

Supplementary Information

Particle on a Hollow Cylinder: the Triple Ring Tubular Cluster B_{27}^+

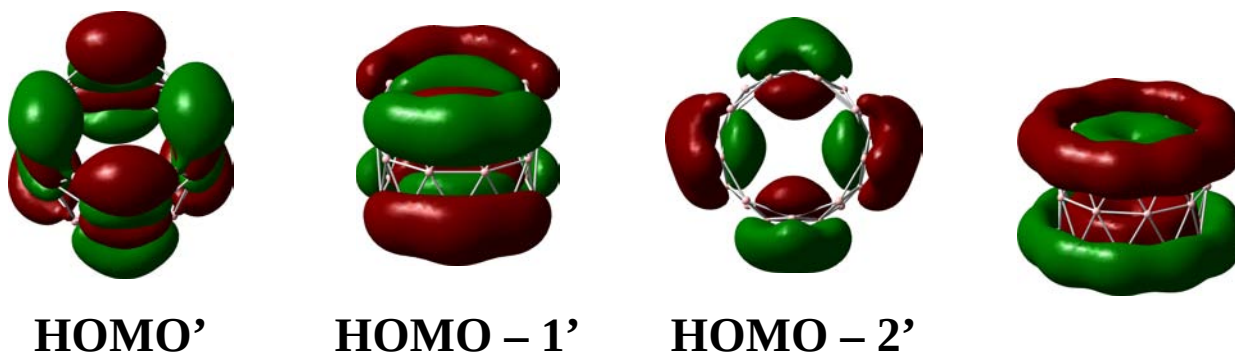
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This file contains:

Figure S1: the shapes of the HOMOs and the ring current maps of these MOs of B_{27}^+ .



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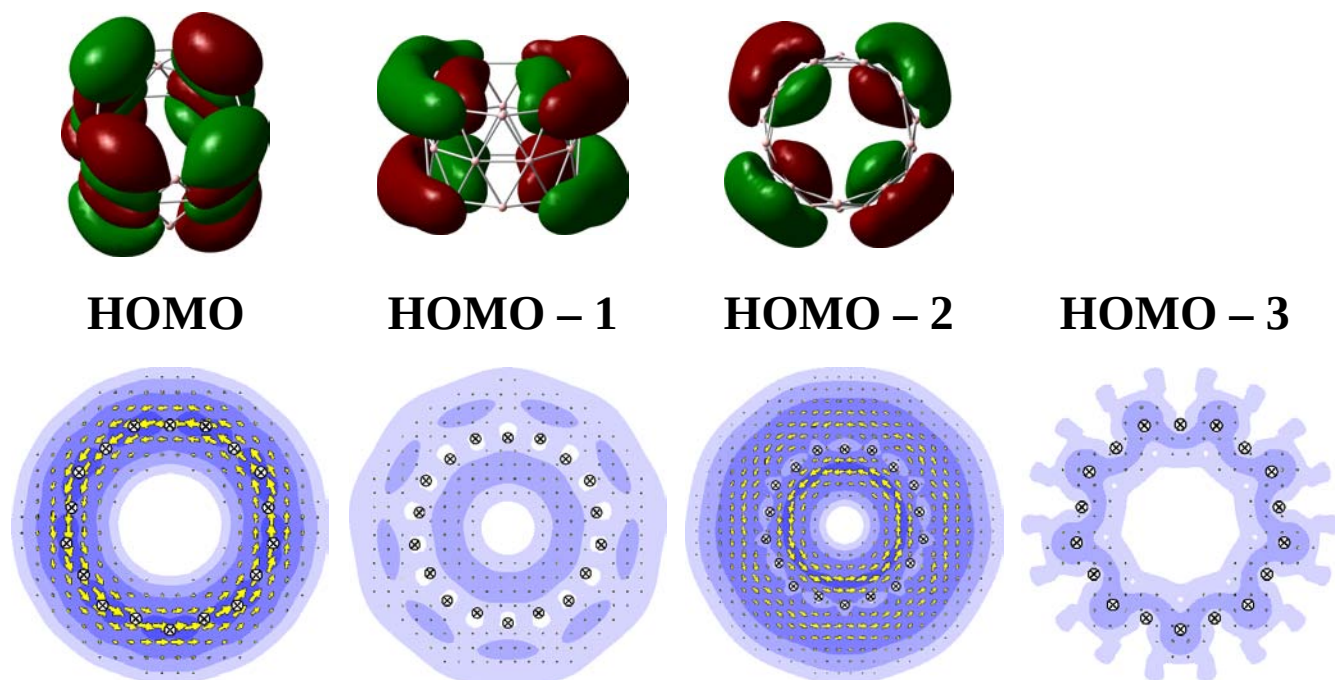


