virt. eigenvalues --	0.10686	0.11012	0.11131	0.11136	0.11331
Alpha virt. eigenvalues --	0.11347	0.11446	0.11605	0.11738	0.11786
Alpha virt. eigenvalues --	0.11906	0.12004	0.12155	0.12188	0.12493
Alpha virt. eigenvalues --	0.12494	0.12533	0.12578	0.12659	0.12660
Alpha virt. eigenvalues --	0.12760	0.12784	0.12837	0.12966	0.12974
Alpha virt. eigenvalues --	0.13008	0.13064	0.13201	0.13268	0.13456
Alpha virt. eigenvalues --	0.13461	0.13593	0.13593	0.13658	0.13743
Alpha virt. eigenvalues --	0.13753	0.13781	0.13784	0.13904	0.13939
Alpha virt. eigenvalues --	0.14063	0.14357	0.14616	0.14846	0.14885
Alpha virt. eigenvalues --	0.15029	0.15222	0.15227	0.15385	0.15498
Alpha virt. eigenvalues --	0.15588	0.15643	0.15720	0.15737	0.15964
Alpha virt. eigenvalues --	0.16004	0.16097	0.16283	0.16413	0.16477
Alpha virt. eigenvalues --	0.16514	0.16670	0.16771	0.16928	0.17051
Alpha virt. eigenvalues --	0.17381	0.18467	0.18923	0.18950	0.19055
Alpha virt. eigenvalues --	0.19180	0.19368	0.19544	0.19709	0.19816
Alpha virt. eigenvalues --	0.19982	0.20071	0.20110	0.20352	0.20380
Alpha virt. eigenvalues --	0.20522	0.20618	0.20805	0.20877	0.21091
Alpha virt. eigenvalues --	0.21171	0.21422	0.21481	0.21680	0.21893
Alpha virt. eigenvalues --	0.22006	0.22013	0.22149	0.22258	0.22475
Alpha virt. eigenvalues --	0.22484	0.22618	0.23235	0.23471	0.23589
Alpha virt. eigenvalues --	0.23741	0.23907	0.24225	0.24347	0.24616
Alpha virt. eigenvalues --	0.24884	0.24979	0.25026	0.25235	0.25511
Alpha virt. eigenvalues --	0.25610	0.25783	0.26415	0.26525	0.26694
Alpha virt. eigenvalues --	0.26752	0.27185	0.27287	0.27582	0.27605
Alpha virt. eigenvalues --	0.27952	0.27994	0.28102	0.28401	0.28403

Alpha virt. eigenvalues --	0.28572	0.28631	0.29168	0.29212	0.30168
Alpha virt. eigenvalues --	0.31074	0.32050	0.33221	0.34081	0.35187
Alpha virt. eigenvalues --	0.35310	0.36923	0.37099	0.37267	0.37874
Alpha virt. eigenvalues --	0.38145	0.39044	0.39146	0.39288	0.39534
Alpha virt. eigenvalues --	0.39759	0.39771	0.40242	0.40366	0.40443
Alpha virt. eigenvalues --	0.40597	0.40829	0.40988	0.41214	0.41320
Alpha virt. eigenvalues --	0.41644	0.41811	0.41991	0.42171	0.42235
Alpha virt. eigenvalues --	0.42326	0.42546	0.42669	0.42720	0.42805
Alpha virt. eigenvalues --	0.42837	0.43342	0.43401	0.43454	0.43505
Alpha virt. eigenvalues --	0.43772	0.43782	0.43939	0.43981	0.44104
Alpha virt. eigenvalues --	0.44128	0.44190	0.44268	0.44419	0.44462
Alpha virt. eigenvalues --	0.44536	0.44561	0.44679	0.44887	0.44973
Alpha virt. eigenvalues --	0.44982	0.45018	0.45198	0.45372	0.45404
Alpha virt. eigenvalues --	0.45524	0.45575	0.45729	0.45878	0.45900
Alpha virt. eigenvalues --	0.45992	0.46041	0.46128	0.46217	0.46269
Alpha virt. eigenvalues --	0.46309	0.46361	0.46499	0.46558	0.46667
Alpha virt. eigenvalues --	0.46698	0.46705	0.46828	0.46994	0.47050
Alpha virt. eigenvalues --	0.47116	0.47358	0.47503	0.47521	0.47594
Alpha virt. eigenvalues --	0.47660	0.47743	0.47759	0.47956	0.47976
Alpha virt. eigenvalues --	0.48384	0.48732	0.48774	0.48916	0.48916
Alpha virt. eigenvalues --	0.48964	0.49279	0.49396	0.49528	0.49707
Alpha virt. eigenvalues --	0.49779	0.49866	0.50143	0.50480	0.50681
Alpha virt. eigenvalues --	0.50695	0.50825	0.51085	0.51114	0.51148
Alpha virt. eigenvalues --	0.51303	0.51450	0.51814	0.51828	0.52126
Alpha virt. eigenvalues --	0.52187	0.52436	0.52592	0.53035	0.53120
Alpha virt. eigenvalues --	0.53324	0.53473	0.53565	0.53615	0.53660
Alpha virt. eigenvalues --	0.53736	0.53858	0.54041	0.54106	0.54244
Alpha virt. eigenvalues --	0.54812	0.54826	0.55391	0.55428	0.55546
Alpha virt. eigenvalues --	0.55813	0.56027	0.56107	0.56953	0.57209
Alpha virt. eigenvalues --	0.57513	0.57717	0.58081	0.58122	0.58283
Alpha virt. eigenvalues --	0.58373	0.58860	0.58868	0.58966	0.59021
Alpha virt. eigenvalues --	0.59264	0.59316	0.59344	0.59734	0.59758
Alpha virt. eigenvalues --	0.59816	0.59928	0.60096	0.60208	0.60304
Alpha virt. eigenvalues --	0.60359	0.60401	0.60583	0.60651	0.60725
Alpha virt. eigenvalues --	0.60872	0.60957	0.61083	0.61114	0.61193
Alpha virt. eigenvalues --	0.61212	0.61596	0.61622	0.61680	0.61699
Alpha virt. eigenvalues --	0.61908	0.61977	0.61985	0.62236	0.62271
Alpha virt. eigenvalues --	0.62295	0.62361	0.62472	0.62652	0.62677
Alpha virt. eigenvalues --	0.62749	0.62845	0.62867	0.62946	0.62972
Alpha virt. eigenvalues --	0.63015	0.63052	0.63140	0.63190	0.63414
Alpha virt. eigenvalues --	0.63535	0.63743	0.63791	0.63885	0.63931
Alpha virt. eigenvalues --	0.64039	0.64152	0.64355	0.64439	0.64541
Alpha virt. eigenvalues --	0.64629	0.64676	0.64752	0.64803	0.64875
Alpha virt. eigenvalues --	0.65011	0.65082	0.65149	0.65264	0.65335
Alpha virt. eigenvalues --	0.65443	0.65539	0.65588	0.65610	0.65777
Alpha virt. eigenvalues --	0.65878	0.65951	0.66034	0.66138	0.66271
Alpha virt. eigenvalues --	0.66315	0.66561	0.66706	0.66716	0.66876
Alpha virt. eigenvalues --	0.66888	0.67049	0.67050	0.67129	0.67163

Alpha virt. eigenvalues --	0.67183	0.67229	0.67385	0.67515	0.67565
Alpha virt. eigenvalues --	0.67598	0.67839	0.67961	0.68007	0.68284
Alpha virt. eigenvalues --	0.68350	0.68583	0.68734	0.68967	0.68982
Alpha virt. eigenvalues --	0.69097	0.69330	0.69415	0.69742	0.69762
Alpha virt. eigenvalues --	0.69937	0.70309	0.70398	0.70405	0.70426
Alpha virt. eigenvalues --	0.70717	0.71000	0.71480	0.71491	0.71717
Alpha virt. eigenvalues --	0.71784	0.71957	0.72107	0.72404	0.72436
Alpha virt. eigenvalues --	0.72566	0.72706	0.72751	0.72790	0.72945
Alpha virt. eigenvalues --	0.72955	0.73395	0.73455	0.73497	0.73601
Alpha virt. eigenvalues --	0.73816	0.74020	0.74200	0.74369	0.74392
Alpha virt. eigenvalues --	0.74436	0.74625	0.74674	0.74719	0.74806
Alpha virt. eigenvalues --	0.74889	0.74975	0.74987	0.75209	0.75379
Alpha virt. eigenvalues --	0.75627	0.76063	0.76299	0.76450	0.76745
Alpha virt. eigenvalues --	0.76906	0.77172	0.77364	0.78799	0.78901
Alpha virt. eigenvalues --	0.79177	0.79233	0.79341	0.79838	0.80305
Alpha virt. eigenvalues --	0.80561	0.80778	0.80830	0.80974	0.82054
Alpha virt. eigenvalues --	0.82094	0.82622	0.83164	0.83804	0.83941
Alpha virt. eigenvalues --	0.84138	0.84754	0.84865	0.85111	0.85311
Alpha virt. eigenvalues --	0.85462	0.85798	0.85977	0.85989	0.86067
Alpha virt. eigenvalues --	0.86079	0.86443	0.86726	0.86741	0.86892
Alpha virt. eigenvalues --	0.87263	0.87369	0.87570	0.87812	0.89201
Alpha virt. eigenvalues --	0.89336	0.89415	0.89451	0.89759	0.89883
Alpha virt. eigenvalues --	0.90016	0.90188	0.90337	0.90380	0.90485
Alpha virt. eigenvalues --	0.90539	0.90769	0.90796	0.91553	0.91672
Alpha virt. eigenvalues --	0.91966	0.92093	0.92441	0.92742	0.93343
Alpha virt. eigenvalues --	0.93386	0.94074	0.94512	0.94845	0.95179
Alpha virt. eigenvalues --	0.95527	0.95568	0.95728	0.96220	0.96365
Alpha virt. eigenvalues --	0.96697	0.97004	0.97105	0.97537	0.97613
Alpha virt. eigenvalues --	0.97805	0.98058	0.98386	0.98438	0.98503
Alpha virt. eigenvalues --	0.98655	0.98689	0.98993	0.99474	0.99515
Alpha virt. eigenvalues --	0.99593	0.99893	1.00390	1.00451	1.00734
Alpha virt. eigenvalues --	1.00850	1.01073	1.01075	1.01158	1.01671
Alpha virt. eigenvalues --	1.01713	1.01940	1.02395	1.02892	1.03264
Alpha virt. eigenvalues --	1.03465	1.04332	1.04458	1.05116	1.05259
Alpha virt. eigenvalues --	1.05378	1.05662	1.06336	1.06894	1.07420
Alpha virt. eigenvalues --	1.07655	1.08097	1.08199	1.08668	1.09002
Alpha virt. eigenvalues --	1.09591	1.09736	1.10142	1.10624	1.10959
Alpha virt. eigenvalues --	1.11017	1.11102	1.11177	1.11651	1.11800
Alpha virt. eigenvalues --	1.12934	1.13540	1.14188	1.14228	1.14490
Alpha virt. eigenvalues --	1.14667	1.14721	1.14753	1.15016	1.15482
Alpha virt. eigenvalues --	1.16356	1.16593	1.16600	1.16762	1.16989
Alpha virt. eigenvalues --	1.17539	1.17556	1.17740	1.17884	1.17990
Alpha virt. eigenvalues --	1.18035	1.18074	1.18145	1.18297	1.18324
Alpha virt. eigenvalues --	1.18404	1.18417	1.20028	1.20044	1.20297
Alpha virt. eigenvalues --	1.20498	1.20611	1.20726	1.21014	1.21176
Alpha virt. eigenvalues --	1.21524	1.22116	1.22232	1.22459	1.22770
Alpha virt. eigenvalues --	1.22930	1.23184	1.23270	1.23284	1.23573
Alpha virt. eigenvalues --	1.23684	1.23904	1.23923	1.24173	1.24420

Alpha virt. eigenvalues --	1.24591	1.25024	1.25113	1.25230	1.25471
Alpha virt. eigenvalues --	1.25618	1.25651	1.25865	1.26726	1.26763
Alpha virt. eigenvalues --	1.27000	1.27094	1.27172	1.27342	1.27481
Alpha virt. eigenvalues --	1.27770	1.28273	1.28719	1.29482	1.29569
Alpha virt. eigenvalues --	1.29691	1.30003	1.30047	1.30155	1.30488
Alpha virt. eigenvalues --	1.30491	1.30543	1.30619	1.31168	1.31952
Alpha virt. eigenvalues --	1.32185	1.32520	1.32837	1.32872	1.32923
Alpha virt. eigenvalues --	1.33202	1.33249	1.33912	1.34758	1.34839
Alpha virt. eigenvalues --	1.35078	1.35152	1.35273	1.35390	1.35497
Alpha virt. eigenvalues --	1.35844	1.36095	1.36104	1.36252	1.36489
Alpha virt. eigenvalues --	1.36530	1.36765	1.37087	1.37347	1.37615
Alpha virt. eigenvalues --	1.37995	1.38694	1.38982	1.39056	1.39214
Alpha virt. eigenvalues --	1.39545	1.39553	1.39597	1.39789	1.39926
Alpha virt. eigenvalues --	1.39986	1.39987	1.40045	1.40068	1.40085
Alpha virt. eigenvalues --	1.40139	1.40227	1.40257	1.40282	1.40331
Alpha virt. eigenvalues --	1.40412	1.40589	1.40613	1.40869	1.41071
Alpha virt. eigenvalues --	1.41128	1.41198	1.41462	1.41472	1.41636
Alpha virt. eigenvalues --	1.41879	1.42029	1.42267	1.42423	1.42599
Alpha virt. eigenvalues --	1.42867	1.42903	1.42945	1.43094	1.43148
Alpha virt. eigenvalues --	1.43337	1.43483	1.43600	1.43801	1.43824
Alpha virt. eigenvalues --	1.44822	1.45094	1.45266	1.45348	1.45396
Alpha virt. eigenvalues --	1.45531	1.45566	1.45740	1.45809	1.46080
Alpha virt. eigenvalues --	1.46216	1.46287	1.46681	1.47084	1.47257
Alpha virt. eigenvalues --	1.47439	1.47519	1.48075	1.48097	1.48684
Alpha virt. eigenvalues --	1.48798	1.48861	1.49691	1.49887	1.50015
Alpha virt. eigenvalues --	1.50113	1.50324	1.50623	1.50801	1.50955
Alpha virt. eigenvalues --	1.51210	1.51355	1.51584	1.51745	1.51774
Alpha virt. eigenvalues --	1.51903	1.51903	1.52166	1.52651	1.52813
Alpha virt. eigenvalues --	1.53260	1.53293	1.53598	1.53822	1.54183
Alpha virt. eigenvalues --	1.54597	1.54888	1.54962	1.54981	1.55176
Alpha virt. eigenvalues --	1.55238	1.55470	1.55607	1.55822	1.56035
Alpha virt. eigenvalues --	1.56198	1.56296	1.56325	1.56556	1.56603
Alpha virt. eigenvalues --	1.56694	1.56844	1.56956	1.57111	1.57480
Alpha virt. eigenvalues --	1.57520	1.57697	1.57857	1.57862	1.57972
Alpha virt. eigenvalues --	1.58173	1.58323	1.58962	1.58975	1.59570
Alpha virt. eigenvalues --	1.59763	1.59981	1.60153	1.60335	1.60738
Alpha virt. eigenvalues --	1.60846	1.60891	1.60919	1.60939	1.61123
Alpha virt. eigenvalues --	1.61241	1.61448	1.61471	1.61494	1.61518
Alpha virt. eigenvalues --	1.61649	1.61656	1.61691	1.61775	1.61922
Alpha virt. eigenvalues --	1.61937	1.62047	1.62165	1.62174	1.62413
Alpha virt. eigenvalues --	1.62442	1.62523	1.62749	1.62795	1.62848
Alpha virt. eigenvalues --	1.62946	1.63012	1.63190	1.63392	1.63620
Alpha virt. eigenvalues --	1.63742	1.63880	1.63896	1.63989	1.64020
Alpha virt. eigenvalues --	1.64383	1.64747	1.64796	1.64974	1.64994
Alpha virt. eigenvalues --	1.65283	1.65535	1.65567	1.66089	1.66452
Alpha virt. eigenvalues --	1.66553	1.66611	1.66832	1.67067	1.67187
Alpha virt. eigenvalues --	1.67280	1.67349	1.67528	1.67542	1.67799
Alpha virt. eigenvalues --	1.67875	1.68143	1.68401	1.68506	1.68993

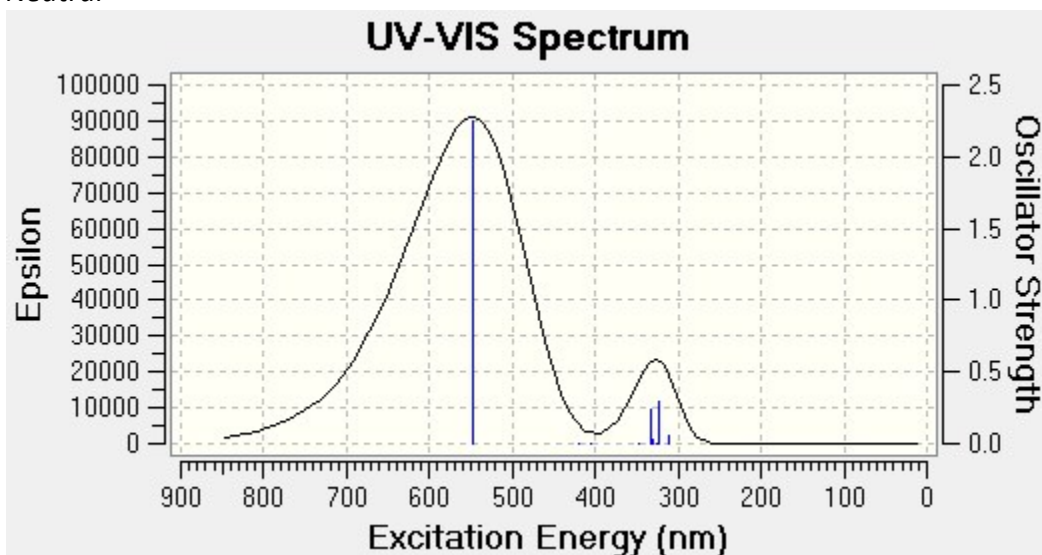
Alpha virt. eigenvalues --	1.69117	1.69247	1.69406	1.69805	1.69905
Alpha virt. eigenvalues --	1.70009	1.70114	1.70294	1.70437	1.70439
Alpha virt. eigenvalues --	1.70559	1.70575	1.70728	1.70778	1.70780
Alpha virt. eigenvalues --	1.71166	1.71400	1.71564	1.71764	1.71944
Alpha virt. eigenvalues --	1.71974	1.72116	1.72223	1.72498	1.72518
Alpha virt. eigenvalues --	1.72830	1.72988	1.73379	1.73668	1.73785
Alpha virt. eigenvalues --	1.73839	1.73951	1.74271	1.74393	1.74746
Alpha virt. eigenvalues --	1.74941	1.75039	1.75244	1.75421	1.75448
Alpha virt. eigenvalues --	1.75457	1.75556	1.75587	1.75713	1.76354
Alpha virt. eigenvalues --	1.76507	1.76710	1.77041	1.77137	1.77400
Alpha virt. eigenvalues --	1.77464	1.77584	1.77615	1.77726	1.77911
Alpha virt. eigenvalues --	1.78137	1.78502	1.78580	1.78790	1.78803
Alpha virt. eigenvalues --	1.79026	1.79197	1.79872	1.80027	1.80167
Alpha virt. eigenvalues --	1.80608	1.80749	1.80862	1.81158	1.81362
Alpha virt. eigenvalues --	1.81389	1.81505	1.81506	1.81775	1.81885
Alpha virt. eigenvalues --	1.82411	1.82488	1.82569	1.82736	1.82825
Alpha virt. eigenvalues --	1.82971	1.83171	1.83371	1.83433	1.83621
Alpha virt. eigenvalues --	1.83867	1.83946	1.84091	1.84138	1.84211
Alpha virt. eigenvalues --	1.84342	1.84793	1.84797	1.85178	1.85179
Alpha virt. eigenvalues --	1.85371	1.85405	1.85580	1.85749	1.85750
Alpha virt. eigenvalues --	1.86069	1.86083	1.86293	1.86446	1.86462
Alpha virt. eigenvalues --	1.86750	1.86914	1.86973	1.87477	1.87764
Alpha virt. eigenvalues --	1.87844	1.88137	1.88239	1.88610	1.89459
Alpha virt. eigenvalues --	1.90538	1.90646	1.91090	1.91097	1.91228
Alpha virt. eigenvalues --	1.91277	1.91895	1.92260	1.92591	1.93099
Alpha virt. eigenvalues --	1.93139	1.93294	1.93959	1.94006	1.95071
Alpha virt. eigenvalues --	1.95168	1.95620	1.96097	1.96174	1.96328
Alpha virt. eigenvalues --	1.96408	1.96611	1.96762	1.96886	1.97358
Alpha virt. eigenvalues --	1.97455	1.97996	1.98063	1.98230	1.98506
Alpha virt. eigenvalues --	1.98562	1.98698	1.98798	1.98800	1.98945
Alpha virt. eigenvalues --	1.98998	1.99014	1.99118	1.99120	1.99176
Alpha virt. eigenvalues --	1.99642	1.99762	2.00165	2.00817	2.01462
Alpha virt. eigenvalues --	2.01679	2.02038	2.02108	2.02131	2.02194
Alpha virt. eigenvalues --	2.02617	2.02728	2.03078	2.03512	2.03558
Alpha virt. eigenvalues --	2.03954	2.04950	2.04985	2.05211	2.05326
Alpha virt. eigenvalues --	2.05560	2.05599	2.06028	2.06034	2.06489
Alpha virt. eigenvalues --	2.06725	2.06982	2.06998	2.07678	2.07778
Alpha virt. eigenvalues --	2.07899	2.07916	2.08017	2.08175	2.08343
Alpha virt. eigenvalues --	2.08357	2.09087	2.10005	2.11025	2.11060
Alpha virt. eigenvalues --	2.11259	2.11427	2.11584	2.11691	2.11731
Alpha virt. eigenvalues --	2.11854	2.11964	2.12222	2.12869	2.12948
Alpha virt. eigenvalues --	2.13181	2.13242	2.13386	2.13425	2.14356
Alpha virt. eigenvalues --	2.14554	2.15169	2.15244	2.15986	2.16228
Alpha virt. eigenvalues --	2.16716	2.16731	2.16918	2.17025	2.17262
Alpha virt. eigenvalues --	2.17389	2.17744	2.17782	2.18193	2.18205
Alpha virt. eigenvalues --	2.18658	2.18672	2.20374	2.20385	2.20846
Alpha virt. eigenvalues --	2.20922	2.21209	2.21239	2.21527	2.21607
Alpha virt. eigenvalues --	2.21831	2.21990	2.22288	2.22335	2.24466

Alpha virt. eigenvalues --	2.24876	2.25500	2.25511	2.25641	2.25854
Alpha virt. eigenvalues --	2.26246	2.26801	2.27951	2.28696	2.28788
Alpha virt. eigenvalues --	2.28922	2.28988	2.29037	2.29293	2.29621
Alpha virt. eigenvalues --	2.30156	2.30334	2.30437	2.31006	2.31239
Alpha virt. eigenvalues --	2.31804	2.32064	2.32545	2.32841	2.32930
Alpha virt. eigenvalues --	2.33164	2.33484	2.34496	2.35128	2.35219
Alpha virt. eigenvalues --	2.35460	2.35750	2.36364	2.36576	2.37074
Alpha virt. eigenvalues --	2.37428	2.37841	2.38644	2.38847	2.38949
Alpha virt. eigenvalues --	2.39162	2.39164	2.39535	2.39935	2.40178
Alpha virt. eigenvalues --	2.40811	2.41028	2.41069	2.41212	2.41307
Alpha virt. eigenvalues --	2.41331	2.41405	2.41429	2.41566	2.41604
Alpha virt. eigenvalues --	2.42086	2.42258	2.42467	2.42486	2.42624
Alpha virt. eigenvalues --	2.42679	2.42734	2.42863	2.43083	2.43114
Alpha virt. eigenvalues --	2.43269	2.43369	2.43778	2.44101	2.44244
Alpha virt. eigenvalues --	2.44263	2.44395	2.44477	2.44557	2.44639
Alpha virt. eigenvalues --	2.44990	2.45072	2.45155	2.45564	2.45829
Alpha virt. eigenvalues --	2.46101	2.46254	2.46294	2.46496	2.46702
Alpha virt. eigenvalues --	2.46776	2.47169	2.47262	2.47304	2.47502
Alpha virt. eigenvalues --	2.47746	2.47835	2.48028	2.48142	2.48222
Alpha virt. eigenvalues --	2.48282	2.48390	2.48503	2.48672	2.48869
Alpha virt. eigenvalues --	2.48897	2.49723	2.50043	2.50241	2.50282
Alpha virt. eigenvalues --	2.50332	2.50640	2.51381	2.51880	2.52109
Alpha virt. eigenvalues --	2.52180	2.52349	2.52571	2.52770	2.53828
Alpha virt. eigenvalues --	2.54093	2.54456	2.54559	2.54746	2.54818
Alpha virt. eigenvalues --	2.54822	2.55136	2.55166	2.56051	2.56301
Alpha virt. eigenvalues --	2.56577	2.56670	2.56670	2.57011	2.57284
Alpha virt. eigenvalues --	2.58328	2.58561	2.58937	2.59485	2.60541
Alpha virt. eigenvalues --	2.61571	2.62660	2.66742	2.67315	2.67509
Alpha virt. eigenvalues --	2.67918	2.68170	2.68322	2.74638	2.75292
Alpha virt. eigenvalues --	2.76034	2.76491	2.78384	2.78412	2.87563
Alpha virt. eigenvalues --	2.87655	2.88094	2.88273	2.89501	2.89559
Alpha virt. eigenvalues --	2.91193	2.91338	2.91706	2.91753	2.92587
Alpha virt. eigenvalues --	2.92597	2.94259	2.94508	2.94915	2.95143
Alpha virt. eigenvalues --	2.96047	2.96072	2.97264	2.97369	2.97533
Alpha virt. eigenvalues --	2.97535	2.97842	2.97845	2.98034	2.98092
Alpha virt. eigenvalues --	2.98267	2.98298	2.98600	2.98604	3.00523
Alpha virt. eigenvalues --	3.00927	3.00986	3.01000	3.01197	3.01207
Alpha virt. eigenvalues --	3.01252	3.01300	3.01502	3.01502	3.01761
Alpha virt. eigenvalues --	3.01768	3.06406	3.06588	3.06730	3.06763
Alpha virt. eigenvalues --	3.07029	3.07032	3.07275	3.07284	3.07375
Alpha virt. eigenvalues --	3.07447	3.07453	3.07719	3.07721	3.07907
Alpha virt. eigenvalues --	3.08308	3.08570	3.09075	3.09075	3.09417
Alpha virt. eigenvalues --	3.09510	3.09730	3.09966	3.10060	3.10520
Alpha virt. eigenvalues --	3.10728	3.10821	3.10915	3.10954	3.11160
Alpha virt. eigenvalues --	3.11200	3.22832	3.22903	3.23042	3.23075
Alpha virt. eigenvalues --	3.23257	3.23259	3.24870	3.24921	3.25072
Alpha virt. eigenvalues --	3.25099	3.25318	3.25320	3.28013	3.28072
Alpha virt. eigenvalues --	3.28477	3.28500	3.29285	3.29287	3.35126

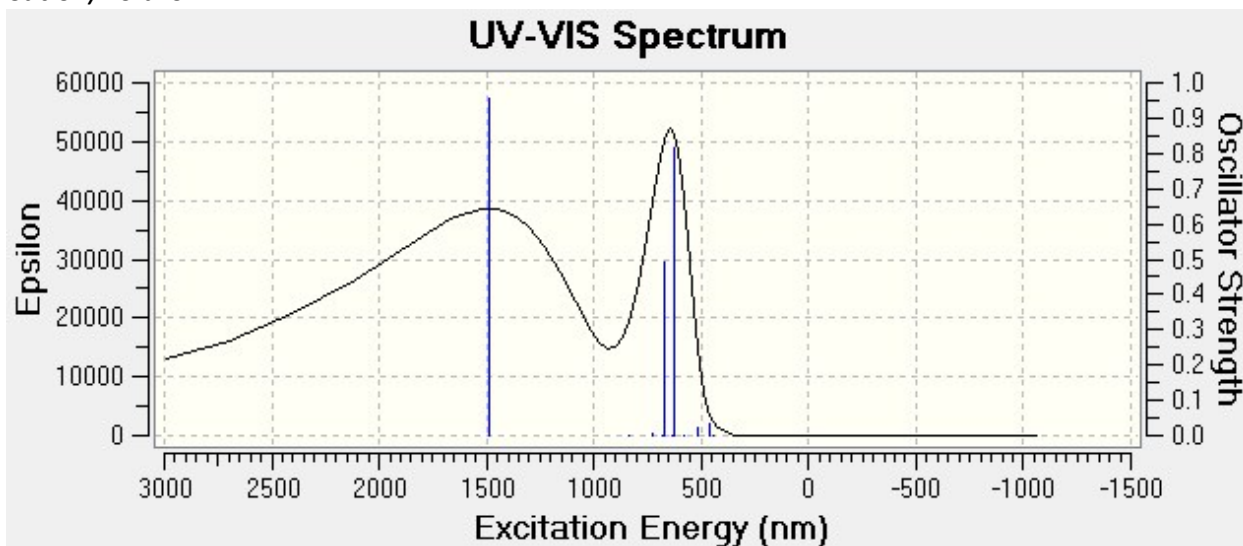
Alpha virt. eigenvalues -- 3.35160 3.35388 3.35487 3.35703 3.35759
Alpha virt. eigenvalues -- 3.35842 3.35894 3.36104 3.36110 3.36156
Alpha virt. eigenvalues -- 3.36181 3.37378 3.37455 3.37559 3.37832
Alpha virt. eigenvalues -- 3.38076 3.38169 3.38979 3.39887 3.40466
Alpha virt. eigenvalues -- 3.40671 3.41005 3.41076 3.46850 3.47366
Alpha virt. eigenvalues -- 3.48091 3.48827 3.49658 3.49890

Magenta UV-Vis Spectrum Epsilon/Oscillator Strength – N = 6

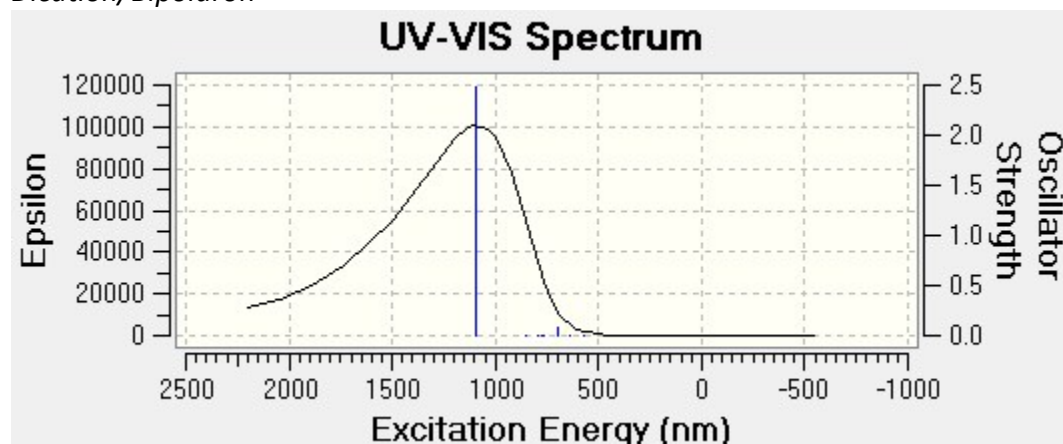
Neutral



Cation/Polaron



Dication/Bipolaron



Magenta Table of Excited States – N = 6

Neutral – 10 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	2.26	458.61	2.2493
2	2.95	419.79	0.0000
3	3.06	405.56	0.0000
4	3.56	348.13	0.0000
5	3.72	333.06	0.2398
6	3.76	329.69	0.0241
7	3.82	324.70	0.0000
8	3.83	324.09	0.2870
9	3.98	311.44	0.0001
10	3.99	310.79	0.0567

Cation/Polaron – 13 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	0.83	1490.47	0.9537
2	1.48	837.93	0.0000
3	1.70	731.08	0.0001
4	1.70	728.82	0.0056
5	1.82	682.63	0.0000
6	1.82	682.34	0.0013
7	1.84	674.06	0.4921
8	1.95	635.98	0.0000
9	1.97	629.19	0.8160
10	2.14	579.38	0.0000
11	2.41	515.46	0.0248
12	2.68	462.61	0.0323
13	2.82	439.73	0.0000
14			
15			

Dication/Bipolaron – 13 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	1.14	1090.97	2.4893
2	1.46	849.09	0.0000
3	1.46	848.88	0.0083
4	1.55	797.48	0.0001
5	1.60	773.13	0.0056
6	1.62	765.83	0.0001
7	1.78	695.20	0.0748
8	1.94	639.22	0.0000
9	2.17	570.73	0.0000
10	2.17	570.73	0.0091
11	2.17	570.27	0.0000
12	2.17	570.27	0.0000
13	2.18	569.10	0.0000

Yellow Cartesian Coordinate – N = 1

```

C      -5.11322  1.51088  1.11567
C      -5.24141  0.12968  0.96605
C      -3.89939  2.12052  0.79895
C      -4.16833 -0.6306  0.51198
H      -6.183   -0.36367  1.21302
C      -2.82471  1.36601  0.33561
H      -3.78679  3.20093  0.90623
C      -2.9395   -0.02859  0.18587
H      -4.28152 -1.71294  0.42166
H      -1.88591  1.85471  0.08155
C      -1.81758 -0.83186 -0.3045
C      -0.46323 -0.56422 -0.25171
S      -2.08856 -2.37637 -1.07103
C      0.34444  -1.60099 -0.83437
O      0.02896  0.57808  0.28721
C      -0.40334 -2.64306 -1.30952
O      1.69992  -1.59748 -0.89005
C      1.2619   0.4589   0.99555
H      -0.04081 -3.53938 -1.80434
C      2.30486  -0.33247 -1.15075
H      1.2674   1.28948  1.71464
H      1.27467  -0.48626  1.55772
C      2.50473  0.5337   0.10091
H      3.27776  -0.56018 -1.60799
H      1.70045  0.22343 -1.88316
C      2.80666  1.96506 -0.352
C      3.71022  0.08009  0.92984
H      3.05572  2.58542  0.53243
H      3.7027   1.96413 -1.00654
O      1.70675  2.50685 -1.03527

```


H	4.63649	0.21525	0.33593
H	3.80702	0.72562	1.82714
O	3.56389	-1.26283	1.30945
C	1.96221	3.80849	-1.50197
C	4.64041	-1.71261	2.09413
H	1.06126	4.15351	-2.02489
H	2.18234	4.50396	-0.67089
H	2.81556	3.82996	-2.20518
H	4.44684	-2.76258	2.34775
H	5.59924	-1.64727	1.54701
H	4.73627	-1.12953	3.02903
H	-5.953	2.10675	1.47621

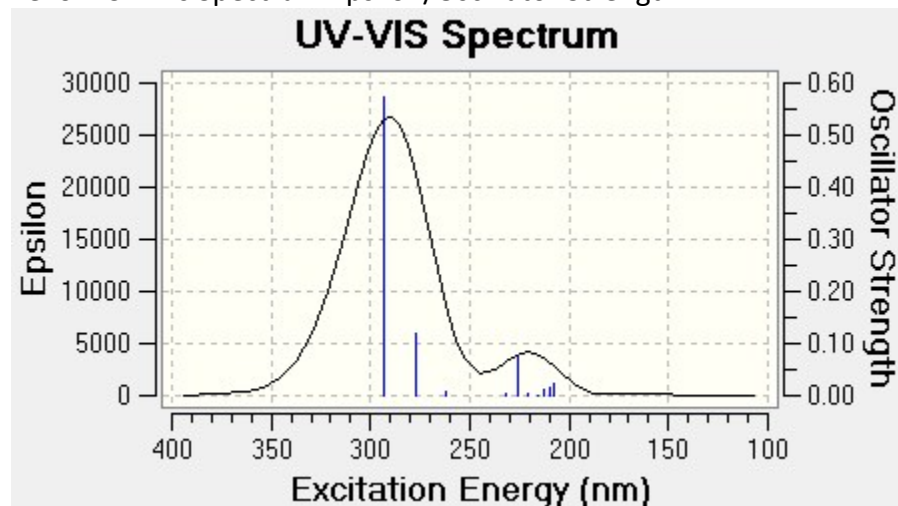
Yellow Energy Levels – N = 1

Alpha occ. eigenvalues --	-89.09520	-19.26280	-19.25919	-19.23688	-19.23651
Alpha occ. eigenvalues --	-10.30718	-10.30579	-10.29702	-10.29604	-10.29336
Alpha occ. eigenvalues --	-10.29328	-10.28230	-10.28221	-10.27675	-10.26785
Alpha occ. eigenvalues --	-10.26675	-10.26428	-10.25000	-10.24921	-10.24842
Alpha occ. eigenvalues --	-10.24723	-10.24644	-8.03916	-5.97787	-5.97431
Alpha occ. eigenvalues --	-5.97040	-1.11652	-1.09281	-1.07828	-1.07654
Alpha occ. eigenvalues --	-0.91687	-0.88476	-0.85844	-0.80288	-0.77453
Alpha occ. eigenvalues --	-0.76293	-0.75548	-0.74566	-0.71478	-0.70532
Alpha occ. eigenvalues --	-0.68224	-0.64591	-0.63900	-0.62864	-0.60123
Alpha occ. eigenvalues --	-0.59007	-0.57952	-0.54228	-0.53173	-0.52472
Alpha occ. eigenvalues --	-0.51964	-0.50313	-0.49813	-0.48726	-0.48599
Alpha occ. eigenvalues --	-0.47363	-0.47079	-0.46674	-0.46207	-0.45027
Alpha occ. eigenvalues --	-0.44008	-0.43774	-0.43065	-0.42571	-0.41164
Alpha occ. eigenvalues --	-0.40942	-0.40101	-0.39631	-0.39123	-0.37807
Alpha occ. eigenvalues --	-0.37210	-0.36937	-0.35987	-0.35046	-0.34557
Alpha occ. eigenvalues --	-0.33605	-0.33159	-0.32250	-0.30600	-0.28579
Alpha occ. eigenvalues --	-0.27871	-0.27083	-0.26851	-0.23150	-0.21784
Alpha virt. eigenvalues --	-0.03774	-0.00552	0.02505	0.04296	0.06141
Alpha virt. eigenvalues --	0.07340	0.07918	0.08251	0.08852	0.09807
Alpha virt. eigenvalues --	0.10390	0.10984	0.11552	0.12185	0.12466
Alpha virt. eigenvalues --	0.13160	0.13820	0.13929	0.14128	0.14353
Alpha virt. eigenvalues --	0.14922	0.15227	0.15660	0.16767	0.16892
Alpha virt. eigenvalues --	0.17254	0.17558	0.18637	0.19541	0.20292
Alpha virt. eigenvalues --	0.21546	0.21916	0.23152	0.23795	0.25543
Alpha virt. eigenvalues --	0.26332	0.27312	0.28173	0.29065	0.29245
Alpha virt. eigenvalues --	0.29733	0.30089	0.30825	0.33648	0.34891
Alpha virt. eigenvalues --	0.35587	0.42482	0.42699	0.43225	0.43502
Alpha virt. eigenvalues --	0.44486	0.45383	0.45916	0.46279	0.46906
Alpha virt. eigenvalues --	0.47147	0.47545	0.47727	0.48717	0.48831
Alpha virt. eigenvalues --	0.49411	0.49841	0.50457	0.50681	0.51281
Alpha virt. eigenvalues --	0.51559	0.51842	0.52359	0.52679	0.53075
Alpha virt. eigenvalues --	0.53405	0.53688	0.55131	0.55485	0.55860
Alpha virt. eigenvalues --	0.56064	0.56352	0.57330	0.59536	0.60130
Alpha virt. eigenvalues --	0.60330	0.60733	0.61558	0.62136	0.63159

Alpha virt. eigenvalues --	0.63297	0.63671	0.63873	0.64111	0.64828
Alpha virt. eigenvalues --	0.65316	0.65614	0.66027	0.66557	0.66678
Alpha virt. eigenvalues --	0.67650	0.67802	0.68438	0.68535	0.68712
Alpha virt. eigenvalues --	0.69432	0.69618	0.70111	0.71062	0.71640
Alpha virt. eigenvalues --	0.72033	0.73037	0.73914	0.74865	0.75519
Alpha virt. eigenvalues --	0.75795	0.76093	0.77328	0.77485	0.77851
Alpha virt. eigenvalues --	0.78774	0.81895	0.84952	0.85846	0.87069
Alpha virt. eigenvalues --	0.87740	0.88356	0.89019	0.90020	0.91330
Alpha virt. eigenvalues --	0.91618	0.92694	0.93193	0.93992	0.95635
Alpha virt. eigenvalues --	0.97631	0.97872	0.99364	0.99822	1.00716
Alpha virt. eigenvalues --	1.00856	1.01877	1.02348	1.02812	1.03847
Alpha virt. eigenvalues --	1.04927	1.05887	1.06940	1.07938	1.08761
Alpha virt. eigenvalues --	1.09688	1.11775	1.13259	1.13503	1.15320
Alpha virt. eigenvalues --	1.16502	1.18433	1.19884	1.20743	1.22026
Alpha virt. eigenvalues --	1.22465	1.23746	1.25218	1.27324	1.27883
Alpha virt. eigenvalues --	1.28543	1.30006	1.30328	1.31273	1.32784
Alpha virt. eigenvalues --	1.33860	1.34401	1.36071	1.36602	1.38440
Alpha virt. eigenvalues --	1.40298	1.41172	1.41384	1.41502	1.42436
Alpha virt. eigenvalues --	1.43986	1.44566	1.44660	1.45591	1.46479
Alpha virt. eigenvalues --	1.47639	1.48955	1.49543	1.50202	1.51114
Alpha virt. eigenvalues --	1.51733	1.52493	1.53376	1.54801	1.55970
Alpha virt. eigenvalues --	1.56087	1.57263	1.58420	1.58843	1.59337
Alpha virt. eigenvalues --	1.60134	1.60592	1.61960	1.62155	1.62588
Alpha virt. eigenvalues --	1.62997	1.63191	1.64052	1.64355	1.64981
Alpha virt. eigenvalues --	1.65329	1.65931	1.66514	1.67250	1.68615
Alpha virt. eigenvalues --	1.68704	1.69322	1.71316	1.71406	1.72087
Alpha virt. eigenvalues --	1.72750	1.73022	1.73558	1.73978	1.75395
Alpha virt. eigenvalues --	1.76291	1.76509	1.77703	1.78620	1.79280
Alpha virt. eigenvalues --	1.79659	1.80449	1.81475	1.82431	1.82829
Alpha virt. eigenvalues --	1.83273	1.84297	1.84934	1.85847	1.86322
Alpha virt. eigenvalues --	1.86807	1.87171	1.87868	1.88977	1.89373
Alpha virt. eigenvalues --	1.90143	1.92896	1.94653	1.95505	1.96279
Alpha virt. eigenvalues --	1.98083	1.98691	1.99683	1.99726	2.00351
Alpha virt. eigenvalues --	2.00907	2.02140	2.02502	2.03408	2.03576
Alpha virt. eigenvalues --	2.06340	2.07116	2.07801	2.10054	2.10348
Alpha virt. eigenvalues --	2.12811	2.13077	2.14654	2.16366	2.17932
Alpha virt. eigenvalues --	2.18369	2.19864	2.21463	2.22749	2.24370
Alpha virt. eigenvalues --	2.26498	2.27899	2.28318	2.30698	2.32717
Alpha virt. eigenvalues --	2.34747	2.36027	2.38880	2.39857	2.40221
Alpha virt. eigenvalues --	2.42613	2.43180	2.43930	2.44872	2.45400
Alpha virt. eigenvalues --	2.45751	2.46346	2.47837	2.48049	2.48746
Alpha virt. eigenvalues --	2.49688	2.50079	2.51325	2.53415	2.55553
Alpha virt. eigenvalues --	2.56392	2.58288	2.60843	2.65746	2.67329
Alpha virt. eigenvalues --	2.70005	2.72281	2.76888	2.82946	2.86048
Alpha virt. eigenvalues --	2.92004	2.94205	2.95344	2.98745	2.99198
Alpha virt. eigenvalues --	3.00193	3.02936	3.05319	3.08315	3.09009
Alpha virt. eigenvalues --	3.11186	3.13012	3.14426	3.24536	3.26647
Alpha virt. eigenvalues --	3.32235	3.37531	3.37653	3.41887	3.43559