Figure S1. the HOMOs and their contributions to the ring current maps of B_{27}^+

Table S1: The coordinates of all structures given in the figure 1.

dc-TR-1 ($C_1 - {}^2A$)

B	2.54020	-0.32977	1.20192
B	-1.42608	0.97519	2.13103
B	0.00000	1.72223	2.24295
B	1.01117	2.29240	1.15889
B	1.30359	2.45339	-0.41756
B	0.59741	2.05586	-1.79050
B	-0.74677	1.35445	-2.31315
B	-2.06684	0.59095	-1.82277
B	-2.71059	0.28604	-0.39741
B	-2.54020	0.32977	1.20192
B	1.42608	-0.97519	2.13103
B	2.71059	-0.28604	-0.39741
B	0.00000	0.00000	2.49603
B	1.39455	0.76231	1.88921
B	2.14300	1.16822	0.43437
B	1.87900	1.03101	-1.24735

B	0.75052	0.40567	-2.31766
B	-0.75052	-0.40567	-2.31766
B	-1.87900	-1.03101	-1.24735
B	-1.01117	-2.29240	1.15889
B	0.00000	-1.72223	2.24295
B	-1.39455	-0.76231	1.88921
B	0.74677	-1.35445	-2.31315
B	2.06684	-0.59095	-1.82277
B	-0.59741	-2.05586	-1.79050
B	-1.30359	-2.45339	-0.41756
B	-2.14300	-1.16822	0.43437

dc-DR-2 ($C_s - {}^2A'$)

B	-1.62044	2.58842	1.03267
B	-2.77223	1.48535	0.80237
B	-3.37850	-0.00000	0.35229
B	-2.77223	-1.48535	0.80237
B	-1.62044	-2.58842	1.03267
B	-0.11327	-3.14640	1.00416
B	1.49135	-3.04878	0.82932
B	2.83393	-2.19980	0.61316
B	3.62538	-0.80127	0.46391
B	3.62538	0.80128	0.46391
B	2.83393	2.19980	0.61316
B	1.49135	3.04878	0.82932
B	-0.11327	3.14640	1.00416
B	-1.07276	3.33049	-0.40404
B	-2.49278	2.60049	-0.42793
B	-3.56693	1.37906	-0.68744
B	-3.56693	-1.37907	-0.68744
B	-2.49278	-2.60050	-0.42793
B	-1.07275	-3.33049	-0.40404
B	0.55129	-3.41054	-0.54106
B	2.03084	-2.80209	-0.76493
B	3.08659	-1.57769	-0.94994
B	3.46637	0.00000	-1.02735
B	3.08658	1.57769	-0.94994
B	2.03084	2.80209	-0.76493
B	0.55129	3.41054	-0.54106
B	-4.04981	-0.00000	-1.26544

dc-QP-3 ($C_1 - {}^2A$)

B	0.64383	0.72909	-0.02770
B	2.08140	-2.42710	-0.05727

B	3.24046	2.00582	0.08619
B	-1.53850	2.54202	0.02170
B	-2.68693	0.99806	0.01969
B	-1.14425	-2.16531	0.03068
B	2.98086	-0.96237	-0.38417
B	-1.97800	-0.55033	-0.15779
B	-3.66675	-0.56548	0.15376
B	3.65543	-2.38530	0.18788
B	-3.10294	2.65673	0.02005
B	-5.33743	-1.06911	0.26525
B	-4.30274	-2.18659	0.05300
B	-5.21798	0.44609	0.24161
B	-2.73923	-2.11818	-0.03503
B	-0.26919	-0.69048	-0.23867
B	1.33818	-0.82513	-0.01694
B	2.30399	0.57744	-0.39013
B	1.64336	2.18191	-0.20855
B	-0.98094	0.86913	-0.39952
B	-4.31646	1.73433	0.11368
B	0.02376	2.30706	-0.08276
B	3.90898	0.39741	-0.01122
B	4.83018	1.67970	0.34765
B	0.44129	-2.26779	-0.16651
B	4.71380	-1.16797	0.23496
B	5.47584	0.25636	0.40018

c-TR-1 ($D_{9h} - {}^1A_1'$)