Alpha virt. eigenvalues -- 3.51711 3.60013

Yellow UV-Vis Spectrum Epsilon/Oscillator Strength – N = 1



Yellow Table of 10 Lowest Excited States – N = 1

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	4.23	292.82	0.5742
2	4.48	276.86	0.1193
3	4.74	261.72	0.0081
4	5.34	232.37	0.0020
5	5.49	225.72	0.0755
6	5.62	220.78	0.0028
7	5.74	216.18	0.0002
8	5.82	212.89	0.0130
9	5.92	209.44	0.0145
10	5.96	207.97	0.0239

Yellow Cartesian Coordinate – N = 2

C -4.05012 1.90126 -0.30068
C -4.28311 0.55837 -0.07554
C -3.09881 -0.24606 -0.13751
C -1.95685 0.47466 -0.43155
S -2.35519 2.16225 -0.61216
O -3.07736 -1.58723 0.05695
O -5.52042 0.07815 0.19477
C -5.83208 -1.21522 -0.3228
H -6.92542 -1.23184 -0.42741
H -5.3855 -1.33225 -1.32096
C -3.94521 -2.0913 1.07297
H -3.47906 -3.02288 1.42165
H -3.97874 -1.38302 1.9136
C -5.37112 -2.36507 0.5798
C -6.2767 -2.54002 1.8024

H	-7.29295	-2.83138	1.46868
H	-5.89424	-3.37124	2.43014
C	-5.46502	-3.66747	-0.21998
H	-5.23081	-4.52377	0.44389
H	-6.50664	-3.81065	-0.57427
O	-6.32821	-1.35205	2.54791
O	-4.57996	-3.63607	-1.30874
C	-7.12227	-1.48454	3.70109
H	-7.10103	-0.52208	4.22768
H	-8.1701	-1.73169	3.44854
H	-6.735	-2.27111	4.37519
C	-4.65641	-4.80424	-2.08807
H	-3.94109	-4.69667	-2.91322
H	-4.39372	-5.7038	-1.50109
H	-5.66925	-4.9494	-2.50773
C	-4.99615	3.0166	-0.32394
C	-6.23189	2.93781	0.34629
C	-4.68931	4.20687	-1.00916
C	-7.12104	4.00877	0.3215
H	-6.48685	2.0314	0.89194
C	-5.5791	5.27594	-1.02384
H	-3.74487	4.2924	-1.55056
C	-6.8032	5.18313	-0.3607
H	-8.07251	3.92489	0.84975
H	-5.31585	6.18637	-1.56483
C	-0.57804	0.01367	-0.56397
C	-0.27432	-1.3333	-0.8395
C	0.50275	0.90438	-0.43082
C	1.04111	-1.75768	-0.95932
H	-1.08253	-2.05218	-0.95759
C	1.8175	0.48194	-0.5632
H	0.31368	1.95723	-0.21114
C	2.12172	-0.86722	-0.8258
H	1.2317	-2.81471	-1.15644
H	2.62578	1.20305	-0.45979
C	3.50175	-1.32541	-0.96588
C	4.66698	-0.74991	-0.49332
S	3.87326	-2.80707	-1.81284
C	5.84666	-1.50046	-0.82481
O	4.66882	0.41564	0.19763
C	5.56412	-2.63805	-1.52975
O	7.11093	-1.1666	-0.46329
C	5.64665	0.5408	1.22947
H	6.27329	-3.3673	-1.91047
C	7.42122	0.22453	-0.52374
H	5.23316	1.27513	1.93423
H	5.75556	-0.41959	1.75424
C	7.02064	1.00715	0.73515

H	8.50914	0.27803	-0.66806
H	6.93343	0.67439	-1.4016
C	7.03935	2.50038	0.39656
C	8.02254	0.81098	1.8771
H	6.85316	3.08906	1.31733
H	8.04882	2.78383	0.03309
O	6.07243	2.79578	-0.57696
H	9.00296	1.23625	1.5824
H	7.68316	1.37517	2.77029
O	8.15281	-0.55247	2.18231
C	6.08333	4.15479	-0.93828
C	9.04643	-0.77532	3.24474
H	5.30817	4.2988	-1.70153
H	5.86103	4.80828	-0.07435
H	7.06073	4.45813	-1.35767
H	9.08949	-1.85823	3.41705
H	10.06263	-0.40986	3.00661
H	8.70965	-0.27756	4.17318
H	-7.50291	6.02006	-0.37496

Yellow Energy Levels – N = 2

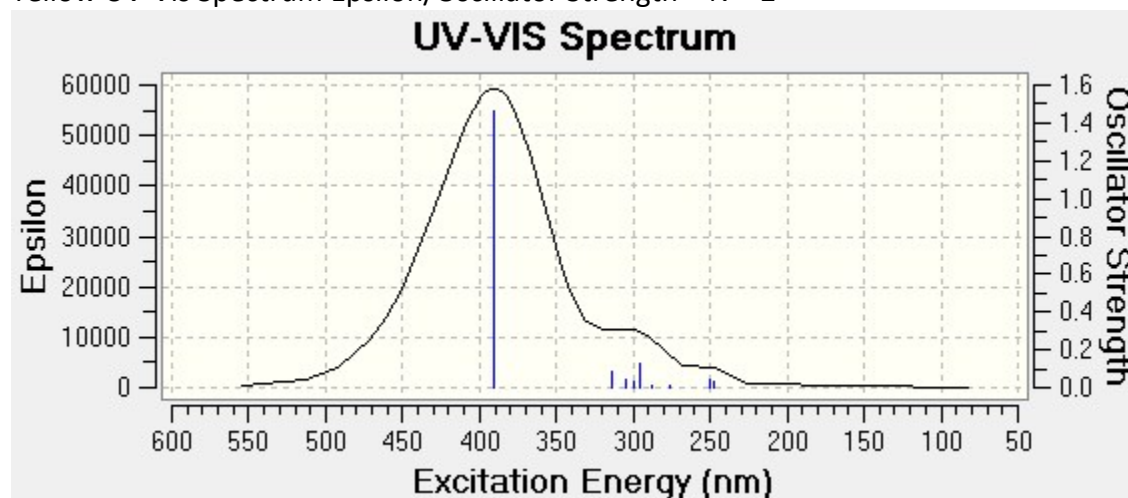
Alpha occ. eigenvalues -- -89.09524 -89.09506 -19.26450 -19.26427 -19.26329
Alpha occ. eigenvalues -- -19.25899 -19.23717 -19.23705 -19.23649 -19.23641
Alpha occ. eigenvalues -- -10.30988 -10.30928 -10.30747 -10.30571 -10.29810
Alpha occ. eigenvalues -- -10.29792 -10.29716 -10.29584 -10.29381 -10.29372
Alpha occ. eigenvalues -- -10.29313 -10.29306 -10.28237 -10.28221 -10.28208
Alpha occ. eigenvalues -- -10.28188 -10.28018 -10.27939 -10.27710 -10.26880
Alpha occ. eigenvalues -- -10.26739 -10.26713 -10.26701 -10.26519 -10.26417
Alpha occ. eigenvalues -- -10.25063 -10.25049 -10.25007 -10.24963 -10.24874
Alpha occ. eigenvalues -- -10.24783 -10.24769 -10.24737 -10.24696 -8.03939
Alpha occ. eigenvalues -- -8.03903 -5.97817 -5.97775 -5.97461 -5.97419
Alpha occ. eigenvalues -- -5.97040 -5.97025 -1.12014 -1.11667 -1.09584
Alpha occ. eigenvalues -- -1.09287 -1.07860 -1.07804 -1.07682 -1.07628
Alpha occ. eigenvalues -- -0.92360 -0.91645 -0.89189 -0.88253 -0.85992
Alpha occ. eigenvalues -- -0.85833 -0.82278 -0.79670 -0.77817 -0.77483
Alpha occ. eigenvalues -- -0.76893 -0.76380 -0.75856 -0.75226 -0.74591
Alpha occ. eigenvalues -- -0.74541 -0.71861 -0.71473 -0.71465 -0.69656
Alpha occ. eigenvalues -- -0.68295 -0.68192 -0.65636 -0.64630 -0.64553
Alpha occ. eigenvalues -- -0.63546 -0.62854 -0.62597 -0.60392 -0.60088
Alpha occ. eigenvalues -- -0.59296 -0.58416 -0.58162 -0.57815 -0.54504
Alpha occ. eigenvalues -- -0.54031 -0.53348 -0.53157 -0.52726 -0.52252
Alpha occ. eigenvalues -- -0.52018 -0.51728 -0.51116 -0.50419 -0.50058
Alpha occ. eigenvalues -- -0.49002 -0.48800 -0.48716 -0.48614 -0.47919
Alpha occ. eigenvalues -- -0.47644 -0.47360 -0.47301 -0.47097 -0.46904
Alpha occ. eigenvalues -- -0.46428 -0.46208 -0.45330 -0.44992 -0.44905
Alpha occ. eigenvalues -- -0.44161 -0.44054 -0.43955 -0.43397 -0.43001
Alpha occ. eigenvalues -- -0.42791 -0.42466 -0.41866 -0.41430 -0.41132
Alpha occ. eigenvalues -- -0.40574 -0.40193 -0.40082 -0.40025 -0.39548

Alpha occ. eigenvalues --	-0.39398	-0.39193	-0.38578	-0.38056	-0.37844
Alpha occ. eigenvalues --	-0.37438	-0.36943	-0.36665	-0.36260	-0.36016
Alpha occ. eigenvalues --	-0.35211	-0.34713	-0.34640	-0.34503	-0.33783
Alpha occ. eigenvalues --	-0.33437	-0.33281	-0.33132	-0.32514	-0.32247
Alpha occ. eigenvalues --	-0.31474	-0.30302	-0.29801	-0.27964	-0.27858
Alpha occ. eigenvalues --	-0.27682	-0.27117	-0.27059	-0.26976	-0.26896
Alpha occ. eigenvalues --	-0.23567	-0.23157	-0.22964	-0.19906	
Alpha virt. eigenvalues --	-0.05972	-0.02463	-0.00675	-0.00571	0.01249
Alpha virt. eigenvalues --	0.03532	0.03956	0.04970	0.06063	0.06257
Alpha virt. eigenvalues --	0.07084	0.07396	0.07657	0.07890	0.08078
Alpha virt. eigenvalues --	0.08521	0.09049	0.09811	0.09837	0.09917
Alpha virt. eigenvalues --	0.10361	0.10552	0.11090	0.11411	0.11599
Alpha virt. eigenvalues --	0.11963	0.12258	0.12738	0.13006	0.13198
Alpha virt. eigenvalues --	0.13466	0.13620	0.13884	0.13980	0.14087
Alpha virt. eigenvalues --	0.14169	0.14361	0.14391	0.14818	0.14885
Alpha virt. eigenvalues --	0.14935	0.15229	0.15264	0.15829	0.16639
Alpha virt. eigenvalues --	0.16717	0.16880	0.17037	0.17365	0.17448
Alpha virt. eigenvalues --	0.17652	0.17845	0.18439	0.19289	0.19443
Alpha virt. eigenvalues --	0.19684	0.20333	0.20659	0.20943	0.21598
Alpha virt. eigenvalues --	0.21969	0.22462	0.23125	0.23178	0.23738
Alpha virt. eigenvalues --	0.23817	0.24923	0.25601	0.25728	0.26358
Alpha virt. eigenvalues --	0.26784	0.26856	0.28120	0.28239	0.28392
Alpha virt. eigenvalues --	0.28787	0.29067	0.29343	0.29499	0.29832
Alpha virt. eigenvalues --	0.30107	0.30740	0.31598	0.32221	0.33477
Alpha virt. eigenvalues --	0.34050	0.34306	0.35296	0.35819	0.38854
Alpha virt. eigenvalues --	0.40132	0.42399	0.42639	0.42814	0.42961
Alpha virt. eigenvalues --	0.43195	0.43500	0.43998	0.44359	0.44880
Alpha virt. eigenvalues --	0.45187	0.45536	0.45589	0.46091	0.46248
Alpha virt. eigenvalues --	0.46658	0.46820	0.46945	0.46969	0.47204
Alpha virt. eigenvalues --	0.47348	0.47615	0.47765	0.48077	0.48464
Alpha virt. eigenvalues --	0.48800	0.49120	0.49387	0.49451	0.49769
Alpha virt. eigenvalues --	0.49811	0.50073	0.50280	0.50374	0.50517
Alpha virt. eigenvalues --	0.50738	0.50987	0.51405	0.51495	0.51681
Alpha virt. eigenvalues --	0.52218	0.52290	0.52371	0.52634	0.52945
Alpha virt. eigenvalues --	0.53123	0.53216	0.53487	0.53623	0.53867
Alpha virt. eigenvalues --	0.54419	0.54710	0.55266	0.55479	0.55532
Alpha virt. eigenvalues --	0.55875	0.55911	0.56062	0.56377	0.56778
Alpha virt. eigenvalues --	0.57150	0.57676	0.58681	0.58944	0.59608
Alpha virt. eigenvalues --	0.60059	0.60307	0.60739	0.61088	0.61338
Alpha virt. eigenvalues --	0.61759	0.62031	0.62162	0.62287	0.62791
Alpha virt. eigenvalues --	0.63139	0.63297	0.63534	0.63753	0.63850
Alpha virt. eigenvalues --	0.63928	0.63968	0.64133	0.64607	0.64817
Alpha virt. eigenvalues --	0.65030	0.65311	0.65401	0.65501	0.65879
Alpha virt. eigenvalues --	0.66121	0.66429	0.66540	0.66721	0.66990
Alpha virt. eigenvalues --	0.67259	0.67464	0.67800	0.67893	0.68442
Alpha virt. eigenvalues --	0.68504	0.68536	0.68715	0.68801	0.69001
Alpha virt. eigenvalues --	0.69302	0.69520	0.69964	0.70106	0.70407
Alpha virt. eigenvalues --	0.70570	0.71072	0.71427	0.71736	0.71923

Alpha virt. eigenvalues --	0.72211	0.72868	0.73337	0.73608	0.73926
Alpha virt. eigenvalues --	0.74130	0.74687	0.75173	0.75327	0.75356
Alpha virt. eigenvalues --	0.75699	0.76039	0.76191	0.76369	0.76794
Alpha virt. eigenvalues --	0.77079	0.77369	0.77595	0.78003	0.78496
Alpha virt. eigenvalues --	0.79383	0.81686	0.81906	0.82160	0.84346
Alpha virt. eigenvalues --	0.84974	0.85542	0.86184	0.86988	0.87361
Alpha virt. eigenvalues --	0.87537	0.87986	0.88223	0.88640	0.88865
Alpha virt. eigenvalues --	0.89166	0.90059	0.91121	0.91481	0.91726
Alpha virt. eigenvalues --	0.91959	0.92130	0.92911	0.93087	0.93731
Alpha virt. eigenvalues --	0.93994	0.94373	0.95124	0.95701	0.96444
Alpha virt. eigenvalues --	0.96839	0.97793	0.98358	0.98862	0.99148
Alpha virt. eigenvalues --	0.99683	0.99915	1.00243	1.00463	1.00516
Alpha virt. eigenvalues --	1.00694	1.00923	1.01855	1.02209	1.02333
Alpha virt. eigenvalues --	1.02955	1.03447	1.03800	1.04288	1.05015
Alpha virt. eigenvalues --	1.05842	1.06223	1.06301	1.06767	1.07603
Alpha virt. eigenvalues --	1.07983	1.08296	1.08954	1.09929	1.10598
Alpha virt. eigenvalues --	1.11509	1.12576	1.12718	1.13366	1.13748
Alpha virt. eigenvalues --	1.13961	1.14209	1.16160	1.16500	1.16944
Alpha virt. eigenvalues --	1.18471	1.18792	1.19553	1.19696	1.20194
Alpha virt. eigenvalues --	1.21060	1.21532	1.21950	1.22323	1.23037
Alpha virt. eigenvalues --	1.23718	1.23790	1.24251	1.25199	1.25728
Alpha virt. eigenvalues --	1.27044	1.27628	1.27816	1.27908	1.28436
Alpha virt. eigenvalues --	1.28582	1.30046	1.30113	1.30657	1.31181
Alpha virt. eigenvalues --	1.32370	1.32665	1.32978	1.33528	1.34010
Alpha virt. eigenvalues --	1.34289	1.34822	1.35285	1.35934	1.36350
Alpha virt. eigenvalues --	1.36683	1.37006	1.38288	1.39571	1.39614
Alpha virt. eigenvalues --	1.40233	1.40697	1.40946	1.41181	1.41201
Alpha virt. eigenvalues --	1.41425	1.41464	1.41519	1.42315	1.42741
Alpha virt. eigenvalues --	1.43429	1.44367	1.44531	1.44748	1.44936
Alpha virt. eigenvalues --	1.45274	1.45779	1.46133	1.46665	1.47319
Alpha virt. eigenvalues --	1.47580	1.48220	1.48792	1.49216	1.49351
Alpha virt. eigenvalues --	1.49516	1.50271	1.50643	1.51113	1.51686
Alpha virt. eigenvalues --	1.52165	1.52403	1.52472	1.53048	1.53351
Alpha virt. eigenvalues --	1.54217	1.54502	1.55499	1.55920	1.56018
Alpha virt. eigenvalues --	1.56407	1.57195	1.57270	1.57735	1.58506
Alpha virt. eigenvalues --	1.58640	1.58711	1.58903	1.59223	1.59721
Alpha virt. eigenvalues --	1.60175	1.60705	1.61048	1.61725	1.61885
Alpha virt. eigenvalues --	1.61992	1.62271	1.62501	1.62719	1.62862
Alpha virt. eigenvalues --	1.63269	1.63469	1.64193	1.64212	1.64579
Alpha virt. eigenvalues --	1.64765	1.64925	1.65133	1.65254	1.65513
Alpha virt. eigenvalues --	1.65760	1.66033	1.66284	1.66862	1.67083
Alpha virt. eigenvalues --	1.67780	1.68205	1.68431	1.68713	1.69111
Alpha virt. eigenvalues --	1.69428	1.69761	1.70210	1.70832	1.71218
Alpha virt. eigenvalues --	1.71629	1.71898	1.72173	1.72311	1.72606
Alpha virt. eigenvalues --	1.72714	1.72994	1.73376	1.73807	1.74141
Alpha virt. eigenvalues --	1.74754	1.75441	1.75641	1.76061	1.76609
Alpha virt. eigenvalues --	1.76953	1.77245	1.77554	1.77930	1.78306
Alpha virt. eigenvalues --	1.78376	1.78994	1.79231	1.79334	1.79750

Alpha virt. eigenvalues --	1.80052	1.80334	1.81134	1.81413	1.82041
Alpha virt. eigenvalues --	1.82465	1.82808	1.83230	1.83387	1.84033
Alpha virt. eigenvalues --	1.84537	1.84619	1.85289	1.85543	1.85989
Alpha virt. eigenvalues --	1.86739	1.86831	1.86974	1.87031	1.87138
Alpha virt. eigenvalues --	1.87776	1.87919	1.88381	1.88677	1.89613
Alpha virt. eigenvalues --	1.90135	1.90281	1.91912	1.92246	1.93111
Alpha virt. eigenvalues --	1.93607	1.94244	1.94675	1.95197	1.95506
Alpha virt. eigenvalues --	1.96913	1.97292	1.97995	1.98447	1.98664
Alpha virt. eigenvalues --	1.99568	1.99634	1.99785	2.00069	2.00252
Alpha virt. eigenvalues --	2.00448	2.00467	2.01372	2.01566	2.01819
Alpha virt. eigenvalues --	2.02605	2.03132	2.03412	2.03815	2.04555
Alpha virt. eigenvalues --	2.05449	2.06632	2.06916	2.07152	2.07477
Alpha virt. eigenvalues --	2.08548	2.09150	2.09585	2.10214	2.10531
Alpha virt. eigenvalues --	2.11074	2.11871	2.12858	2.13079	2.13338
Alpha virt. eigenvalues --	2.14259	2.14778	2.14997	2.17209	2.17619
Alpha virt. eigenvalues --	2.17956	2.18182	2.18582	2.19707	2.20085
Alpha virt. eigenvalues --	2.21961	2.22264	2.22571	2.22811	2.23264
Alpha virt. eigenvalues --	2.23763	2.25741	2.26776	2.27458	2.27807
Alpha virt. eigenvalues --	2.28070	2.28572	2.29539	2.30621	2.30764
Alpha virt. eigenvalues --	2.32854	2.33750	2.34722	2.34927	2.36075
Alpha virt. eigenvalues --	2.36874	2.39345	2.39756	2.40271	2.40407
Alpha virt. eigenvalues --	2.40741	2.41892	2.42500	2.42778	2.43254
Alpha virt. eigenvalues --	2.43309	2.43586	2.43928	2.44170	2.44992
Alpha virt. eigenvalues --	2.45391	2.45504	2.45854	2.45958	2.46505
Alpha virt. eigenvalues --	2.47319	2.47938	2.48025	2.48135	2.48845
Alpha virt. eigenvalues --	2.49398	2.49700	2.50085	2.50179	2.50252
Alpha virt. eigenvalues --	2.51151	2.51929	2.53400	2.53969	2.54587
Alpha virt. eigenvalues --	2.55707	2.56316	2.56413	2.58277	2.58346
Alpha virt. eigenvalues --	2.59594	2.60878	2.65810	2.67936	2.68576
Alpha virt. eigenvalues --	2.69058	2.69930	2.71354	2.72369	2.73364
Alpha virt. eigenvalues --	2.76117	2.77601	2.80810	2.82846	2.84798
Alpha virt. eigenvalues --	2.86360	2.91944	2.92548	2.93634	2.94869
Alpha virt. eigenvalues --	2.95467	2.96422	2.98648	2.98850	2.99126
Alpha virt. eigenvalues --	2.99234	3.00229	3.00314	3.02937	3.03019
Alpha virt. eigenvalues --	3.05348	3.06634	3.08297	3.08339	3.08973
Alpha virt. eigenvalues --	3.09025	3.11151	3.11242	3.13207	3.14203
Alpha virt. eigenvalues --	3.14521	3.15030	3.24558	3.24601	3.26681
Alpha virt. eigenvalues --	3.26723	3.32254	3.32458	3.37532	3.37593
Alpha virt. eigenvalues --	3.37648	3.37686	3.40946	3.41885	3.43489
Alpha virt. eigenvalues --	3.44473	3.49251	3.51893	3.54878	3.60068

Yellow UV-Vis Spectrum Epsilon/Oscillator Strength – N = 2



Yellow Table of 10 Lowest Excited States – N = 2

Excited state	Energy (eV)	Wavelength (nm)	Oscillator Strength
1	3.17	390.74	1.4634
2	3.95	313.51	0.0883
3	4.07	304.27	0.0476
4	4.14	299.55	0.0279
5	4.19	295.99	0.1264
6	4.31	287.53	0.0100
7	4.49	276.37	0.0058
8	4.96	249.79	0.0417
9	5.01	247.55	0.0301
10	5.02	247.02	0.0269

Yellow Cartesian Coordinate – N = 3

C	-0.51647	0.74699	-0.14466
C	0.29835	1.88192	0.03417
C	1.67798	1.60565	-0.07198
C	1.96097	0.24513	-0.28098
S	0.47804	-0.66875	-0.38527
O	2.65162	2.52763	0.00233
O	-0.22681	3.08665	0.28948
C	0.53281	3.96794	1.13173
H	-0.20886	4.65106	1.56399
H	0.98829	3.38297	1.94296
C	2.36423	3.81353	-0.56708
H	3.34321	4.23321	-0.83035
H	1.78066	3.67549	-1.48842
C	1.61636	4.75016	0.38689
C	1.03498	5.9031	-0.4361
H	0.58786	6.65252	0.2468
H	1.85157	6.41431	-0.98551

C	2.55122	5.37058	1.42915
H	3.28167	6.02882	0.91819
H	1.96641	6.0124	2.11915
O	0.07169	5.41511	-1.3314
O	3.21217	4.35837	2.14087
C	-0.47438	6.43447	-2.13442
H	-1.21096	5.96798	-2.80034
H	-0.97921	7.20561	-1.52423
H	0.30138	6.92965	-2.74688
C	4.06256	4.87511	3.13672
H	4.53186	4.02186	3.64206
H	4.8529	5.51549	2.70413
H	3.5025	5.47027	3.88113
C	-1.94287	0.64281	-0.12257
C	-2.78221	1.78883	-0.1335
C	-2.57839	-0.62599	-0.11203
C	-4.15152	1.66008	-0.12917
H	-2.33686	2.77958	-0.15964
C	-3.94769	-0.75335	-0.09621
H	-1.97536	-1.53558	-0.10868
C	-4.78655	0.3924	-0.10199
H	-4.75555	2.56869	-0.13994
H	-4.39495	-1.74368	-0.09259
C	-6.21843	0.28671	-0.10174
C	-7.02901	-0.83226	0.1205
S	-7.21873	1.69647	-0.36397
C	-8.42046	-0.54858	0.03207
O	-6.51128	-2.04047	0.386
C	-8.69475	0.78989	-0.21863
O	-9.39908	-1.4687	0.16589
C	-7.26799	-2.90768	1.24321
C	-9.98688	1.44599	-0.38405
C	-9.13986	-2.75235	-0.41213
H	-6.52691	-3.59314	1.67349
H	-7.71084	-2.31437	2.05527
C	-8.36646	-3.69122	0.52099
C	-10.08331	2.67267	-1.06873
C	-11.16244	0.88049	0.14742
H	-10.12729	-3.17175	-0.64482
H	-8.5841	-2.62292	-1.35223
C	-9.27521	-4.31493	1.58454
C	-7.80441	-4.84532	-0.31332
C	-11.30875	3.30993	-1.21944
H	-9.19023	3.12515	-1.50402
C	-12.38557	1.5246	-0.00855
H	-11.10778	-0.06098	0.68981
H	-10.0158	-4.974	1.08929
H	-8.67329	-4.95691	2.25978

O	-9.92322	-3.30751	2.31514
H	-7.34104	-5.59427	0.3594
H	-8.63461	-5.35734	-0.84151
O	-6.86256	-4.36248	-1.23436
C	-12.46732	2.73843	-0.69101
H	-11.36041	4.25689	-1.75831
H	-13.28494	1.07389	0.41367
C	-10.75021	-3.83215	3.326
C	-6.34046	-5.38621	-2.04687
H	-13.42953	3.23825	-0.81057
H	-11.21083	-2.98334	3.84668
H	-11.54825	-4.47235	2.90727
H	-10.17277	-4.43038	4.05472
H	-5.61987	-4.92488	-2.73371
H	-5.82215	-6.15683	-1.44712
H	-7.13289	-5.88203	-2.6373
C	3.2321	-0.40689	-0.43699
C	3.30532	-1.75623	-0.8617
C	4.45471	0.25491	-0.16748
C	4.51496	-2.39538	-1.01464
H	2.39249	-2.31099	-1.08509
C	5.66685	-0.38902	-0.31802
H	4.43952	1.28779	0.17023
C	5.7384	-1.73451	-0.7486
H	4.51708	-3.43692	-1.33923
H	6.58632	0.15162	-0.10851
C	7.00121	-2.41481	-0.92522
C	8.27404	-2.04126	-0.49756
S	7.08187	-3.95228	-1.75872
C	9.2901	-2.98062	-0.86763
O	8.49502	-0.90515	0.18677
C	8.78281	-4.05774	-1.54609
O	10.60717	-2.86022	-0.58076
C	9.57737	-0.90675	1.12487
H	9.34534	-4.89493	-1.95001
C	11.14554	-1.54507	-0.73288
H	9.3331	-0.10825	1.83751
H	9.59006	-1.86431	1.66412
C	10.95314	-0.65379	0.50297
H	12.21575	-1.68703	-0.93399
H	10.68788	-1.06097	-1.60842
C	11.14304	0.80557	0.08127
C	12.00544	-0.94001	1.57914
H	11.1043	1.45644	0.9776
H	12.15126	0.93147	-0.36414
O	10.15333	1.1799	-0.84084
H	13.00758	-0.66886	1.19093
H	11.81873	-0.2989	2.46498

O	11.96802	-2.29548	1.93842
C	10.32428	2.50018	-1.29561
C	12.91434	-2.60965	2.93092
H	9.51967	2.70779	-2.01223
H	10.26208	3.22825	-0.46586
H	11.29861	2.6343	-1.80098
H	12.81723	-3.68037	3.15016
H	13.9457	-2.4057	2.58875
H	12.73792	-2.03564	3.85942

Yellow Energy Levels – N = 3

Neutral

Alpha occ. eigenvalues -- -89.09557 -89.09484 -89.09483 -19.26512 -19.26470
Alpha occ. eigenvalues -- -19.26452 -19.26418 -19.26364 -19.25881 -19.23722
Alpha occ. eigenvalues -- -19.23713 -19.23693 -19.23673 -19.23645 -19.23639
Alpha occ. eigenvalues -- -10.31028 -10.31007 -10.30958 -10.30943 -10.30772
Alpha occ. eigenvalues -- -10.30560 -10.29832 -10.29827 -10.29806 -10.29776
Alpha occ. eigenvalues -- -10.29728 -10.29569 -10.29383 -10.29377 -10.29359
Alpha occ. eigenvalues -- -10.29357 -10.29309 -10.29305 -10.28237 -10.28224
Alpha occ. eigenvalues -- -10.28207 -10.28205 -10.28195 -10.28189 -10.28036
Alpha occ. eigenvalues -- -10.28035 -10.28020 -10.27976 -10.27719 -10.26888
Alpha occ. eigenvalues -- -10.26816 -10.26813 -10.26720 -10.26712 -10.26674
Alpha occ. eigenvalues -- -10.26532 -10.26510 -10.26416 -10.25102 -10.25093
Alpha occ. eigenvalues -- -10.25074 -10.24995 -10.24971 -10.24955 -10.24886
Alpha occ. eigenvalues -- -10.24837 -10.24832 -10.24781 -10.24715 -10.24682
Alpha occ. eigenvalues -- -10.24663 -8.03970 -8.03903 -8.03882 -5.97848
Alpha occ. eigenvalues -- -5.97782 -5.97754 -5.97492 -5.97426 -5.97398
Alpha occ. eigenvalues -- -5.97072 -5.97003 -5.97001 -1.12038 -1.12034
Alpha occ. eigenvalues -- -1.11679 -1.09606 -1.09600 -1.09287 -1.07864
Alpha occ. eigenvalues -- -1.07837 -1.07806 -1.07686 -1.07658 -1.07630
Alpha occ. eigenvalues -- -0.92495 -0.92208 -0.91628 -0.89481 -0.88728
Alpha occ. eigenvalues -- -0.88179 -0.86034 -0.85963 -0.85830 -0.82891
Alpha occ. eigenvalues -- -0.81310 -0.79470 -0.77923 -0.77718 -0.77520
Alpha occ. eigenvalues -- -0.77294 -0.76551 -0.76317 -0.75922 -0.75573
Alpha occ. eigenvalues -- -0.75142 -0.74586 -0.74566 -0.74541 -0.72170
Alpha occ. eigenvalues -- -0.71694 -0.71517 -0.71469 -0.70883 -0.69297
Alpha occ. eigenvalues -- -0.68319 -0.68262 -0.68190 -0.66281 -0.64637
Alpha occ. eigenvalues -- -0.64624 -0.64547 -0.64118 -0.63731 -0.63310
Alpha occ. eigenvalues -- -0.62866 -0.62180 -0.60569 -0.60196 -0.60068
Alpha occ. eigenvalues -- -0.59376 -0.58686 -0.58431 -0.58133 -0.58033
Alpha occ. eigenvalues -- -0.57750 -0.54565 -0.54367 -0.53961 -0.53389
Alpha occ. eigenvalues -- -0.53308 -0.53158 -0.52798 -0.52339 -0.52250
Alpha occ. eigenvalues -- -0.52057 -0.51880 -0.51657 -0.51290 -0.51134
Alpha occ. eigenvalues -- -0.50353 -0.50150 -0.49080 -0.49036 -0.48789
Alpha occ. eigenvalues -- -0.48771 -0.48753 -0.48701 -0.48085 -0.48065
Alpha occ. eigenvalues -- -0.47644 -0.47553 -0.47383 -0.47321 -0.47139
Alpha occ. eigenvalues -- -0.47073 -0.46956 -0.46626 -0.46391 -0.46194

Alpha occ. eigenvalues --	-0.45512	-0.45118	-0.45025	-0.44965	-0.44845
Alpha occ. eigenvalues --	-0.44342	-0.44075	-0.44060	-0.44028	-0.43428
Alpha occ. eigenvalues --	-0.43263	-0.43054	-0.42802	-0.42652	-0.42413
Alpha occ. eigenvalues --	-0.42194	-0.41559	-0.41358	-0.41289	-0.41125
Alpha occ. eigenvalues --	-0.40435	-0.40239	-0.40161	-0.40134	-0.40069
Alpha occ. eigenvalues --	-0.39955	-0.39701	-0.39362	-0.39281	-0.39207
Alpha occ. eigenvalues --	-0.38923	-0.38285	-0.38196	-0.37862	-0.37763
Alpha occ. eigenvalues --	-0.37555	-0.37196	-0.36866	-0.36528	-0.36332
Alpha occ. eigenvalues --	-0.36181	-0.36054	-0.35259	-0.34893	-0.34683
Alpha occ. eigenvalues --	-0.34627	-0.34537	-0.34469	-0.33862	-0.33601
Alpha occ. eigenvalues --	-0.33371	-0.33311	-0.33250	-0.33121	-0.32572
Alpha occ. eigenvalues --	-0.32494	-0.32290	-0.31933	-0.30745	-0.30202
Alpha occ. eigenvalues --	-0.30034	-0.29170	-0.27953	-0.27904	-0.27852
Alpha occ. eigenvalues --	-0.27390	-0.27119	-0.27089	-0.27054	-0.27026
Alpha occ. eigenvalues --	-0.26936	-0.26902	-0.23899	-0.23441	-0.23214
Alpha occ. eigenvalues --	-0.23160	-0.21285	-0.19205		
Alpha virt. eigenvalues --	-0.06779	-0.04533	-0.01927	-0.00725	-0.00588
Alpha virt. eigenvalues --	-0.00558	0.00717	0.03045	0.03461	0.03768
Alpha virt. eigenvalues --	0.04152	0.05494	0.06028	0.06199	0.06341
Alpha virt. eigenvalues --	0.07066	0.07146	0.07391	0.07653	0.07771
Alpha virt. eigenvalues --	0.07848	0.08021	0.08386	0.08556	0.09195
Alpha virt. eigenvalues --	0.09645	0.09824	0.09865	0.09906	0.10129
Alpha virt. eigenvalues --	0.10342	0.10483	0.10613	0.11111	0.11390
Alpha virt. eigenvalues --	0.11475	0.11634	0.11903	0.12134	0.12574
Alpha virt. eigenvalues --	0.12707	0.12976	0.13084	0.13220	0.13325
Alpha virt. eigenvalues --	0.13570	0.13599	0.13824	0.13973	0.14025
Alpha virt. eigenvalues --	0.14051	0.14129	0.14193	0.14267	0.14392
Alpha virt. eigenvalues --	0.14435	0.14789	0.14861	0.14922	0.14934
Alpha virt. eigenvalues --	0.14957	0.15164	0.15264	0.15306	0.15854
Alpha virt. eigenvalues --	0.16601	0.16676	0.16718	0.16899	0.16965
Alpha virt. eigenvalues --	0.17271	0.17353	0.17440	0.17499	0.17647
Alpha virt. eigenvalues --	0.17769	0.17900	0.18492	0.19223	0.19369
Alpha virt. eigenvalues --	0.19418	0.19584	0.19756	0.20340	0.20521
Alpha virt. eigenvalues --	0.20726	0.20887	0.21326	0.21634	0.21998
Alpha virt. eigenvalues --	0.22346	0.22697	0.23118	0.23151	0.23179
Alpha virt. eigenvalues --	0.23716	0.23759	0.23834	0.24621	0.25198
Alpha virt. eigenvalues --	0.25587	0.25698	0.25752	0.26386	0.26428
Alpha virt. eigenvalues --	0.26804	0.26858	0.27993	0.28261	0.28286
Alpha virt. eigenvalues --	0.28443	0.28491	0.28672	0.28783	0.29290
Alpha virt. eigenvalues --	0.29342	0.29629	0.29771	0.29992	0.30108
Alpha virt. eigenvalues --	0.30513	0.31352	0.31737	0.32130	0.32460
Alpha virt. eigenvalues --	0.33516	0.34033	0.34048	0.34372	0.34649
Alpha virt. eigenvalues --	0.35462	0.35957	0.37948	0.38946	0.40220
Alpha virt. eigenvalues --	0.41529	0.42367	0.42574	0.42732	0.42837
Alpha virt. eigenvalues --	0.42927	0.43041	0.43305	0.43586	0.43899
Alpha virt. eigenvalues --	0.44120	0.44184	0.44541	0.44845	0.45270
Alpha virt. eigenvalues --	0.45400	0.45553	0.45580	0.45903	0.46102
Alpha virt. eigenvalues --	0.46237	0.46552	0.46660	0.46825	0.46908

Alpha virt. eigenvalues --	0.46988	0.47000	0.47062	0.47184	0.47287
Alpha virt. eigenvalues --	0.47576	0.47643	0.47752	0.47864	0.48119
Alpha virt. eigenvalues --	0.48610	0.48742	0.48847	0.49161	0.49257
Alpha virt. eigenvalues --	0.49318	0.49517	0.49626	0.49730	0.49892
Alpha virt. eigenvalues --	0.49920	0.50108	0.50129	0.50224	0.50343
Alpha virt. eigenvalues --	0.50579	0.50661	0.50780	0.50898	0.51329
Alpha virt. eigenvalues --	0.51441	0.51572	0.51712	0.52008	0.52107
Alpha virt. eigenvalues --	0.52282	0.52447	0.52550	0.52702	0.52884
Alpha virt. eigenvalues --	0.52986	0.53048	0.53261	0.53317	0.53522
Alpha virt. eigenvalues --	0.53558	0.53812	0.54022	0.54076	0.54371
Alpha virt. eigenvalues --	0.54767	0.55197	0.55293	0.55394	0.55530
Alpha virt. eigenvalues --	0.55572	0.55796	0.55958	0.56029	0.56194
Alpha virt. eigenvalues --	0.56378	0.56418	0.56870	0.57192	0.57304
Alpha virt. eigenvalues --	0.57892	0.58489	0.58712	0.59291	0.59458
Alpha virt. eigenvalues --	0.59976	0.60060	0.60257	0.60447	0.60696
Alpha virt. eigenvalues --	0.61134	0.61278	0.61573	0.61652	0.61942
Alpha virt. eigenvalues --	0.62094	0.62168	0.62206	0.62334	0.62697
Alpha virt. eigenvalues --	0.63080	0.63273	0.63284	0.63549	0.63654
Alpha virt. eigenvalues --	0.63815	0.63818	0.63869	0.63918	0.63935
Alpha virt. eigenvalues --	0.64036	0.64130	0.64452	0.64651	0.64834
Alpha virt. eigenvalues --	0.64976	0.65076	0.65244	0.65380	0.65413
Alpha virt. eigenvalues --	0.65552	0.65841	0.65911	0.66278	0.66380
Alpha virt. eigenvalues --	0.66483	0.66593	0.66680	0.66809	0.67025
Alpha virt. eigenvalues --	0.67342	0.67407	0.67643	0.67807	0.67887
Alpha virt. eigenvalues --	0.68057	0.68219	0.68479	0.68523	0.68581
Alpha virt. eigenvalues --	0.68660	0.68740	0.68773	0.69011	0.69239
Alpha virt. eigenvalues --	0.69286	0.69549	0.69769	0.69911	0.70149
Alpha virt. eigenvalues --	0.70304	0.70506	0.70584	0.70791	0.71113
Alpha virt. eigenvalues --	0.71383	0.71455	0.71710	0.71767	0.72087
Alpha virt. eigenvalues --	0.72221	0.72906	0.73058	0.73378	0.73624
Alpha virt. eigenvalues --	0.73899	0.74062	0.74123	0.74185	0.74547
Alpha virt. eigenvalues --	0.74942	0.75093	0.75287	0.75378	0.75447
Alpha virt. eigenvalues --	0.75734	0.76017	0.76120	0.76163	0.76459
Alpha virt. eigenvalues --	0.76559	0.76869	0.76931	0.77144	0.77302
Alpha virt. eigenvalues --	0.77636	0.77898	0.78042	0.78202	0.78730
Alpha virt. eigenvalues --	0.80261	0.81059	0.81857	0.81983	0.82182
Alpha virt. eigenvalues --	0.82697	0.83993	0.84488	0.84963	0.85310
Alpha virt. eigenvalues --	0.85929	0.86382	0.86986	0.87102	0.87397
Alpha virt. eigenvalues --	0.87551	0.87796	0.88038	0.88177	0.88577
Alpha virt. eigenvalues --	0.88627	0.88830	0.89242	0.89334	0.90064
Alpha virt. eigenvalues --	0.90951	0.91154	0.91446	0.91710	0.91895
Alpha virt. eigenvalues --	0.92053	0.92115	0.92281	0.92858	0.93139
Alpha virt. eigenvalues --	0.93439	0.93759	0.94108	0.94357	0.95013
Alpha virt. eigenvalues --	0.95062	0.95538	0.95729	0.96054	0.96735
Alpha virt. eigenvalues --	0.97117	0.97611	0.97947	0.98183	0.98372
Alpha virt. eigenvalues --	0.99058	0.99219	0.99496	0.99604	0.99970
Alpha virt. eigenvalues --	1.00053	1.00398	1.00462	1.00469	1.00642
Alpha virt. eigenvalues --	1.00819	1.00969	1.01094	1.01476	1.01924