B	2.02281	1.16787	1.53403
B	-0.79887	2.19488	-1.53403
B	0.79887	2.19488	-1.53403
B	2.02281	1.16787	-1.53403
B	2.30025	-0.40560	-1.53403
B	1.50138	-1.78928	-1.53403
B	0.00000	-2.33574	-1.53403
B	-1.50138	-1.78928	-1.53403
B	-2.30025	-0.40560	-1.53403
B	-2.02281	1.16787	-1.53403
B	0.79887	2.19488	1.53403
B	2.30025	-0.40560	1.53403
B	0.00000	2.45786	0.00000
B	1.57988	1.88283	0.00000
B	2.42052	0.42680	0.00000
B	2.12857	-1.22893	0.00000
B	0.84064	-2.30963	0.00000
B	-0.84064	-2.30963	0.00000

B	-2.12857	-1.22893	0.00000
B	-2.02281	1.16787	1.53403
B	-0.79887	2.19488	1.53403
B	-1.57988	1.88283	0.00000
B	0.00000	-2.33574	1.53403
B	1.50138	-1.78928	1.53403
B	-1.50138	-1.78928	1.53403
B	-2.30025	-0.40560	1.53403
B	-2.42052	0.42680	0.00000

c-DR-2 ($C_s - {}^1A'$)

B	-1.61469	2.56231	1.03525
B	-2.75074	1.45662	0.81140
B	-3.39789	-0.00001	0.34484
B	-2.75074	-1.45663	0.81140
B	-1.61468	-2.56230	1.03524
B	-0.10623	-3.10542	1.00573
B	1.49886	-3.04152	0.82998
B	2.82671	-2.19034	0.61508
B	3.64046	-0.79394	0.46234
B	3.64048	0.79396	0.46233
B	2.82669	2.19034	0.61508
B	1.49885	3.04153	0.82998
B	-0.10624	3.10541	1.00573
B	-1.07908	3.30789	-0.40186
B	-2.48676	2.58237	-0.42959
B	-3.58262	1.37474	-0.68585
B	-3.58262	-1.37475	-0.68584
B	-2.48675	-2.58238	-0.42959
B	-1.07907	-3.30790	-0.40186
B	0.55399	-3.37516	-0.55005
B	2.02729	-2.79576	-0.76954
B	3.07952	-1.56384	-0.95380
B	3.47438	0.00001	-1.03390
B	3.07952	1.56385	-0.95380
B	2.02728	2.79576	-0.76954
B	0.55398	3.37517	-0.55005
B	-4.08992	-0.00001	-1.24909

c-QP-3 ($C_s - {}^1A'$)

B	-0.90251	0.35752	1.69936
B	-0.48337	1.70306	0.89398
B	-1.09930	-1.05581	2.52201
B	-1.35780	-1.16934	0.85230
B	-1.35780	-1.16934	-0.85230

B	-1.09930	-1.05581	-2.52201
B	-0.48337	1.70306	-0.89398
B	-0.90251	0.35752	-1.69936
B	-0.08905	0.09321	3.21252
B	-0.00071	1.60859	2.56877
B	-0.13446	-2.17211	1.65525
B	-0.74174	0.26311	0.00000
B	-0.13446	-2.17211	-1.65525
B	-0.08905	0.09321	-3.21252
B	0.03644	3.03856	0.00000
B	-0.00071	1.60859	-2.56877
B	1.33382	-2.60174	-2.35478
B	0.56860	-1.38582	-3.07881
B	1.09804	-3.01494	-0.85554
B	1.09804	-3.01494	0.85554
B	1.33382	-2.60174	2.35478
B	0.56860	-1.38582	3.07881
B	1.05296	4.09665	-0.78357
B	0.42977	2.96816	-1.74111
B	1.05296	4.09665	0.78357
B	0.42977	2.96816	1.74111
B	-0.12668	-2.15655	0.00000

c-QP-4 ($C_s - {}^1A'$)