Alpha virt. eigenvalues --	1.02472	1.02509	1.02733	1.03104	1.03498
Alpha virt. eigenvalues --	1.03991	1.04259	1.04969	1.05433	1.05755
Alpha virt. eigenvalues --	1.05910	1.06140	1.06410	1.06643	1.06850
Alpha virt. eigenvalues --	1.07223	1.07332	1.07911	1.08201	1.08648
Alpha virt. eigenvalues --	1.09282	1.09760	1.09998	1.10982	1.11420
Alpha virt. eigenvalues --	1.12043	1.12256	1.12469	1.13032	1.13575
Alpha virt. eigenvalues --	1.13788	1.14066	1.14283	1.14851	1.16091
Alpha virt. eigenvalues --	1.16201	1.16510	1.16924	1.16994	1.18471
Alpha virt. eigenvalues --	1.18934	1.19154	1.19473	1.19718	1.19755
Alpha virt. eigenvalues --	1.19933	1.20334	1.21198	1.21296	1.21735
Alpha virt. eigenvalues --	1.22175	1.22335	1.22802	1.23279	1.23599
Alpha virt. eigenvalues --	1.23765	1.23983	1.24054	1.24789	1.25283
Alpha virt. eigenvalues --	1.25627	1.26295	1.26942	1.27321	1.27660
Alpha virt. eigenvalues --	1.27796	1.27836	1.28220	1.28360	1.28585
Alpha virt. eigenvalues --	1.29688	1.29835	1.30207	1.30383	1.30679
Alpha virt. eigenvalues --	1.31321	1.31818	1.32179	1.32547	1.32933
Alpha virt. eigenvalues --	1.33177	1.33374	1.34050	1.34165	1.34519
Alpha virt. eigenvalues --	1.34758	1.34974	1.35123	1.35733	1.36063
Alpha virt. eigenvalues --	1.36353	1.36546	1.36878	1.36946	1.37529
Alpha virt. eigenvalues --	1.38542	1.39201	1.39409	1.39735	1.40004
Alpha virt. eigenvalues --	1.40479	1.40623	1.40934	1.41004	1.41178
Alpha virt. eigenvalues --	1.41197	1.41282	1.41366	1.41411	1.41470
Alpha virt. eigenvalues --	1.41484	1.41551	1.42284	1.42692	1.42848
Alpha virt. eigenvalues --	1.43374	1.44091	1.44320	1.44461	1.44844
Alpha virt. eigenvalues --	1.44900	1.44969	1.45149	1.45544	1.45776
Alpha virt. eigenvalues --	1.46089	1.46317	1.46731	1.47286	1.47380
Alpha virt. eigenvalues --	1.47512	1.48155	1.48478	1.48611	1.48962
Alpha virt. eigenvalues --	1.49098	1.49413	1.49730	1.50052	1.50155
Alpha virt. eigenvalues --	1.50524	1.50798	1.51215	1.51681	1.51849
Alpha virt. eigenvalues --	1.52134	1.52331	1.52455	1.52617	1.52747
Alpha virt. eigenvalues --	1.53047	1.53332	1.54128	1.54303	1.54513
Alpha virt. eigenvalues --	1.55012	1.55690	1.55923	1.56006	1.56087
Alpha virt. eigenvalues --	1.56458	1.57152	1.57212	1.57267	1.57521
Alpha virt. eigenvalues --	1.58236	1.58401	1.58585	1.58681	1.58750
Alpha virt. eigenvalues --	1.58855	1.59151	1.59327	1.59564	1.59814
Alpha virt. eigenvalues --	1.60445	1.60536	1.60749	1.61118	1.61641
Alpha virt. eigenvalues --	1.61801	1.61923	1.61964	1.62170	1.62456
Alpha virt. eigenvalues --	1.62691	1.62768	1.62803	1.63221	1.63311
Alpha virt. eigenvalues --	1.63466	1.63631	1.63914	1.64128	1.64194
Alpha virt. eigenvalues --	1.64255	1.64565	1.64763	1.65037	1.65098
Alpha virt. eigenvalues --	1.65266	1.65329	1.65583	1.65720	1.65771
Alpha virt. eigenvalues --	1.65983	1.66169	1.66323	1.66627	1.66885
Alpha virt. eigenvalues --	1.67044	1.67383	1.67674	1.68098	1.68307
Alpha virt. eigenvalues --	1.68385	1.68907	1.68949	1.69211	1.69469
Alpha virt. eigenvalues --	1.69767	1.69871	1.70127	1.70337	1.70827
Alpha virt. eigenvalues --	1.71062	1.71364	1.71648	1.71928	1.72066
Alpha virt. eigenvalues --	1.72196	1.72260	1.72401	1.72543	1.72748
Alpha virt. eigenvalues --	1.72958	1.73127	1.73326	1.73649	1.73893

Alpha virt. eigenvalues --	1.74311	1.74654	1.74917	1.75241	1.75639
Alpha virt. eigenvalues --	1.75768	1.76119	1.76250	1.76507	1.76965
Alpha virt. eigenvalues --	1.77169	1.77315	1.77598	1.77819	1.77889
Alpha virt. eigenvalues --	1.78334	1.78435	1.78504	1.78826	1.79071
Alpha virt. eigenvalues --	1.79269	1.79396	1.79474	1.79751	1.79951
Alpha virt. eigenvalues --	1.80216	1.80532	1.80597	1.81168	1.81632
Alpha virt. eigenvalues --	1.81882	1.82339	1.82432	1.82761	1.83055
Alpha virt. eigenvalues --	1.83203	1.83593	1.84015	1.84189	1.84537
Alpha virt. eigenvalues --	1.84658	1.84842	1.85463	1.85503	1.85912
Alpha virt. eigenvalues --	1.86303	1.86551	1.86828	1.86927	1.86996
Alpha virt. eigenvalues --	1.87096	1.87276	1.87375	1.87742	1.87765
Alpha virt. eigenvalues --	1.88250	1.88405	1.88634	1.88850	1.89143
Alpha virt. eigenvalues --	1.89508	1.89974	1.90980	1.91308	1.91860
Alpha virt. eigenvalues --	1.92329	1.92645	1.93167	1.93757	1.94023
Alpha virt. eigenvalues --	1.94445	1.94578	1.94877	1.95316	1.95617
Alpha virt. eigenvalues --	1.96246	1.97250	1.97383	1.97788	1.98087
Alpha virt. eigenvalues --	1.98351	1.98491	1.98975	1.99123	1.99657
Alpha virt. eigenvalues --	1.99767	1.99806	2.00069	2.00241	2.00261
Alpha virt. eigenvalues --	2.00392	2.00470	2.00608	2.00812	2.01268
Alpha virt. eigenvalues --	2.01552	2.01766	2.01908	2.02808	2.03076
Alpha virt. eigenvalues --	2.03321	2.03560	2.03851	2.04237	2.04818
Alpha virt. eigenvalues --	2.05476	2.05681	2.06418	2.06836	2.07114
Alpha virt. eigenvalues --	2.07161	2.07445	2.08099	2.08816	2.09203
Alpha virt. eigenvalues --	2.09256	2.09513	2.09774	2.10328	2.10706
Alpha virt. eigenvalues --	2.10885	2.11644	2.12076	2.12319	2.12875
Alpha virt. eigenvalues --	2.13117	2.13130	2.13443	2.14369	2.14515
Alpha virt. eigenvalues --	2.14893	2.15488	2.16458	2.17139	2.17638
Alpha virt. eigenvalues --	2.17763	2.18027	2.18163	2.18343	2.18603
Alpha virt. eigenvalues --	2.19343	2.19909	2.20220	2.21961	2.22098
Alpha virt. eigenvalues --	2.22340	2.22553	2.22624	2.23149	2.23369
Alpha virt. eigenvalues --	2.23622	2.24053	2.25225	2.26369	2.26825
Alpha virt. eigenvalues --	2.27451	2.27461	2.27714	2.27936	2.28568
Alpha virt. eigenvalues --	2.28809	2.29442	2.29754	2.30559	2.30731
Alpha virt. eigenvalues --	2.30806	2.32902	2.33703	2.33906	2.34753
Alpha virt. eigenvalues --	2.34832	2.35083	2.36099	2.37210	2.37609
Alpha virt. eigenvalues --	2.39570	2.39745	2.40172	2.40429	2.40651
Alpha virt. eigenvalues --	2.40827	2.41290	2.41796	2.41995	2.42479
Alpha virt. eigenvalues --	2.42665	2.43128	2.43209	2.43299	2.43401
Alpha virt. eigenvalues --	2.43645	2.43906	2.43941	2.44131	2.44377
Alpha virt. eigenvalues --	2.44981	2.45392	2.45450	2.45504	2.45885
Alpha virt. eigenvalues --	2.45947	2.46112	2.46485	2.47335	2.47710
Alpha virt. eigenvalues --	2.48023	2.48089	2.48163	2.48221	2.48937
Alpha virt. eigenvalues --	2.49292	2.49563	2.49783	2.50093	2.50131
Alpha virt. eigenvalues --	2.50195	2.50263	2.50449	2.51208	2.51745
Alpha virt. eigenvalues --	2.52002	2.53426	2.53904	2.54141	2.54416
Alpha virt. eigenvalues --	2.55326	2.55924	2.56343	2.56389	2.56474
Alpha virt. eigenvalues --	2.58274	2.58307	2.58384	2.59459	2.60143
Alpha virt. eigenvalues --	2.60957	2.65792	2.67838	2.68541	2.68944

Alpha virt. eigenvalues --	2.69119	2.69768	2.69898	2.70527	2.72207
Alpha virt. eigenvalues --	2.72369	2.73125	2.75301	2.76127	2.77067
Alpha virt. eigenvalues --	2.77681	2.79471	2.82066	2.82778	2.84167
Alpha virt. eigenvalues --	2.85961	2.86448	2.91911	2.92347	2.92656
Alpha virt. eigenvalues --	2.93573	2.94456	2.95172	2.95414	2.96300
Alpha virt. eigenvalues --	2.96795	2.98672	2.98720	2.98905	2.99139
Alpha virt. eigenvalues --	2.99183	2.99261	3.00248	3.00301	3.00404
Alpha virt. eigenvalues --	3.02925	3.03042	3.03051	3.05356	3.06510
Alpha virt. eigenvalues --	3.06727	3.08264	3.08333	3.08367	3.08947
Alpha virt. eigenvalues --	3.09006	3.09047	3.11108	3.11188	3.11299
Alpha virt. eigenvalues --	3.13334	3.14168	3.14392	3.14689	3.14845
Alpha virt. eigenvalues --	3.15369	3.24535	3.24583	3.24641	3.26687
Alpha virt. eigenvalues --	3.26705	3.26757	3.32228	3.32400	3.32492
Alpha virt. eigenvalues --	3.37536	3.37591	3.37625	3.37632	3.37703
Alpha virt. eigenvalues --	3.37717	3.40622	3.41235	3.41841	3.43403
Alpha virt. eigenvalues --	3.44162	3.44792	3.48858	3.49947	3.51958
Alpha virt. eigenvalues --	3.53978	3.55832	3.60061		

Cation/Polaron

Alpha occ. eigenvalues --	-89.12740	-89.11761	-89.11364	-19.29470	-19.29373
Alpha occ. eigenvalues --	-19.28712	-19.28360	-19.28170	-19.27247	-19.24709
Alpha occ. eigenvalues --	-19.24693	-19.24540	-19.24484	-19.24403	-19.24307
Alpha occ. eigenvalues --	-10.34980	-10.34934	-10.33923	-10.33313	-10.33269
Alpha occ. eigenvalues --	-10.32985	-10.32917	-10.32410	-10.31597	-10.31561
Alpha occ. eigenvalues --	-10.31163	-10.31124	-10.31035	-10.31010	-10.30922
Alpha occ. eigenvalues --	-10.30565	-10.30447	-10.30445	-10.30359	-10.30351
Alpha occ. eigenvalues --	-10.30226	-10.30207	-10.30160	-10.30069	-10.30040
Alpha occ. eigenvalues --	-10.30021	-10.30019	-10.29138	-10.29031	-10.29018
Alpha occ. eigenvalues --	-10.28939	-10.28871	-10.28857	-10.28765	-10.28526
Alpha occ. eigenvalues --	-10.28235	-10.28041	-10.28014	-10.27992	-10.27879
Alpha occ. eigenvalues --	-10.27724	-10.27645	-10.27626	-10.27500	-10.27374
Alpha occ. eigenvalues --	-10.27243	-10.26698	-10.26349	-10.26333	-10.26225
Alpha occ. eigenvalues --	-10.26115	-8.07203	-8.06195	-8.05775	-6.01090
Alpha occ. eigenvalues --	-6.00720	-6.00259	-6.00078	-5.99713	-5.99650
Alpha occ. eigenvalues --	-5.99286	-5.99275	-5.98883	-1.14909	-1.13987
Alpha occ. eigenvalues --	-1.13392	-1.12453	-1.11504	-1.10840	-1.08871
Alpha occ. eigenvalues --	-1.08675	-1.08674	-1.08534	-1.08478	-1.08341
Alpha occ. eigenvalues --	-0.96277	-0.94944	-0.94005	-0.92441	-0.91440
Alpha occ. eigenvalues --	-0.90207	-0.87658	-0.87218	-0.86901	-0.86124
Alpha occ. eigenvalues --	-0.84115	-0.81994	-0.80714	-0.80371	-0.79981
Alpha occ. eigenvalues --	-0.79305	-0.78920	-0.78292	-0.77970	-0.77554
Alpha occ. eigenvalues --	-0.77285	-0.75574	-0.75371	-0.75251	-0.74443
Alpha occ. eigenvalues --	-0.73562	-0.72926	-0.72864	-0.72628	-0.71692
Alpha occ. eigenvalues --	-0.69576	-0.69325	-0.69126	-0.68844	-0.66704
Alpha occ. eigenvalues --	-0.66625	-0.66070	-0.65512	-0.65386	-0.65212
Alpha occ. eigenvalues --	-0.64538	-0.64439	-0.63011	-0.61940	-0.61856
Alpha occ. eigenvalues --	-0.61216	-0.60851	-0.60756	-0.60462	-0.59802
Alpha occ. eigenvalues --	-0.59743	-0.56878	-0.56236	-0.55700	-0.55226

Alpha occ. eigenvalues --	-0.54817	-0.54648	-0.54468	-0.54201	-0.54102
Alpha occ. eigenvalues --	-0.53791	-0.53429	-0.52933	-0.52883	-0.52685
Alpha occ. eigenvalues --	-0.51878	-0.51796	-0.50881	-0.50625	-0.50364
Alpha occ. eigenvalues --	-0.50060	-0.49828	-0.49647	-0.49512	-0.49458
Alpha occ. eigenvalues --	-0.49373	-0.49273	-0.48847	-0.48722	-0.48507
Alpha occ. eigenvalues --	-0.48327	-0.48303	-0.48098	-0.47808	-0.47703
Alpha occ. eigenvalues --	-0.47431	-0.47328	-0.47010	-0.46833	-0.46670
Alpha occ. eigenvalues --	-0.46420	-0.46233	-0.45834	-0.45597	-0.45483
Alpha occ. eigenvalues --	-0.45219	-0.44851	-0.44816	-0.44656	-0.44173
Alpha occ. eigenvalues --	-0.43968	-0.43603	-0.43315	-0.42934	-0.42631
Alpha occ. eigenvalues --	-0.42366	-0.42286	-0.42095	-0.41835	-0.41299
Alpha occ. eigenvalues --	-0.41183	-0.41046	-0.41012	-0.40842	-0.40667
Alpha occ. eigenvalues --	-0.40616	-0.40531	-0.40402	-0.40032	-0.39712
Alpha occ. eigenvalues --	-0.39366	-0.38953	-0.38578	-0.38332	-0.38133
Alpha occ. eigenvalues --	-0.37778	-0.37550	-0.37304	-0.37084	-0.36589
Alpha occ. eigenvalues --	-0.36018	-0.35754	-0.35511	-0.35459	-0.35131
Alpha occ. eigenvalues --	-0.34893	-0.34769	-0.34723	-0.34466	-0.34253
Alpha occ. eigenvalues --	-0.34048	-0.33976	-0.33579	-0.32918	-0.32428
Alpha occ. eigenvalues --	-0.31876	-0.31269	-0.29851	-0.29654	-0.29536
Alpha occ. eigenvalues --	-0.28985	-0.28768	-0.28600	-0.28261	-0.28069
Alpha occ. eigenvalues --	-0.27890	-0.27747	-0.26894	-0.26421	-0.25380
Alpha occ. eigenvalues --	-0.24883	-0.23881	-0.22507		
Alpha virt. eigenvalues --	-0.09869	-0.07086	-0.04510	-0.03474	-0.03165
Alpha virt. eigenvalues --	-0.02028	-0.01815	0.00312	0.00616	0.01465
Alpha virt. eigenvalues --	0.02225	0.02930	0.04444	0.04721	0.05166
Alpha virt. eigenvalues --	0.05356	0.05539	0.05672	0.06002	0.06360
Alpha virt. eigenvalues --	0.06687	0.06800	0.06969	0.07352	0.07464
Alpha virt. eigenvalues --	0.07846	0.08206	0.08858	0.09016	0.09108
Alpha virt. eigenvalues --	0.09318	0.09405	0.09579	0.09750	0.10093
Alpha virt. eigenvalues --	0.10308	0.10721	0.10743	0.11077	0.11233
Alpha virt. eigenvalues --	0.11496	0.11667	0.11933	0.12089	0.12218
Alpha virt. eigenvalues --	0.12376	0.12492	0.12662	0.12794	0.12981
Alpha virt. eigenvalues --	0.13152	0.13171	0.13228	0.13364	0.13443
Alpha virt. eigenvalues --	0.13514	0.13566	0.13683	0.13943	0.13962
Alpha virt. eigenvalues --	0.14167	0.14267	0.14364	0.14402	0.14851
Alpha virt. eigenvalues --	0.14973	0.15266	0.15424	0.15610	0.15755
Alpha virt. eigenvalues --	0.15779	0.15934	0.16040	0.16084	0.16227
Alpha virt. eigenvalues --	0.16408	0.16554	0.17404	0.17502	0.17844
Alpha virt. eigenvalues --	0.18046	0.18185	0.18590	0.19088	0.19391
Alpha virt. eigenvalues --	0.19712	0.19905	0.19948	0.20358	0.21011
Alpha virt. eigenvalues --	0.21217	0.21335	0.21785	0.21891	0.22190
Alpha virt. eigenvalues --	0.22339	0.22529	0.22622	0.22930	0.23121
Alpha virt. eigenvalues --	0.23968	0.24017	0.24389	0.24650	0.24688
Alpha virt. eigenvalues --	0.25147	0.25283	0.25953	0.26251	0.26658
Alpha virt. eigenvalues --	0.26901	0.27080	0.27191	0.27366	0.27474
Alpha virt. eigenvalues --	0.28082	0.28110	0.28346	0.28575	0.28893
Alpha virt. eigenvalues --	0.29029	0.29289	0.29739	0.29890	0.30269
Alpha virt. eigenvalues --	0.31546	0.31638	0.31968	0.32255	0.32724

Alpha virt. eigenvalues --	0.33396	0.33817	0.35431	0.36666	0.37886
Alpha virt. eigenvalues --	0.39257	0.40612	0.40660	0.40803	0.41021
Alpha virt. eigenvalues --	0.41202	0.41628	0.41835	0.41998	0.42094
Alpha virt. eigenvalues --	0.42171	0.42313	0.42632	0.42917	0.43415
Alpha virt. eigenvalues --	0.43542	0.43781	0.43984	0.44121	0.44291
Alpha virt. eigenvalues --	0.44561	0.44771	0.44979	0.45078	0.45332
Alpha virt. eigenvalues --	0.45665	0.45745	0.45918	0.45961	0.46034
Alpha virt. eigenvalues --	0.46241	0.46430	0.46529	0.46721	0.46779
Alpha virt. eigenvalues --	0.46925	0.47165	0.47192	0.47335	0.47437
Alpha virt. eigenvalues --	0.47596	0.47706	0.47913	0.47987	0.48120
Alpha virt. eigenvalues --	0.48216	0.48267	0.48454	0.48509	0.48701
Alpha virt. eigenvalues --	0.48818	0.48860	0.49011	0.49126	0.49287
Alpha virt. eigenvalues --	0.49440	0.49710	0.49809	0.50026	0.50107
Alpha virt. eigenvalues --	0.50327	0.50528	0.50638	0.50817	0.51030
Alpha virt. eigenvalues --	0.51090	0.51205	0.51246	0.51523	0.51567
Alpha virt. eigenvalues --	0.51772	0.51954	0.52049	0.52070	0.52589
Alpha virt. eigenvalues --	0.52939	0.53395	0.53503	0.53573	0.53756
Alpha virt. eigenvalues --	0.53881	0.54180	0.54449	0.54559	0.54691
Alpha virt. eigenvalues --	0.54773	0.54945	0.55178	0.55451	0.55773
Alpha virt. eigenvalues --	0.55995	0.56508	0.56922	0.57401	0.57934
Alpha virt. eigenvalues --	0.58295	0.58409	0.58689	0.58918	0.59070
Alpha virt. eigenvalues --	0.59588	0.59789	0.59993	0.60357	0.60564
Alpha virt. eigenvalues --	0.60742	0.61112	0.61142	0.61293	0.61433
Alpha virt. eigenvalues --	0.61592	0.61986	0.62084	0.62171	0.62255
Alpha virt. eigenvalues --	0.62417	0.62481	0.62623	0.62777	0.62926
Alpha virt. eigenvalues --	0.62974	0.62988	0.63020	0.63099	0.63452
Alpha virt. eigenvalues --	0.63677	0.63888	0.64161	0.64250	0.64310
Alpha virt. eigenvalues --	0.64431	0.64554	0.64637	0.64707	0.64875
Alpha virt. eigenvalues --	0.65043	0.65179	0.65455	0.65551	0.65862
Alpha virt. eigenvalues --	0.65949	0.66115	0.66268	0.66477	0.66675
Alpha virt. eigenvalues --	0.66746	0.66861	0.67031	0.67187	0.67243
Alpha virt. eigenvalues --	0.67364	0.67415	0.67653	0.67690	0.67778
Alpha virt. eigenvalues --	0.67904	0.68136	0.68295	0.68510	0.68563
Alpha virt. eigenvalues --	0.68592	0.68808	0.68905	0.69258	0.69456
Alpha virt. eigenvalues --	0.69823	0.70004	0.70225	0.70312	0.70501
Alpha virt. eigenvalues --	0.70692	0.71245	0.71754	0.72081	0.72173
Alpha virt. eigenvalues --	0.72239	0.72632	0.72718	0.72788	0.72981
Alpha virt. eigenvalues --	0.73054	0.73376	0.73772	0.73813	0.74007
Alpha virt. eigenvalues --	0.74360	0.74638	0.74784	0.75083	0.75144
Alpha virt. eigenvalues --	0.75282	0.75471	0.75682	0.75699	0.75794
Alpha virt. eigenvalues --	0.76082	0.76297	0.76538	0.76863	0.77038
Alpha virt. eigenvalues --	0.78109	0.78844	0.79966	0.80670	0.80857
Alpha virt. eigenvalues --	0.80952	0.81193	0.82266	0.82659	0.83534
Alpha virt. eigenvalues --	0.83793	0.84094	0.84631	0.85105	0.85478
Alpha virt. eigenvalues --	0.85749	0.86024	0.86662	0.86906	0.87127
Alpha virt. eigenvalues --	0.87291	0.87402	0.87620	0.87949	0.88499
Alpha virt. eigenvalues --	0.88946	0.89201	0.89986	0.90210	0.90347
Alpha virt. eigenvalues --	0.90636	0.90956	0.91211	0.91462	0.91565

Alpha virt. eigenvalues --	0.91758	0.92025	0.92420	0.92636	0.93035
Alpha virt. eigenvalues --	0.93139	0.93433	0.93899	0.94019	0.94840
Alpha virt. eigenvalues --	0.95068	0.95268	0.96019	0.96190	0.96569
Alpha virt. eigenvalues --	0.96668	0.97221	0.97459	0.97639	0.97859
Alpha virt. eigenvalues --	0.98140	0.98304	0.98641	0.98872	0.98926
Alpha virt. eigenvalues --	0.99134	0.99330	0.99511	0.99656	0.99989
Alpha virt. eigenvalues --	1.00567	1.00708	1.01152	1.01371	1.01804
Alpha virt. eigenvalues --	1.02128	1.02675	1.03115	1.03320	1.03641
Alpha virt. eigenvalues --	1.03885	1.03937	1.04449	1.04646	1.04787
Alpha virt. eigenvalues --	1.05142	1.05368	1.05772	1.06137	1.06690
Alpha virt. eigenvalues --	1.07459	1.07637	1.08083	1.09025	1.09274
Alpha virt. eigenvalues --	1.10152	1.10324	1.10653	1.11245	1.11982
Alpha virt. eigenvalues --	1.12094	1.12401	1.12546	1.12827	1.13990
Alpha virt. eigenvalues --	1.14230	1.15386	1.15538	1.15833	1.16723
Alpha virt. eigenvalues --	1.16863	1.17492	1.17634	1.18174	1.18489
Alpha virt. eigenvalues --	1.18809	1.19019	1.19433	1.19833	1.20172
Alpha virt. eigenvalues --	1.20389	1.20522	1.21085	1.21553	1.21910
Alpha virt. eigenvalues --	1.22235	1.22473	1.22759	1.22903	1.23592
Alpha virt. eigenvalues --	1.24044	1.24589	1.25339	1.25684	1.25748
Alpha virt. eigenvalues --	1.26459	1.26576	1.26649	1.26712	1.26842
Alpha virt. eigenvalues --	1.27672	1.27871	1.28125	1.28423	1.29145
Alpha virt. eigenvalues --	1.29666	1.30040	1.30492	1.30995	1.31087
Alpha virt. eigenvalues --	1.31434	1.31557	1.32208	1.32447	1.32847
Alpha virt. eigenvalues --	1.32957	1.33392	1.33510	1.33843	1.34174
Alpha virt. eigenvalues --	1.34420	1.35175	1.35207	1.35445	1.35739
Alpha virt. eigenvalues --	1.36811	1.37050	1.37443	1.37626	1.38215
Alpha virt. eigenvalues --	1.38764	1.39091	1.39169	1.39370	1.39538
Alpha virt. eigenvalues --	1.39935	1.40339	1.40477	1.40513	1.40693
Alpha virt. eigenvalues --	1.40802	1.40890	1.40928	1.41324	1.41505
Alpha virt. eigenvalues --	1.41711	1.42251	1.42553	1.43016	1.43362
Alpha virt. eigenvalues --	1.43497	1.43605	1.43812	1.43894	1.44141
Alpha virt. eigenvalues --	1.44302	1.44721	1.45117	1.45956	1.46113
Alpha virt. eigenvalues --	1.46205	1.46350	1.46611	1.46647	1.47121
Alpha virt. eigenvalues --	1.47235	1.47894	1.48002	1.48218	1.48437
Alpha virt. eigenvalues --	1.48777	1.48907	1.49444	1.49951	1.50248
Alpha virt. eigenvalues --	1.50577	1.50681	1.50886	1.51017	1.51323
Alpha virt. eigenvalues --	1.51430	1.51731	1.52220	1.52531	1.52915
Alpha virt. eigenvalues --	1.53172	1.53688	1.54051	1.54192	1.54353
Alpha virt. eigenvalues --	1.55004	1.55464	1.55917	1.56179	1.56339
Alpha virt. eigenvalues --	1.56498	1.56859	1.57090	1.57313	1.57431
Alpha virt. eigenvalues --	1.57682	1.57811	1.57970	1.58011	1.58184
Alpha virt. eigenvalues --	1.58528	1.58890	1.59101	1.59480	1.60002
Alpha virt. eigenvalues --	1.60298	1.60635	1.60705	1.60805	1.61199
Alpha virt. eigenvalues --	1.61351	1.61593	1.61768	1.61805	1.62038
Alpha virt. eigenvalues --	1.62291	1.62358	1.62480	1.62680	1.62728
Alpha virt. eigenvalues --	1.63185	1.63249	1.63337	1.63490	1.63500
Alpha virt. eigenvalues --	1.63589	1.63881	1.63931	1.64071	1.64181
Alpha virt. eigenvalues --	1.64418	1.64492	1.64816	1.65190	1.65199

Alpha virt. eigenvalues --	1.65578	1.65758	1.65999	1.66385	1.66637
Alpha virt. eigenvalues --	1.66772	1.67305	1.67531	1.67838	1.67992
Alpha virt. eigenvalues --	1.68121	1.68509	1.68550	1.68739	1.68942
Alpha virt. eigenvalues --	1.69335	1.69786	1.70194	1.70483	1.70514
Alpha virt. eigenvalues --	1.70703	1.71037	1.71156	1.71298	1.71365
Alpha virt. eigenvalues --	1.71494	1.71629	1.71763	1.72080	1.72131
Alpha virt. eigenvalues --	1.72717	1.73100	1.73154	1.73813	1.74119
Alpha virt. eigenvalues --	1.74249	1.74547	1.74636	1.74847	1.75223
Alpha virt. eigenvalues --	1.75458	1.75583	1.75731	1.76080	1.76257
Alpha virt. eigenvalues --	1.76586	1.76644	1.76905	1.77164	1.77382
Alpha virt. eigenvalues --	1.77710	1.77809	1.78082	1.78198	1.78377
Alpha virt. eigenvalues --	1.78674	1.78847	1.78962	1.79415	1.79665
Alpha virt. eigenvalues --	1.80075	1.80697	1.81055	1.81400	1.81613
Alpha virt. eigenvalues --	1.81837	1.82250	1.82620	1.82707	1.82988
Alpha virt. eigenvalues --	1.83342	1.83632	1.83948	1.84100	1.84304
Alpha virt. eigenvalues --	1.84676	1.85191	1.85444	1.85515	1.85690
Alpha virt. eigenvalues --	1.85696	1.85839	1.85931	1.86140	1.86287
Alpha virt. eigenvalues --	1.86339	1.86793	1.87125	1.87365	1.87469
Alpha virt. eigenvalues --	1.87674	1.88346	1.88773	1.89381	1.89872
Alpha virt. eigenvalues --	1.90609	1.90729	1.90947	1.91735	1.92082
Alpha virt. eigenvalues --	1.92472	1.92579	1.93248	1.93503	1.93835
Alpha virt. eigenvalues --	1.94337	1.95290	1.95550	1.95712	1.96147
Alpha virt. eigenvalues --	1.96584	1.96761	1.96902	1.97265	1.97602
Alpha virt. eigenvalues --	1.97987	1.98318	1.98420	1.98666	1.98911
Alpha virt. eigenvalues --	1.99000	1.99351	1.99566	1.99635	1.99692
Alpha virt. eigenvalues --	1.99884	2.00094	2.00300	2.01181	2.01517
Alpha virt. eigenvalues --	2.02004	2.02269	2.02638	2.02764	2.02886
Alpha virt. eigenvalues --	2.03894	2.03973	2.04635	2.05548	2.05751
Alpha virt. eigenvalues --	2.06071	2.06322	2.06529	2.07164	2.07375
Alpha virt. eigenvalues --	2.07575	2.08122	2.08531	2.08677	2.09138
Alpha virt. eigenvalues --	2.09298	2.09542	2.10067	2.10462	2.11350
Alpha virt. eigenvalues --	2.12136	2.12185	2.12306	2.12899	2.12939
Alpha virt. eigenvalues --	2.13661	2.14032	2.14440	2.14585	2.15401
Alpha virt. eigenvalues --	2.15994	2.16692	2.16992	2.17141	2.17170
Alpha virt. eigenvalues --	2.17657	2.18492	2.18887	2.20077	2.20237
Alpha virt. eigenvalues --	2.20502	2.20800	2.21178	2.21313	2.21729
Alpha virt. eigenvalues --	2.21998	2.22257	2.23093	2.24170	2.25379
Alpha virt. eigenvalues --	2.25526	2.25838	2.26219	2.26420	2.26505
Alpha virt. eigenvalues --	2.26894	2.27496	2.27571	2.29391	2.29689
Alpha virt. eigenvalues --	2.29914	2.31601	2.31918	2.32375	2.33514
Alpha virt. eigenvalues --	2.33815	2.33903	2.34172	2.34921	2.35944
Alpha virt. eigenvalues --	2.37976	2.38152	2.38523	2.38698	2.39223
Alpha virt. eigenvalues --	2.39387	2.39551	2.39905	2.40417	2.40741
Alpha virt. eigenvalues --	2.41121	2.42005	2.42049	2.42267	2.42385
Alpha virt. eigenvalues --	2.42520	2.42656	2.43046	2.43276	2.43450
Alpha virt. eigenvalues --	2.43703	2.44179	2.44536	2.44564	2.45033
Alpha virt. eigenvalues --	2.45133	2.45219	2.45285	2.45710	2.46145
Alpha virt. eigenvalues --	2.46274	2.46721	2.47069	2.47106	2.47680

Alpha virt. eigenvalues --	2.47989	2.48175	2.48522	2.48831	2.48866
Alpha virt. eigenvalues --	2.49113	2.49261	2.49363	2.50068	2.50243
Alpha virt. eigenvalues --	2.50833	2.51996	2.52351	2.52788	2.53083
Alpha virt. eigenvalues --	2.53326	2.54540	2.55349	2.55613	2.55709
Alpha virt. eigenvalues --	2.57025	2.57319	2.57446	2.57706	2.58233
Alpha virt. eigenvalues --	2.59716	2.64435	2.65384	2.66416	2.66866
Alpha virt. eigenvalues --	2.67147	2.67888	2.68109	2.68792	2.70244
Alpha virt. eigenvalues --	2.70921	2.71040	2.72738	2.73565	2.74532
Alpha virt. eigenvalues --	2.75163	2.76890	2.79486	2.81066	2.81783
Alpha virt. eigenvalues --	2.83824	2.84393	2.89565	2.90194	2.90782
Alpha virt. eigenvalues --	2.91585	2.92321	2.93339	2.93670	2.93942
Alpha virt. eigenvalues --	2.94610	2.96573	2.97188	2.97483	2.98038
Alpha virt. eigenvalues --	2.98262	2.98482	2.98965	2.99227	2.99330
Alpha virt. eigenvalues --	3.01835	3.02082	3.02120	3.03864	3.04262
Alpha virt. eigenvalues --	3.04986	3.07272	3.07446	3.07624	3.07963
Alpha virt. eigenvalues --	3.08137	3.08325	3.09219	3.09793	3.09909
Alpha virt. eigenvalues --	3.11860	3.12222	3.12500	3.12881	3.12952
Alpha virt. eigenvalues --	3.13116	3.23563	3.23710	3.23844	3.25605
Alpha virt. eigenvalues --	3.25817	3.25942	3.29874	3.30670	3.30741
Alpha virt. eigenvalues --	3.36165	3.36552	3.36624	3.36761	3.36775
Alpha virt. eigenvalues --	3.36873	3.38383	3.39357	3.40006	3.41415
Alpha virt. eigenvalues --	3.42183	3.42501	3.46166	3.47632	3.49755
Alpha virt. eigenvalues --	3.51648	3.53173	3.58585		
Beta occ. eigenvalues --	-89.12758	-89.11769	-89.11367	-19.29423	-19.29326
Beta occ. eigenvalues --	-19.28661	-19.28310	-19.28169	-19.27251	-19.24708
Beta occ. eigenvalues --	-19.24692	-19.24540	-19.24483	-19.24402	-19.24307
Beta occ. eigenvalues --	-10.34951	-10.34893	-10.33831	-10.33310	-10.33221
Beta occ. eigenvalues --	-10.32696	-10.32661	-10.32454	-10.31597	-10.31561
Beta occ. eigenvalues --	-10.31161	-10.31011	-10.30972	-10.30927	-10.30921
Beta occ. eigenvalues --	-10.30567	-10.30447	-10.30445	-10.30315	-10.30228
Beta occ. eigenvalues --	-10.30226	-10.30207	-10.30145	-10.30069	-10.30040
Beta occ. eigenvalues --	-10.30016	-10.29873	-10.29031	-10.29018	-10.28997
Beta occ. eigenvalues --	-10.28938	-10.28871	-10.28857	-10.28765	-10.28561
Beta occ. eigenvalues --	-10.28168	-10.28011	-10.27954	-10.27938	-10.27879
Beta occ. eigenvalues --	-10.27657	-10.27641	-10.27624	-10.27532	-10.27372
Beta occ. eigenvalues --	-10.27276	-10.26646	-10.26298	-10.26289	-10.26238
Beta occ. eigenvalues --	-10.26140	-8.07221	-8.06203	-8.05779	-6.01116
Beta occ. eigenvalues --	-6.00741	-6.00295	-6.00089	-5.99722	-5.99655
Beta occ. eigenvalues --	-5.99291	-5.99291	-5.98890	-1.14815	-1.13924
Beta occ. eigenvalues --	-1.13324	-1.12352	-1.11457	-1.10813	-1.08868
Beta occ. eigenvalues --	-1.08673	-1.08673	-1.08533	-1.08477	-1.08340
Beta occ. eigenvalues --	-0.95894	-0.94732	-0.93843	-0.92218	-0.91242
Beta occ. eigenvalues --	-0.90119	-0.87637	-0.87199	-0.86883	-0.85793
Beta occ. eigenvalues --	-0.83874	-0.81773	-0.80619	-0.80289	-0.79770
Beta occ. eigenvalues --	-0.79264	-0.78863	-0.78170	-0.77917	-0.77492
Beta occ. eigenvalues --	-0.77177	-0.75569	-0.75370	-0.75250	-0.74308
Beta occ. eigenvalues --	-0.73537	-0.72889	-0.72805	-0.72603	-0.71425
Beta occ. eigenvalues --	-0.69554	-0.69300	-0.69102	-0.68712	-0.66557

Beta occ. eigenvalues --	-0.66486	-0.65951	-0.65503	-0.65379	-0.65208
Beta occ. eigenvalues --	-0.64410	-0.64389	-0.62886	-0.61884	-0.61800
Beta occ. eigenvalues --	-0.61162	-0.60736	-0.60687	-0.60396	-0.59742
Beta occ. eigenvalues --	-0.59677	-0.56831	-0.56188	-0.55644	-0.55136
Beta occ. eigenvalues --	-0.54735	-0.54597	-0.54399	-0.54171	-0.54055
Beta occ. eigenvalues --	-0.53705	-0.53373	-0.52921	-0.52867	-0.52663
Beta occ. eigenvalues --	-0.51813	-0.51754	-0.50804	-0.50534	-0.50299
Beta occ. eigenvalues --	-0.50024	-0.49814	-0.49634	-0.49478	-0.49454
Beta occ. eigenvalues --	-0.49304	-0.49114	-0.48752	-0.48639	-0.48448
Beta occ. eigenvalues --	-0.48273	-0.48230	-0.48067	-0.47773	-0.47648
Beta occ. eigenvalues --	-0.47401	-0.47261	-0.46953	-0.46746	-0.46582
Beta occ. eigenvalues --	-0.46331	-0.46193	-0.45760	-0.45514	-0.45369
Beta occ. eigenvalues --	-0.44992	-0.44744	-0.44620	-0.44569	-0.44045
Beta occ. eigenvalues --	-0.43851	-0.43359	-0.43210	-0.42776	-0.42540
Beta occ. eigenvalues --	-0.42269	-0.41983	-0.41853	-0.41731	-0.41263
Beta occ. eigenvalues --	-0.41076	-0.41012	-0.40905	-0.40827	-0.40593
Beta occ. eigenvalues --	-0.40538	-0.40472	-0.40343	-0.39866	-0.39548
Beta occ. eigenvalues --	-0.39285	-0.38760	-0.38405	-0.38186	-0.38048
Beta occ. eigenvalues --	-0.37706	-0.37496	-0.37254	-0.37044	-0.36557
Beta occ. eigenvalues --	-0.35978	-0.35664	-0.35435	-0.35414	-0.34892
Beta occ. eigenvalues --	-0.34729	-0.34679	-0.34525	-0.34447	-0.34187
Beta occ. eigenvalues --	-0.34003	-0.33876	-0.33477	-0.32524	-0.32188
Beta occ. eigenvalues --	-0.31668	-0.30852	-0.29612	-0.29351	-0.29037
Beta occ. eigenvalues --	-0.28972	-0.28758	-0.28593	-0.28144	-0.28069
Beta occ. eigenvalues --	-0.27889	-0.27746	-0.26105	-0.25499	-0.24899
Beta occ. eigenvalues --	-0.24718	-0.22426			
Beta virt. eigenvalues --	-0.18342	-0.09130	-0.06479	-0.03870	-0.03016
Beta virt. eigenvalues --	-0.02738	-0.01852	-0.01242	0.00537	0.01111
Beta virt. eigenvalues --	0.01677	0.02346	0.03516	0.04772	0.04818
Beta virt. eigenvalues --	0.05259	0.05432	0.05615	0.05831	0.06060
Beta virt. eigenvalues --	0.06583	0.06751	0.06825	0.07068	0.07393
Beta virt. eigenvalues --	0.07660	0.08245	0.08254	0.08865	0.09025
Beta virt. eigenvalues --	0.09122	0.09335	0.09456	0.09595	0.09768
Beta virt. eigenvalues --	0.10146	0.10336	0.10736	0.10763	0.11094
Beta virt. eigenvalues --	0.11254	0.11514	0.11704	0.11964	0.12128
Beta virt. eigenvalues --	0.12241	0.12385	0.12521	0.12677	0.12827
Beta virt. eigenvalues --	0.12998	0.13173	0.13181	0.13235	0.13375
Beta virt. eigenvalues --	0.13474	0.13539	0.13583	0.13730	0.13969
Beta virt. eigenvalues --	0.13991	0.14180	0.14279	0.14376	0.14416
Beta virt. eigenvalues --	0.14984	0.15215	0.15542	0.15599	0.15637
Beta virt. eigenvalues --	0.15784	0.15822	0.15957	0.16066	0.16122
Beta virt. eigenvalues --	0.16246	0.16430	0.16573	0.17434	0.17593
Beta virt. eigenvalues --	0.17908	0.18094	0.18231	0.18613	0.19130
Beta virt. eigenvalues --	0.19421	0.19723	0.19927	0.19957	0.20396
Beta virt. eigenvalues --	0.21028	0.21269	0.21375	0.21892	0.21909
Beta virt. eigenvalues --	0.22199	0.22348	0.22579	0.22661	0.22949
Beta virt. eigenvalues --	0.23203	0.24057	0.24102	0.24449	0.24681
Beta virt. eigenvalues --	0.24772	0.25228	0.25338	0.26054	0.26329

Beta virt. eigenvalues --	0.26720	0.26947	0.27099	0.27218	0.27390
Beta virt. eigenvalues --	0.27528	0.28119	0.28144	0.28387	0.28611
Beta virt. eigenvalues --	0.28910	0.29044	0.29331	0.29794	0.29928
Beta virt. eigenvalues --	0.30316	0.31618	0.31718	0.32046	0.32317
Beta virt. eigenvalues --	0.32796	0.33481	0.33901	0.35575	0.36774
Beta virt. eigenvalues --	0.38034	0.39353	0.40710	0.40802	0.40876
Beta virt. eigenvalues --	0.41094	0.41255	0.41716	0.41895	0.42067
Beta virt. eigenvalues --	0.42135	0.42284	0.42367	0.42736	0.43039
Beta virt. eigenvalues --	0.43561	0.43657	0.43920	0.44051	0.44203
Beta virt. eigenvalues --	0.44410	0.44676	0.44886	0.45117	0.45188
Beta virt. eigenvalues --	0.45494	0.45765	0.45798	0.45961	0.45998
Beta virt. eigenvalues --	0.46079	0.46349	0.46496	0.46659	0.46754
Beta virt. eigenvalues --	0.46822	0.46982	0.47249	0.47290	0.47494
Beta virt. eigenvalues --	0.47513	0.47671	0.47790	0.47989	0.48107
Beta virt. eigenvalues --	0.48228	0.48321	0.48368	0.48547	0.48667
Beta virt. eigenvalues --	0.48791	0.48895	0.48977	0.49114	0.49266
Beta virt. eigenvalues --	0.49352	0.49597	0.49852	0.49995	0.50151
Beta virt. eigenvalues --	0.50249	0.50432	0.50626	0.50764	0.50920
Beta virt. eigenvalues --	0.51051	0.51213	0.51275	0.51379	0.51607
Beta virt. eigenvalues --	0.51709	0.51832	0.52052	0.52122	0.52158
Beta virt. eigenvalues --	0.52641	0.53015	0.53486	0.53600	0.53642
Beta virt. eigenvalues --	0.53848	0.53957	0.54241	0.54506	0.54641
Beta virt. eigenvalues --	0.54736	0.54841	0.55023	0.55239	0.55499
Beta virt. eigenvalues --	0.55879	0.56119	0.56591	0.56991	0.57510
Beta virt. eigenvalues --	0.57998	0.58400	0.58470	0.58748	0.58980
Beta virt. eigenvalues --	0.59105	0.59636	0.59914	0.60077	0.60380
Beta virt. eigenvalues --	0.60671	0.60780	0.61143	0.61198	0.61313
Beta virt. eigenvalues --	0.61436	0.61712	0.62044	0.62121	0.62244
Beta virt. eigenvalues --	0.62344	0.62454	0.62526	0.62664	0.62797
Beta virt. eigenvalues --	0.62968	0.63008	0.63044	0.63092	0.63123
Beta virt. eigenvalues --	0.63540	0.63779	0.63932	0.64189	0.64266
Beta virt. eigenvalues --	0.64347	0.64483	0.64599	0.64670	0.64760
Beta virt. eigenvalues --	0.64915	0.65081	0.65223	0.65481	0.65588
Beta virt. eigenvalues --	0.65908	0.65998	0.66149	0.66309	0.66539
Beta virt. eigenvalues --	0.66715	0.66764	0.66917	0.67091	0.67246
Beta virt. eigenvalues --	0.67288	0.67407	0.67465	0.67696	0.67748
Beta virt. eigenvalues --	0.67812	0.67941	0.68175	0.68355	0.68571
Beta virt. eigenvalues --	0.68610	0.68658	0.68857	0.68963	0.69297
Beta virt. eigenvalues --	0.69506	0.69880	0.70062	0.70307	0.70375
Beta virt. eigenvalues --	0.70591	0.70752	0.71340	0.71777	0.72138
Beta virt. eigenvalues --	0.72258	0.72368	0.72697	0.72748	0.72822
Beta virt. eigenvalues --	0.73029	0.73152	0.73430	0.73828	0.73866
Beta virt. eigenvalues --	0.74041	0.74428	0.74678	0.74854	0.75111
Beta virt. eigenvalues --	0.75187	0.75328	0.75513	0.75700	0.75744
Beta virt. eigenvalues --	0.75808	0.76140	0.76357	0.76594	0.76889
Beta virt. eigenvalues --	0.77108	0.78192	0.79033	0.80137	0.80739
Beta virt. eigenvalues --	0.80884	0.80999	0.81505	0.82442	0.82784
Beta virt. eigenvalues --	0.83634	0.83915	0.84234	0.84753	0.85235