B	-4.25774	0.80767	-0.60679
B	1.29457	-2.84924	-0.27962
B	3.08864	0.00017	0.56095
B	-0.17888	0.00000	1.26401
B	-1.09381	1.35725	0.45946
B	2.12301	1.37159	-0.02809
B	3.78585	1.45685	-0.39944
B	-0.40595	2.72552	-0.18135
B	-3.53033	2.16929	-0.58260
B	-2.01139	-2.59327	-0.33521
B	-1.78640	-0.00021	1.26856
B	-2.78128	-0.99613	0.34103
B	2.85425	-2.77041	-0.48474
B	-1.09350	-1.35764	0.45961
B	-2.01171	2.59306	-0.33525
B	1.29406	2.84921	-0.27981
B	2.85380	2.77078	-0.48458
B	4.41674	0.00034	-0.47416
B	1.46340	0.00004	0.83741
B	0.52051	1.45451	0.36967
B	-2.78165	0.99511	0.34043
B	0.52082	-1.45469	0.36996

B	2.12325	-1.37146	-0.02794
B	-3.52986	-2.16928	-0.58320
B	3.78601	-1.45626	-0.39951
B	-4.25697	-0.80737	-0.60684
B	-0.40546	-2.72545	-0.18195

n-TR-1 ($C_1 - {}^2A$)

B	2.19386	-0.39383	-1.51330
B	-0.08021	-2.28842	1.52157
B	1.41008	-1.71445	1.56667
B	2.35992	-0.43209	1.53457
B	1.89978	1.10607	1.56175
B	0.82136	2.29476	1.50292
B	-0.75827	2.03626	1.53013
B	-2.15216	1.24414	1.46539
B	-2.19936	-0.36435	1.51479
B	-1.64142	-1.85367	1.47184
B	1.62399	-1.87904	-1.46811
B	2.16423	1.21450	-1.46751
B	0.81518	-2.27335	0.02589
B	2.20371	-1.28549	0.02549
B	2.41523	0.40701	0.02343
B	1.58144	1.85365	0.01145
B	0.01455	2.50104	-0.00139
B	-1.56218	1.87393	-0.01376
B	-2.40639	0.43278	-0.02393
B	-1.43204	-1.70532	-1.56399
B	0.05431	-2.28636	-1.52045
B	-0.84279	-2.27010	-0.02457
B	-0.79477	2.29926	-1.50639
B	0.78276	2.02875	-1.53304
B	-1.88686	1.12414	-1.56326
B	-2.36431	-0.40897	-1.53298
B	-2.21963	-1.26087	-0.02320

n-DR-2 ($C_s - {}^2A'$)

B	1.61462	-2.59770	1.02296
B	2.73835	-1.48666	0.82704
B	3.34234	0.00013	0.36883
B	2.73822	1.48688	0.82703
B	1.61436	2.59779	1.02295
B	0.10424	3.16217	0.99436
B	-1.48481	3.05899	0.82287
B	-2.82724	2.19841	0.62239
B	-3.61238	0.80236	0.48773
B	-3.61245	-0.80270	0.48768

B	-2.82693	-2.19852	0.62243
B	-1.48458	-3.05921	0.82284
B	0.10450	-3.16206	0.99436
B	1.06982	-3.31563	-0.43497
B	2.48889	-2.58916	-0.43967
B	3.56650	-1.38055	-0.68577
B	3.56633	1.38082	-0.68580
B	2.48867	2.58936	-0.43966
B	1.06952	3.31570	-0.43499
B	-0.55190	3.38852	-0.57353
B	-2.02586	2.78972	-0.77717
B	-3.07477	1.56418	-0.94637
B	-3.46181	-0.00014	-1.01658
B	-3.07463	-1.56442	-0.94638
B	-2.02561	-2.78989	-0.77718
B	-0.55160	-3.38854	-0.57354
B	4.10822	0.00016	-1.19185

n-BB-1 ($C_s - {}^2A'$)

B	0.18389	-1.58552	0.73548
B	1.61918	-0.83733	0.33687
B	-1.17929	-2.41123	1.02330
B	-1.32350	-0.81256	1.35118
B	-1.32351	0.81259	1.35118
B	-1.17925	2.41125	1.02329
B	1.61918	0.83730	0.33688
B	0.18393	1.58554	0.73550
B	-0.13186	-3.08355	-0.04454
B	1.36789	-2.45695	-0.18633
B	-2.46206	-1.64674	0.26793
B	4.30164	1.37368	-0.43976
B	-2.46202	1.64679	0.26790
B	-0.13177	3.08358	-0.04452
B	3.19809	0.00002	-0.09011
B	1.36796	2.45694	-0.18630
B	-2.96639	2.32699	-1.18863
B	-1.68760	3.03126	-0.57841
B	-3.39027	0.84610	-0.90205
B	-3.39031	-0.84604	-0.90201
B	-2.96649	-2.32696	-1.18857
B	-1.68770	-3.03126	-0.57837
B	4.95807	-0.00005	-0.42879
B	2.83697	1.87890	-0.28644
B	4.30158	-1.37375	-0.43977
B	2.83693	-1.87901	-0.28647
B	-2.49330	0.00002	0.34156

n-QP-4 ($C_s - {}^2A'$)

B	-0.84503	0.37873	1.71125
B	-0.55640	1.75473	0.89196
B	-1.08192	-1.04122	2.51682
B	-1.33469	-1.13264	0.85210
B	-1.33469	-1.13264	-0.85210
B	-1.08192	-1.04122	-2.51682
B	-0.55640	1.75473	-0.89196
B	-0.84503	0.37873	-1.71125
B	-0.02476	0.09834	3.19869
B	0.01784	1.62358	2.57674
B	-0.11734	-2.14746	1.64654
B	-0.82996	0.34009	0.00000
B	-0.11734	-2.14746	-1.64654
B	-0.02476	0.09834	-3.19869
B	0.04144	3.05504	0.00000
B	0.01784	1.62358	-2.57674
B	1.27963	-2.68393	-2.38041
B	0.56140	-1.42692	-3.09203
B	1.03960	-3.08044	-0.85440
B	1.03960	-3.08044	0.85440
B	1.27963	-2.68393	2.38041
B	0.56140	-1.42692	3.09203
B	1.06713	4.09178	-0.78125
B	0.46262	2.95729	-1.74775
B	1.06713	4.09178	0.78125
B	0.46262	2.95729	1.74775
B	-0.14765	-2.17882	0.00000

a-QP-1 ($C_s - {}^1A'$)

B	-4.24842	0.79978	-0.67535
B	1.28374	-2.84381	-0.25279
B	3.11811	-0.00015	0.41682
B	-0.18067	0.00040	1.18551
B	-1.10743	1.36134	0.51934
B	2.15206	1.45359	0.14330
B	3.78892	1.45402	-0.43751
B	-0.41215	2.72143	-0.15462
B	-3.53602	2.15934	-0.57425
B	-2.01763	-2.57495	-0.31454
B	-1.82660	0.00038	1.28192
B	-2.79700	-0.96026	0.32014
B	2.85855	-2.78623	-0.49599
B	-1.10763	-1.36131	0.52095
B	-2.01692	2.57631	-0.31466

B	1.28452	2.84323	-0.25198
B	2.85950	2.78626	-0.49407
B	4.46737	-0.00020	-0.53222
B	1.46532	-0.00053	0.84049
B	0.51401	1.39385	0.32320
B	-2.79729	0.95943	0.32009
B	0.51362	-1.39471	0.32459
B	2.15165	-1.45411	0.14289
B	-3.53721	-2.15916	-0.57356
B	3.78795	-1.45411	-0.43855
B	-4.24764	-0.79836	-0.67546
B	-0.41268	-2.72148	-0.15369

a-QP-2 ($C_1 - {}^1A$)