Beta virt. eigenvalues --	0.85564	0.85800	0.86081	0.86703	0.86987
Beta virt. eigenvalues --	0.87163	0.87322	0.87451	0.87675	0.87966
Beta virt. eigenvalues --	0.88571	0.89056	0.89324	0.90077	0.90291
Beta virt. eigenvalues --	0.90396	0.90700	0.90990	0.91237	0.91506
Beta virt. eigenvalues --	0.91618	0.91812	0.92100	0.92508	0.92734
Beta virt. eigenvalues --	0.93166	0.93258	0.93546	0.93979	0.94123
Beta virt. eigenvalues --	0.94914	0.95200	0.95403	0.96122	0.96319
Beta virt. eigenvalues --	0.96650	0.96791	0.97362	0.97545	0.97789
Beta virt. eigenvalues --	0.97983	0.98215	0.98368	0.98695	0.98947
Beta virt. eigenvalues --	0.98975	0.99195	0.99366	0.99554	0.99701
Beta virt. eigenvalues --	1.00039	1.00679	1.00767	1.01197	1.01455
Beta virt. eigenvalues --	1.01900	1.02229	1.02750	1.03221	1.03445
Beta virt. eigenvalues --	1.03763	1.04001	1.04055	1.04586	1.04724
Beta virt. eigenvalues --	1.04860	1.05199	1.05422	1.05863	1.06231
Beta virt. eigenvalues --	1.06774	1.07560	1.07748	1.08155	1.09128
Beta virt. eigenvalues --	1.09376	1.10244	1.10397	1.10750	1.11315
Beta virt. eigenvalues --	1.12042	1.12167	1.12459	1.12606	1.12909
Beta virt. eigenvalues --	1.14081	1.14312	1.15413	1.15560	1.15848
Beta virt. eigenvalues --	1.16845	1.16935	1.17553	1.17723	1.18285
Beta virt. eigenvalues --	1.18534	1.18828	1.19051	1.19533	1.19912
Beta virt. eigenvalues --	1.20264	1.20496	1.20650	1.21147	1.21651
Beta virt. eigenvalues --	1.22051	1.22302	1.22513	1.22830	1.22977
Beta virt. eigenvalues --	1.23681	1.24132	1.24650	1.25412	1.25739
Beta virt. eigenvalues --	1.25838	1.26544	1.26655	1.26686	1.26751
Beta virt. eigenvalues --	1.26976	1.27818	1.27999	1.28245	1.28506
Beta virt. eigenvalues --	1.29219	1.29773	1.30111	1.30576	1.31072
Beta virt. eigenvalues --	1.31163	1.31511	1.31632	1.32330	1.32517
Beta virt. eigenvalues --	1.32942	1.33019	1.33461	1.33562	1.33938
Beta virt. eigenvalues --	1.34304	1.34595	1.35257	1.35295	1.35476
Beta virt. eigenvalues --	1.35788	1.36929	1.37241	1.37505	1.37764
Beta virt. eigenvalues --	1.38279	1.38852	1.39176	1.39270	1.39459
Beta virt. eigenvalues --	1.39601	1.39986	1.40359	1.40494	1.40520
Beta virt. eigenvalues --	1.40694	1.40803	1.40892	1.41008	1.41381
Beta virt. eigenvalues --	1.41572	1.41743	1.42350	1.42651	1.43064
Beta virt. eigenvalues --	1.43419	1.43538	1.43655	1.43847	1.43925
Beta virt. eigenvalues --	1.44192	1.44357	1.44760	1.45173	1.46005
Beta virt. eigenvalues --	1.46168	1.46260	1.46446	1.46672	1.46740
Beta virt. eigenvalues --	1.47171	1.47308	1.47950	1.48065	1.48305
Beta virt. eigenvalues --	1.48489	1.48831	1.48973	1.49517	1.50014
Beta virt. eigenvalues --	1.50303	1.50623	1.50725	1.50933	1.51075
Beta virt. eigenvalues --	1.51363	1.51478	1.51775	1.52281	1.52593
Beta virt. eigenvalues --	1.52947	1.53241	1.53803	1.54134	1.54255
Beta virt. eigenvalues --	1.54428	1.55061	1.55519	1.55947	1.56199
Beta virt. eigenvalues --	1.56363	1.56559	1.56904	1.57190	1.57378
Beta virt. eigenvalues --	1.57472	1.57718	1.57869	1.58011	1.58054
Beta virt. eigenvalues --	1.58234	1.58590	1.58932	1.59145	1.59517
Beta virt. eigenvalues --	1.60097	1.60371	1.60644	1.60737	1.60826
Beta virt. eigenvalues --	1.61245	1.61409	1.61626	1.61822	1.61827

Beta virt. eigenvalues --	1.62087	1.62320	1.62396	1.62497	1.62716
Beta virt. eigenvalues --	1.62794	1.63230	1.63313	1.63366	1.63495
Beta virt. eigenvalues --	1.63528	1.63633	1.63919	1.64017	1.64130
Beta virt. eigenvalues --	1.64223	1.64458	1.64517	1.64846	1.65231
Beta virt. eigenvalues --	1.65239	1.65620	1.65806	1.66052	1.66449
Beta virt. eigenvalues --	1.66720	1.66837	1.67350	1.67582	1.67896
Beta virt. eigenvalues --	1.68080	1.68158	1.68540	1.68583	1.68784
Beta virt. eigenvalues --	1.69027	1.69393	1.69842	1.70269	1.70521
Beta virt. eigenvalues --	1.70564	1.70763	1.71076	1.71185	1.71324
Beta virt. eigenvalues --	1.71412	1.71529	1.71684	1.71816	1.72144
Beta virt. eigenvalues --	1.72175	1.72765	1.73146	1.73213	1.73880
Beta virt. eigenvalues --	1.74180	1.74311	1.74595	1.74679	1.74910
Beta virt. eigenvalues --	1.75343	1.75527	1.75651	1.75798	1.76147
Beta virt. eigenvalues --	1.76333	1.76646	1.76718	1.76960	1.77243
Beta virt. eigenvalues --	1.77489	1.77764	1.77873	1.78116	1.78264
Beta virt. eigenvalues --	1.78413	1.78730	1.78892	1.79018	1.79479
Beta virt. eigenvalues --	1.79741	1.80167	1.80733	1.81111	1.81452
Beta virt. eigenvalues --	1.81669	1.81866	1.82276	1.82674	1.82759
Beta virt. eigenvalues --	1.83046	1.83369	1.83653	1.83988	1.84130
Beta virt. eigenvalues --	1.84380	1.84721	1.85229	1.85527	1.85559
Beta virt. eigenvalues --	1.85722	1.85740	1.85883	1.85967	1.86158
Beta virt. eigenvalues --	1.86350	1.86419	1.86835	1.87181	1.87413
Beta virt. eigenvalues --	1.87541	1.87721	1.88425	1.88870	1.89478
Beta virt. eigenvalues --	1.89948	1.90670	1.90815	1.91057	1.91863
Beta virt. eigenvalues --	1.92169	1.92549	1.92649	1.93337	1.93558
Beta virt. eigenvalues --	1.93950	1.94396	1.95347	1.95626	1.95829
Beta virt. eigenvalues --	1.96236	1.96668	1.96868	1.96940	1.97311
Beta virt. eigenvalues --	1.97706	1.98085	1.98424	1.98499	1.98767
Beta virt. eigenvalues --	1.99006	1.99093	1.99370	1.99594	1.99651
Beta virt. eigenvalues --	1.99720	1.99955	2.00174	2.00349	2.01269
Beta virt. eigenvalues --	2.01630	2.02086	2.02329	2.02726	2.02786
Beta virt. eigenvalues --	2.02920	2.03929	2.04069	2.04747	2.05591
Beta virt. eigenvalues --	2.05826	2.06118	2.06386	2.06609	2.07259
Beta virt. eigenvalues --	2.07463	2.07620	2.08218	2.08575	2.08799
Beta virt. eigenvalues --	2.09166	2.09320	2.09627	2.10166	2.10539
Beta virt. eigenvalues --	2.11411	2.12144	2.12212	2.12314	2.12944
Beta virt. eigenvalues --	2.12986	2.13692	2.14039	2.14477	2.14714
Beta virt. eigenvalues --	2.15477	2.16056	2.16742	2.17014	2.17161
Beta virt. eigenvalues --	2.17204	2.17695	2.18530	2.18913	2.20164
Beta virt. eigenvalues --	2.20318	2.20568	2.20902	2.21238	2.21368
Beta virt. eigenvalues --	2.21754	2.22055	2.22290	2.23191	2.24287
Beta virt. eigenvalues --	2.25524	2.25611	2.25986	2.26232	2.26498
Beta virt. eigenvalues --	2.26568	2.27021	2.27589	2.27634	2.29406
Beta virt. eigenvalues --	2.29699	2.29922	2.31659	2.32023	2.32427
Beta virt. eigenvalues --	2.33538	2.33825	2.33916	2.34300	2.35168
Beta virt. eigenvalues --	2.35991	2.38062	2.38236	2.38558	2.38797
Beta virt. eigenvalues --	2.39251	2.39459	2.39577	2.39994	2.40474
Beta virt. eigenvalues --	2.40808	2.41286	2.42016	2.42052	2.42282

Beta virt. eigenvalues --	2.42398	2.42529	2.42670	2.43049	2.43279
Beta virt. eigenvalues --	2.43454	2.43733	2.44192	2.44545	2.44572
Beta virt. eigenvalues --	2.45042	2.45140	2.45225	2.45297	2.45724
Beta virt. eigenvalues --	2.46166	2.46293	2.46731	2.47082	2.47110
Beta virt. eigenvalues --	2.47694	2.48002	2.48186	2.48547	2.48839
Beta virt. eigenvalues --	2.48878	2.49122	2.49266	2.49366	2.50093
Beta virt. eigenvalues --	2.50276	2.50848	2.52055	2.52392	2.52809
Beta virt. eigenvalues --	2.53092	2.53370	2.54568	2.55351	2.55614
Beta virt. eigenvalues --	2.55710	2.57037	2.57327	2.57454	2.57734
Beta virt. eigenvalues --	2.58256	2.59742	2.64455	2.65464	2.66483
Beta virt. eigenvalues --	2.66935	2.67189	2.67937	2.68138	2.68823
Beta virt. eigenvalues --	2.70302	2.70985	2.71072	2.72805	2.73691
Beta virt. eigenvalues --	2.74690	2.75217	2.76948	2.79552	2.81102
Beta virt. eigenvalues --	2.81834	2.83875	2.84431	2.89653	2.90248
Beta virt. eigenvalues --	2.90836	2.91634	2.92394	2.93406	2.93737
Beta virt. eigenvalues --	2.93996	2.94655	2.96671	2.97241	2.97524
Beta virt. eigenvalues --	2.98050	2.98268	2.98488	2.98985	2.99242
Beta virt. eigenvalues --	2.99341	3.01847	3.02084	3.02129	3.03926
Beta virt. eigenvalues --	3.04357	3.05039	3.07276	3.07448	3.07627
Beta virt. eigenvalues --	3.07965	3.08137	3.08326	3.09291	3.09835
Beta virt. eigenvalues --	3.09959	3.11908	3.12270	3.12583	3.12941
Beta virt. eigenvalues --	3.12983	3.13201	3.23568	3.23712	3.23846
Beta virt. eigenvalues --	3.25610	3.25819	3.25944	3.29941	3.30708
Beta virt. eigenvalues --	3.30773	3.36180	3.36557	3.36629	3.36767
Beta virt. eigenvalues --	3.36778	3.36875	3.38408	3.39383	3.40028
Beta virt. eigenvalues --	3.41441	3.42206	3.42529	3.46235	3.47682
Beta virt. eigenvalues --	3.49800	3.51699	3.53230	3.58608	

Dication/Bipolaron

Alpha occ. eigenvalues --	-89.15255	-89.14325	-89.13528	-19.31725	-19.31616
Alpha occ. eigenvalues --	-19.31134	-19.30615	-19.30342	-19.28882	-19.25593
Alpha occ. eigenvalues --	-19.25577	-19.25422	-19.25321	-19.25201	-19.25019
Alpha occ. eigenvalues --	-10.37850	-10.37806	-10.36984	-10.36353	-10.36237
Alpha occ. eigenvalues --	-10.36130	-10.36034	-10.34749	-10.34645	-10.34594
Alpha occ. eigenvalues --	-10.33567	-10.33564	-10.33127	-10.33099	-10.33085
Alpha occ. eigenvalues --	-10.33021	-10.32992	-10.32633	-10.32390	-10.32238
Alpha occ. eigenvalues --	-10.31929	-10.31686	-10.31380	-10.31378	-10.31147
Alpha occ. eigenvalues --	-10.31110	-10.30893	-10.30883	-10.30825	-10.30817
Alpha occ. eigenvalues --	-10.30653	-10.30630	-10.30588	-10.30374	-10.30294
Alpha occ. eigenvalues --	-10.30038	-10.29803	-10.29771	-10.29753	-10.29678
Alpha occ. eigenvalues --	-10.29553	-10.29540	-10.29348	-10.29251	-10.28854
Alpha occ. eigenvalues --	-10.28782	-10.28439	-10.28437	-10.28390	-10.27940
Alpha occ. eigenvalues --	-10.27816	-8.09738	-8.08785	-8.07956	-6.03637
Alpha occ. eigenvalues --	-6.03255	-6.02781	-6.02677	-6.02300	-6.01846
Alpha occ. eigenvalues --	-6.01836	-6.01463	-6.01052	-1.17043	-1.16189
Alpha occ. eigenvalues --	-1.15330	-1.14568	-1.13654	-1.12572	-1.09759
Alpha occ. eigenvalues --	-1.09552	-1.09547	-1.09324	-1.09315	-1.09075
Alpha occ. eigenvalues --	-0.98948	-0.97753	-0.96471	-0.95097	-0.93991

Alpha occ. eigenvalues --	-0.92310	-0.89039	-0.88909	-0.88463	-0.87989
Alpha occ. eigenvalues --	-0.86704	-0.84413	-0.83192	-0.82771	-0.82350
Alpha occ. eigenvalues --	-0.81613	-0.80954	-0.80374	-0.80094	-0.79627
Alpha occ. eigenvalues --	-0.79329	-0.76583	-0.76307	-0.76174	-0.75994
Alpha occ. eigenvalues --	-0.75275	-0.74681	-0.74363	-0.73991	-0.73591
Alpha occ. eigenvalues --	-0.71511	-0.70482	-0.70238	-0.69944	-0.69194
Alpha occ. eigenvalues --	-0.69019	-0.68487	-0.66915	-0.66436	-0.66341
Alpha occ. eigenvalues --	-0.66108	-0.65941	-0.65230	-0.63886	-0.63815
Alpha occ. eigenvalues --	-0.63130	-0.62912	-0.62511	-0.62421	-0.61728
Alpha occ. eigenvalues --	-0.61615	-0.58997	-0.58256	-0.57583	-0.57005
Alpha occ. eigenvalues --	-0.56671	-0.56319	-0.56259	-0.55902	-0.55746
Alpha occ. eigenvalues --	-0.55430	-0.55183	-0.54395	-0.54191	-0.53914
Alpha occ. eigenvalues --	-0.53537	-0.53172	-0.52959	-0.52446	-0.52030
Alpha occ. eigenvalues --	-0.51663	-0.51180	-0.50936	-0.50717	-0.50591
Alpha occ. eigenvalues --	-0.50533	-0.50523	-0.50258	-0.50147	-0.50076
Alpha occ. eigenvalues --	-0.50046	-0.49772	-0.49583	-0.49195	-0.49137
Alpha occ. eigenvalues --	-0.48949	-0.48811	-0.48744	-0.48509	-0.48267
Alpha occ. eigenvalues --	-0.48071	-0.47900	-0.47565	-0.47441	-0.47146
Alpha occ. eigenvalues --	-0.46954	-0.46815	-0.46513	-0.46365	-0.45839
Alpha occ. eigenvalues --	-0.45513	-0.45465	-0.45139	-0.44767	-0.44540
Alpha occ. eigenvalues --	-0.44049	-0.43965	-0.43751	-0.43530	-0.43252
Alpha occ. eigenvalues --	-0.43061	-0.42510	-0.42402	-0.42192	-0.41926
Alpha occ. eigenvalues --	-0.41873	-0.41760	-0.41681	-0.41594	-0.41396
Alpha occ. eigenvalues --	-0.41218	-0.40601	-0.40208	-0.40132	-0.39792
Alpha occ. eigenvalues --	-0.39558	-0.39409	-0.38908	-0.38660	-0.38453
Alpha occ. eigenvalues --	-0.37329	-0.37150	-0.36912	-0.36688	-0.36413
Alpha occ. eigenvalues --	-0.36316	-0.36236	-0.36036	-0.35659	-0.35528
Alpha occ. eigenvalues --	-0.35240	-0.35114	-0.34881	-0.34688	-0.33996
Alpha occ. eigenvalues --	-0.33460	-0.32812	-0.32112	-0.31740	-0.31384
Alpha occ. eigenvalues --	-0.29997	-0.29918	-0.29694	-0.29410	-0.28922
Alpha occ. eigenvalues --	-0.28717	-0.28472	-0.28376	-0.28231	-0.27335
Alpha occ. eigenvalues --	-0.26640	-0.24994			
Alpha virt. eigenvalues --	-0.21677	-0.12030	-0.09163	-0.06494	-0.05583
Alpha virt. eigenvalues --	-0.05176	-0.03890	-0.03567	-0.01996	-0.01436
Alpha virt. eigenvalues --	-0.00814	0.00203	0.00883	0.02639	0.02743
Alpha virt. eigenvalues --	0.03571	0.03720	0.04088	0.04273	0.04429
Alpha virt. eigenvalues --	0.04958	0.05304	0.05768	0.05845	0.06134
Alpha virt. eigenvalues --	0.06247	0.06530	0.06987	0.07529	0.08008
Alpha virt. eigenvalues --	0.08148	0.08328	0.08432	0.08629	0.08732
Alpha virt. eigenvalues --	0.08949	0.09032	0.09548	0.09767	0.09932
Alpha virt. eigenvalues --	0.10045	0.10325	0.10418	0.10740	0.10905
Alpha virt. eigenvalues --	0.11092	0.11209	0.11361	0.11536	0.11645
Alpha virt. eigenvalues --	0.11859	0.12003	0.12111	0.12224	0.12427
Alpha virt. eigenvalues --	0.12499	0.12526	0.12668	0.12722	0.12858
Alpha virt. eigenvalues --	0.12894	0.13114	0.13369	0.13414	0.13506
Alpha virt. eigenvalues --	0.13590	0.13728	0.13854	0.14172	0.14386
Alpha virt. eigenvalues --	0.14555	0.14661	0.14750	0.14974	0.15178
Alpha virt. eigenvalues --	0.15242	0.15416	0.15520	0.16157	0.16318

Alpha virt. eigenvalues --	0.16511	0.16648	0.16979	0.17422	0.17628
Alpha virt. eigenvalues --	0.17972	0.18566	0.18876	0.19066	0.19238
Alpha virt. eigenvalues --	0.19434	0.20115	0.20319	0.20454	0.20557
Alpha virt. eigenvalues --	0.20810	0.21139	0.21377	0.21462	0.21646
Alpha virt. eigenvalues --	0.21802	0.22266	0.22499	0.22665	0.22976
Alpha virt. eigenvalues --	0.23362	0.23400	0.23740	0.24203	0.24506
Alpha virt. eigenvalues --	0.24972	0.25234	0.25518	0.25847	0.25857
Alpha virt. eigenvalues --	0.26276	0.26427	0.26635	0.26843	0.26928
Alpha virt. eigenvalues --	0.27524	0.27677	0.27877	0.27933	0.28227
Alpha virt. eigenvalues --	0.28508	0.29488	0.29594	0.29938	0.30365
Alpha virt. eigenvalues --	0.30859	0.31521	0.31768	0.33217	0.34600
Alpha virt. eigenvalues --	0.35859	0.37079	0.38604	0.38646	0.38938
Alpha virt. eigenvalues --	0.39149	0.39410	0.39943	0.40159	0.40351
Alpha virt. eigenvalues --	0.40455	0.40604	0.40797	0.41020	0.41246
Alpha virt. eigenvalues --	0.41573	0.41712	0.41918	0.42327	0.42463
Alpha virt. eigenvalues --	0.42521	0.42859	0.43030	0.43141	0.43529
Alpha virt. eigenvalues --	0.43699	0.44242	0.44383	0.44601	0.44742
Alpha virt. eigenvalues --	0.44892	0.44936	0.44996	0.45153	0.45338
Alpha virt. eigenvalues --	0.45410	0.45616	0.45722	0.45770	0.45875
Alpha virt. eigenvalues --	0.46094	0.46125	0.46241	0.46336	0.46462
Alpha virt. eigenvalues --	0.46585	0.46688	0.46695	0.46804	0.46885
Alpha virt. eigenvalues --	0.47002	0.47196	0.47220	0.47398	0.47491
Alpha virt. eigenvalues --	0.47559	0.47639	0.47803	0.47927	0.48173
Alpha virt. eigenvalues --	0.48523	0.48621	0.48756	0.48887	0.49112
Alpha virt. eigenvalues --	0.49154	0.49345	0.49450	0.49569	0.49580
Alpha virt. eigenvalues --	0.49668	0.50194	0.50234	0.50620	0.50649
Alpha virt. eigenvalues --	0.50961	0.51270	0.51558	0.51808	0.52050
Alpha virt. eigenvalues --	0.52064	0.52153	0.52580	0.52832	0.53010
Alpha virt. eigenvalues --	0.53224	0.53321	0.53377	0.53685	0.54212
Alpha virt. eigenvalues --	0.54258	0.54383	0.54845	0.55303	0.55817
Alpha virt. eigenvalues --	0.56297	0.56483	0.56810	0.57135	0.57218
Alpha virt. eigenvalues --	0.57751	0.58093	0.58471	0.58566	0.59032
Alpha virt. eigenvalues --	0.59250	0.59462	0.59701	0.59979	0.60167
Alpha virt. eigenvalues --	0.60293	0.60540	0.60643	0.60662	0.60765
Alpha virt. eigenvalues --	0.60854	0.61060	0.61225	0.61435	0.61567
Alpha virt. eigenvalues --	0.61616	0.61662	0.61829	0.61958	0.62059
Alpha virt. eigenvalues --	0.62117	0.62320	0.62536	0.62815	0.63096
Alpha virt. eigenvalues --	0.63361	0.63440	0.63499	0.63574	0.63629
Alpha virt. eigenvalues --	0.63713	0.63904	0.63953	0.64145	0.64289
Alpha virt. eigenvalues --	0.64455	0.64562	0.64898	0.65013	0.65156
Alpha virt. eigenvalues --	0.65308	0.65402	0.65509	0.65625	0.65790
Alpha virt. eigenvalues --	0.65837	0.66000	0.66118	0.66221	0.66539
Alpha virt. eigenvalues --	0.66632	0.66723	0.66907	0.66943	0.67085
Alpha virt. eigenvalues --	0.67149	0.67330	0.67430	0.67672	0.67894
Alpha virt. eigenvalues --	0.68058	0.68312	0.68639	0.68751	0.68893
Alpha virt. eigenvalues --	0.69037	0.69092	0.69543	0.70418	0.70477
Alpha virt. eigenvalues --	0.70548	0.70859	0.71151	0.71492	0.71519
Alpha virt. eigenvalues --	0.71781	0.71833	0.72012	0.72244	0.72320

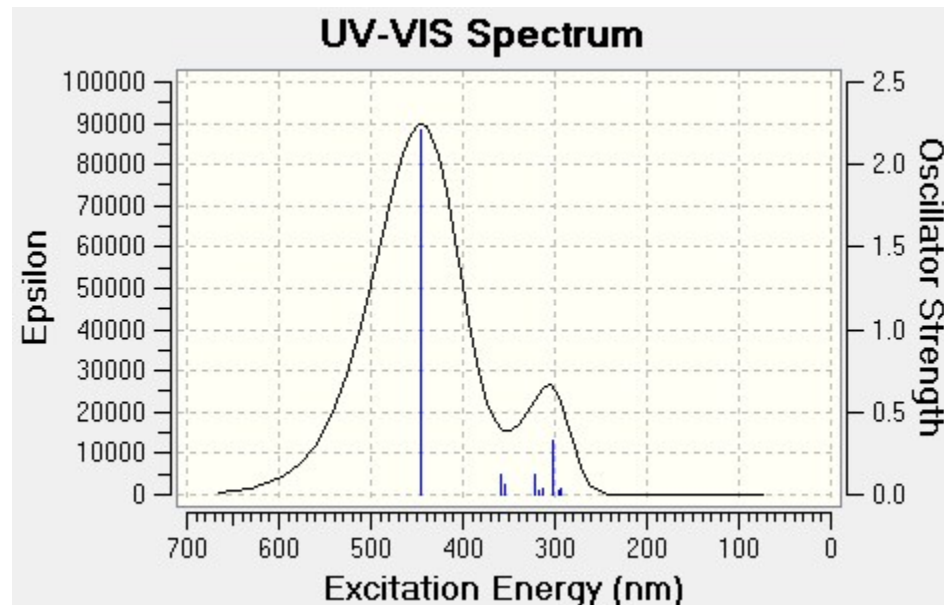
Alpha virt. eigenvalues --	0.72569	0.72819	0.73240	0.73446	0.73619
Alpha virt. eigenvalues --	0.73914	0.73963	0.74208	0.74467	0.74667
Alpha virt. eigenvalues --	0.74832	0.74984	0.75052	0.75307	0.75536
Alpha virt. eigenvalues --	0.75558	0.76115	0.76865	0.78120	0.79067
Alpha virt. eigenvalues --	0.79162	0.79651	0.79788	0.80093	0.80633
Alpha virt. eigenvalues --	0.81604	0.81804	0.82017	0.82479	0.83153
Alpha virt. eigenvalues --	0.83434	0.83831	0.84316	0.85167	0.85299
Alpha virt. eigenvalues --	0.85855	0.86031	0.86159	0.86360	0.86728
Alpha virt. eigenvalues --	0.86832	0.87165	0.87386	0.88181	0.88598
Alpha virt. eigenvalues --	0.88728	0.89024	0.89668	0.89856	0.90290
Alpha virt. eigenvalues --	0.90400	0.90442	0.90526	0.90785	0.90921
Alpha virt. eigenvalues --	0.91221	0.91403	0.91781	0.92215	0.92278
Alpha virt. eigenvalues --	0.93004	0.93128	0.93226	0.94118	0.94429
Alpha virt. eigenvalues --	0.94579	0.94947	0.95118	0.95443	0.95604
Alpha virt. eigenvalues --	0.95787	0.96247	0.96301	0.96744	0.97144
Alpha virt. eigenvalues --	0.97502	0.97681	0.97719	0.98065	0.98446
Alpha virt. eigenvalues --	0.98529	0.98718	0.99066	0.99586	0.99684
Alpha virt. eigenvalues --	0.99961	1.00500	1.00943	1.01202	1.01391
Alpha virt. eigenvalues --	1.01714	1.01943	1.02042	1.02422	1.02897
Alpha virt. eigenvalues --	1.03054	1.03421	1.03586	1.03871	1.04179
Alpha virt. eigenvalues --	1.04646	1.05552	1.05733	1.06285	1.07149
Alpha virt. eigenvalues --	1.07346	1.08352	1.08665	1.08820	1.09635
Alpha virt. eigenvalues --	1.10070	1.10362	1.10689	1.11080	1.11263
Alpha virt. eigenvalues --	1.11984	1.12460	1.14144	1.14309	1.14620
Alpha virt. eigenvalues --	1.14850	1.15050	1.15717	1.16028	1.16468
Alpha virt. eigenvalues --	1.17065	1.17685	1.17841	1.18070	1.18303
Alpha virt. eigenvalues --	1.18521	1.18688	1.18807	1.19656	1.20004
Alpha virt. eigenvalues --	1.20302	1.20859	1.21179	1.21264	1.21800
Alpha virt. eigenvalues --	1.21888	1.22423	1.23333	1.23600	1.24069
Alpha virt. eigenvalues --	1.24268	1.24800	1.25056	1.25180	1.25473
Alpha virt. eigenvalues --	1.25636	1.25791	1.26157	1.26348	1.26725
Alpha virt. eigenvalues --	1.27542	1.27898	1.28657	1.28789	1.29402
Alpha virt. eigenvalues --	1.29495	1.29775	1.29849	1.30378	1.30765
Alpha virt. eigenvalues --	1.31204	1.31344	1.31846	1.31915	1.32126
Alpha virt. eigenvalues --	1.32298	1.32658	1.33449	1.33817	1.34197
Alpha virt. eigenvalues --	1.34497	1.34812	1.35296	1.35519	1.36019
Alpha virt. eigenvalues --	1.36701	1.37214	1.37324	1.37700	1.37878
Alpha virt. eigenvalues --	1.38119	1.38483	1.38813	1.39459	1.39712
Alpha virt. eigenvalues --	1.39778	1.39987	1.40120	1.40127	1.40214
Alpha virt. eigenvalues --	1.40310	1.40531	1.40567	1.40897	1.41196
Alpha virt. eigenvalues --	1.41546	1.42169	1.42243	1.42451	1.42648
Alpha virt. eigenvalues --	1.42781	1.43005	1.43386	1.43572	1.44194
Alpha virt. eigenvalues --	1.44484	1.44623	1.44859	1.45071	1.45261
Alpha virt. eigenvalues --	1.45461	1.45689	1.46257	1.46341	1.46668
Alpha virt. eigenvalues --	1.46923	1.47002	1.47098	1.47608	1.48050
Alpha virt. eigenvalues --	1.48713	1.48970	1.49177	1.49280	1.49527
Alpha virt. eigenvalues --	1.49802	1.50052	1.50404	1.50535	1.50916
Alpha virt. eigenvalues --	1.51246	1.51607	1.51710	1.52221	1.52512

Alpha virt. eigenvalues --	1.52740	1.53508	1.53680	1.54594	1.55056
Alpha virt. eigenvalues --	1.55142	1.55303	1.55410	1.55560	1.55732
Alpha virt. eigenvalues --	1.56053	1.56149	1.56409	1.56617	1.56835
Alpha virt. eigenvalues --	1.57038	1.57308	1.57349	1.57445	1.57914
Alpha virt. eigenvalues --	1.58103	1.58460	1.58966	1.59116	1.59527
Alpha virt. eigenvalues --	1.59713	1.59998	1.60104	1.60364	1.60451
Alpha virt. eigenvalues --	1.60745	1.60949	1.61057	1.61346	1.61383
Alpha virt. eigenvalues --	1.61453	1.61628	1.61661	1.61711	1.62131
Alpha virt. eigenvalues --	1.62265	1.62372	1.62546	1.62669	1.62751
Alpha virt. eigenvalues --	1.62830	1.62949	1.63135	1.63350	1.63739
Alpha virt. eigenvalues --	1.64086	1.64189	1.64455	1.64611	1.64653
Alpha virt. eigenvalues --	1.64954	1.65195	1.65524	1.65903	1.66424
Alpha virt. eigenvalues --	1.66586	1.66852	1.67154	1.67248	1.67326
Alpha virt. eigenvalues --	1.67474	1.67883	1.68236	1.68549	1.68866
Alpha virt. eigenvalues --	1.69027	1.69090	1.69302	1.69883	1.69934
Alpha virt. eigenvalues --	1.70072	1.70311	1.70439	1.70578	1.70793
Alpha virt. eigenvalues --	1.70835	1.71178	1.71493	1.71667	1.72193
Alpha virt. eigenvalues --	1.72426	1.72771	1.72987	1.73195	1.73321
Alpha virt. eigenvalues --	1.73561	1.73728	1.74013	1.74119	1.74469
Alpha virt. eigenvalues --	1.74782	1.74858	1.75136	1.75386	1.75485
Alpha virt. eigenvalues --	1.75730	1.76173	1.76252	1.76425	1.76913
Alpha virt. eigenvalues --	1.77096	1.77267	1.77501	1.77642	1.77762
Alpha virt. eigenvalues --	1.78072	1.78504	1.79106	1.79486	1.79987
Alpha virt. eigenvalues --	1.80087	1.80579	1.80848	1.80982	1.81349
Alpha virt. eigenvalues --	1.81535	1.82052	1.82413	1.82451	1.82599
Alpha virt. eigenvalues --	1.82888	1.83383	1.83490	1.83845	1.83879
Alpha virt. eigenvalues --	1.84148	1.84190	1.84270	1.84580	1.84721
Alpha virt. eigenvalues --	1.84922	1.85170	1.85497	1.85656	1.85743
Alpha virt. eigenvalues --	1.86124	1.86406	1.86719	1.86886	1.87472
Alpha virt. eigenvalues --	1.88091	1.88683	1.88900	1.89144	1.89894
Alpha virt. eigenvalues --	1.90093	1.90667	1.90954	1.91615	1.91890
Alpha virt. eigenvalues --	1.92182	1.92542	1.93405	1.93671	1.93830
Alpha virt. eigenvalues --	1.94232	1.94636	1.94956	1.95372	1.95547
Alpha virt. eigenvalues --	1.95729	1.96108	1.96510	1.96761	1.96948
Alpha virt. eigenvalues --	1.97110	1.97359	1.98258	1.98353	1.98527
Alpha virt. eigenvalues --	1.98668	1.98754	1.98952	1.99032	1.99484
Alpha virt. eigenvalues --	1.99864	2.00362	2.00928	2.01151	2.01790
Alpha virt. eigenvalues --	2.01865	2.02355	2.02554	2.03054	2.03920
Alpha virt. eigenvalues --	2.04341	2.04618	2.04851	2.05426	2.05668
Alpha virt. eigenvalues --	2.05930	2.06323	2.06470	2.07138	2.07378
Alpha virt. eigenvalues --	2.07727	2.07805	2.08173	2.08439	2.08789
Alpha virt. eigenvalues --	2.09672	2.10639	2.11046	2.11299	2.11475
Alpha virt. eigenvalues --	2.11753	2.12272	2.12393	2.12971	2.13110
Alpha virt. eigenvalues --	2.13371	2.14191	2.15098	2.15807	2.15920
Alpha virt. eigenvalues --	2.16155	2.16198	2.16896	2.17515	2.18181
Alpha virt. eigenvalues --	2.18304	2.18602	2.18822	2.19368	2.20029
Alpha virt. eigenvalues --	2.20239	2.20619	2.21011	2.21358	2.22314
Alpha virt. eigenvalues --	2.23290	2.23584	2.23982	2.24495	2.24907

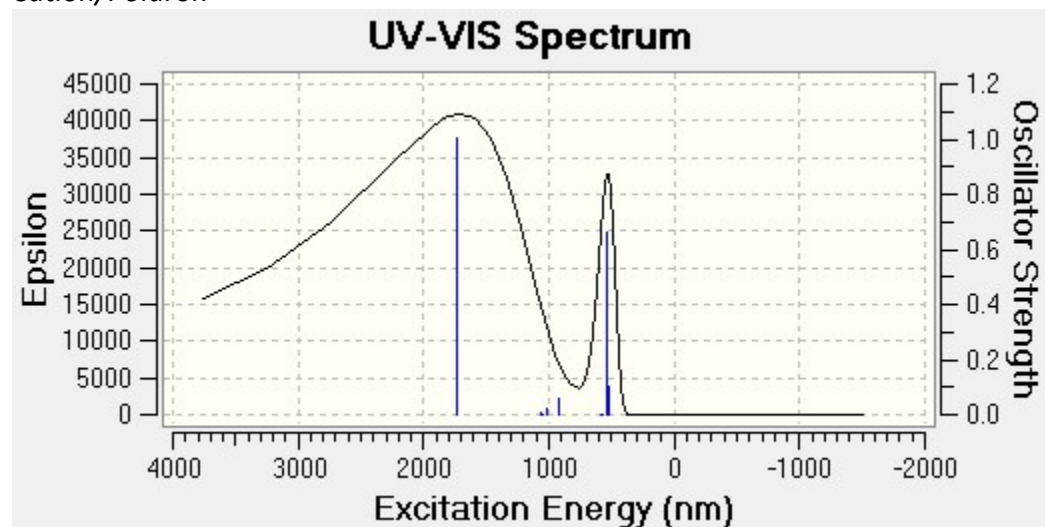
Alpha virt. eigenvalues --	2.25237	2.25496	2.25573	2.26294	2.28348
Alpha virt. eigenvalues --	2.28671	2.28991	2.30075	2.30366	2.30745
Alpha virt. eigenvalues --	2.32200	2.32412	2.32756	2.32823	2.33138
Alpha virt. eigenvalues --	2.34485	2.35947	2.36356	2.36684	2.37095
Alpha virt. eigenvalues --	2.37770	2.38040	2.38183	2.38501	2.38826
Alpha virt. eigenvalues --	2.39000	2.39306	2.41036	2.41295	2.41394
Alpha virt. eigenvalues --	2.41449	2.41516	2.41769	2.42044	2.42093
Alpha virt. eigenvalues --	2.42373	2.42672	2.43037	2.43392	2.43569
Alpha virt. eigenvalues --	2.43718	2.43903	2.44160	2.44392	2.44410
Alpha virt. eigenvalues --	2.44679	2.44777	2.45572	2.45977	2.46011
Alpha virt. eigenvalues --	2.46512	2.46762	2.46912	2.47141	2.47526
Alpha virt. eigenvalues --	2.47664	2.48123	2.48261	2.48425	2.48818
Alpha virt. eigenvalues --	2.49026	2.49595	2.50252	2.50560	2.51714
Alpha virt. eigenvalues --	2.52091	2.52111	2.53185	2.54487	2.54782
Alpha virt. eigenvalues --	2.54939	2.55933	2.55965	2.56275	2.56496
Alpha virt. eigenvalues --	2.56588	2.58390	2.62700	2.63090	2.64257
Alpha virt. eigenvalues --	2.64765	2.65261	2.65974	2.66595	2.67162
Alpha virt. eigenvalues --	2.68458	2.68973	2.69406	2.70461	2.71388
Alpha virt. eigenvalues --	2.72355	2.72781	2.74509	2.77147	2.78985
Alpha virt. eigenvalues --	2.79593	2.81643	2.82357	2.87398	2.88134
Alpha virt. eigenvalues --	2.88805	2.89538	2.90372	2.91422	2.91645
Alpha virt. eigenvalues --	2.91951	2.92748	2.94714	2.95313	2.95923
Alpha virt. eigenvalues --	2.97063	2.97314	2.97650	2.97972	2.98221
Alpha virt. eigenvalues --	2.98456	3.00859	3.01156	3.01170	3.02255
Alpha virt. eigenvalues --	3.02457	3.03143	3.06313	3.06537	3.06808
Alpha virt. eigenvalues --	3.07062	3.07261	3.07558	3.07625	3.08192
Alpha virt. eigenvalues --	3.08507	3.10243	3.10641	3.10790	3.11027
Alpha virt. eigenvalues --	3.11218	3.11355	3.22648	3.22818	3.23055
Alpha virt. eigenvalues --	3.24597	3.24850	3.25114	3.27949	3.28686
Alpha virt. eigenvalues --	3.29067	3.34665	3.35328	3.35622	3.35749
Alpha virt. eigenvalues --	3.35863	3.36042	3.36823	3.37527	3.38201
Alpha virt. eigenvalues --	3.39459	3.40223	3.40387	3.43863	3.45323
Alpha virt. eigenvalues --	3.47597	3.49387	3.50881	3.56703	

Yellow UV-Vis Spectrum Epsilon/Oscillator Strength – N = 3

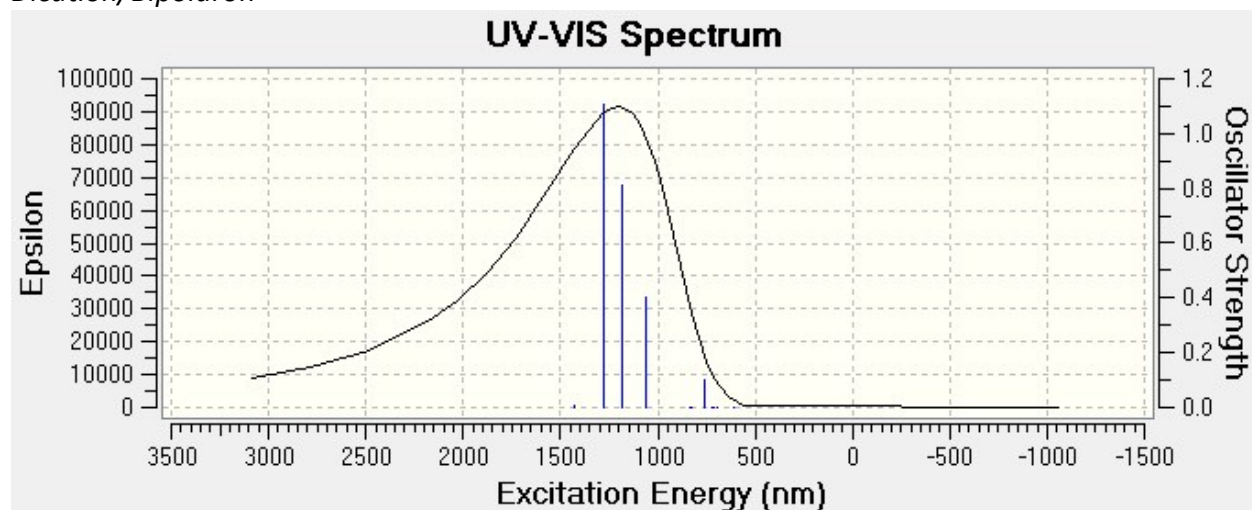
Neutral



Cation/Polaron



Dication/Bipolaron



Yellow Table of Excited States – N = 3

Neutral – 10 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	2.78	445.87	2.2136
2	3.45	358.97	0.1178
3	3.51	353.40	0.0570
4	3.86	321.53	0.1200
5	3.91	317.20	0.0187
6	3.97	312.03	0.0330
7	4.10	302.70	0.3307
8	4.12	301.27	0.1157
9	4.20	295.05	0.0259
10	4.24	292.50	0.0383

Cation/Polaron – 15 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	0.72	1728.42	1.0002
2	1.16	1069.93	0.0075
3	1.18	1050.66	0.0014
4	1.21	1023.74	0.0196
5	1.34	927.49	0.0593
6	2.12	585.44	0.0027
7	2.12	583.52	0.0008
8	2.13	581.76	0.0000
9	2.18	567.64	0.0004
10	2.19	566.67	0.0011
11	2.19	566.24	0.0001
12	2.28	544.79	0.0351
13	2.33	531.07	0.6633
14	2.36	525.09	0.1021
15	2.41	514.58	0.0118

Dication/Bipolaron – 13 Lowest ES

<u>Excited state</u>	<u>Energy (eV)</u>	<u>Wavelength (nm)</u>	<u>Oscillator Strength</u>
1	0.87	1424.08	0.0073
2	0.97	1278.69	1.1071
3	1.04	1185.55	0.8093
4	1.16	1064.47	0.4019
5	1.48	838.37	0.0001
6	1.49	833.41	0.0000
7	1.49	829.82	0.0000
8	1.62	763.15	0.1038
9	1.72	721.01	0.0002
10	1.74	713.03	0.0018
11	1.74	710.97	0.0013
12	1.78	695.75	0.0017
13	2.04	607.22	0.0021