B	0.64383	0.72909	-0.02770
B	2.08140	-2.42710	-0.05727
B	3.24046	2.00582	0.08619
B	-1.53850	2.54202	0.02170
B	-2.68693	0.99806	0.01969
B	-1.14425	-2.16531	0.03068
B	2.98086	-0.96237	-0.38417
B	-1.97800	-0.55033	-0.15779
B	-3.66675	-0.56548	0.15376
B	3.65543	-2.38530	0.18788
B	-3.10294	2.65673	0.02005
B	-5.33743	-1.06911	0.26525
B	-4.30274	-2.18659	0.05300
B	-5.21798	0.44609	0.24161
B	-2.73923	-2.11818	-0.03503
B	-0.26919	-0.69048	-0.23867
B	1.33818	-0.82513	-0.01694
B	2.30399	0.57744	-0.39013
B	1.64336	2.18191	-0.20855
B	-0.98094	0.86913	-0.39952
B	-4.31646	1.73433	0.11368
B	0.02376	2.30706	-0.08276
B	3.90898	0.39741	-0.01122
B	4.83018	1.67970	0.34765
B	0.44129	-2.26779	-0.16651
B	4.71380	-1.16797	0.23496
B	5.47584	0.25636	0.40018

a-DR-3 ($C_s - {}^1A'$)

B	1.60000	-2.61624	1.00542
B	2.73889	-1.52466	0.84232
B	3.26835	-0.00209	0.39719

B	2.74122	1.52118	0.84254
B	1.60392	2.61447	1.00540
B	0.10914	3.24355	0.96968
B	-1.46760	3.07747	0.81232
B	-2.83149	2.21687	0.62913
B	-3.58871	0.81397	0.52083
B	-3.58877	-0.80893	0.52133
B	-2.83536	-2.21392	0.62895
B	-1.47165	-3.07474	0.81265
B	0.10471	-3.24427	0.96957
B	1.06211	-3.32955	-0.46987
B	2.48325	-2.57974	-0.46571
B	3.57690	-1.39095	-0.66552
B	3.57994	1.38661	-0.66480
B	2.48701	2.57654	-0.46584
B	1.06697	3.32830	-0.46976
B	-0.54579	3.37731	-0.60961
B	-2.03783	2.79478	-0.78411
B	-3.07057	1.56131	-0.93346
B	-3.47901	0.00226	-0.99064
B	-3.07298	-1.55747	-0.93333
B	-2.04180	-2.79217	-0.78397
B	-0.55066	-3.37720	-0.60947
B	4.15981	-0.00266	-1.11123

a-TR-4 ($C_1 - {}^1A$)

B	0.72866	1.96477	1.53119
B	-2.11782	1.19498	-1.47339
B	-0.70919	1.97101	-1.53088
B	0.84930	2.34686	-1.48102
B	1.88336	1.09994	-1.54284
B	2.41664	-0.42949	-1.52835
B	1.32897	-1.60641	-1.59937
B	-0.16295	-2.17643	-1.51046
B	-1.79849	-1.96145	-1.39180
B	-2.14773	-0.41056	-1.50976
B	-0.82675	2.35329	1.48130
B	2.13014	1.17567	1.47321
B	-1.53475	1.83469	-0.00787
B	0.01174	2.55556	-0.00022
B	1.55159	1.82044	0.00764
B	2.38019	0.37983	-0.01732
B	2.31706	-1.35015	-0.05887
B	0.80545	-2.18545	-0.05987
B	-0.82697	-2.18049	0.06019
B	-2.42146	-0.40689	1.52814

B	-1.87391	1.11747	1.54323
B	-2.37467	0.40119	0.01702
B	1.77967	-1.97751	1.39178
B	2.14361	-0.42987	1.50957
B	0.14192	-2.17908	1.51029
B	-1.34403	-1.59353	1.59923
B	-2.32958	-1.32838	0.05923

da-QP-1 ($C_1 - {}^2A$)

B	-6.06533	-1.28145	-0.07874
B	4.94827	2.13282	0.26704
B	3.58523	-1.93088	0.01273
B	-1.23373	-1.66062	0.17855
B	-1.97915	-0.05055	0.22951
B	1.26103	-0.18870	0.26707
B	3.85053	1.02971	-0.30025
B	-1.09217	1.44322	-0.06617
B	-4.33312	1.59931	-0.15082
B	-5.17213	0.09584	0.20444
B	-2.85191	-1.57235	0.13799
B	-4.47549	-1.51492	0.09308
B	-6.77053	0.14305	-0.13124
B	-5.93845	1.48866	-0.28884
B	-2.71072	1.51060	-0.10038
B	0.50890	1.33041	-0.07838
B	2.12667	1.44220	0.10679
B	2.86286	-0.33962	-0.19123
B	1.96266	-1.76669	0.05968
B	-0.35403	-0.15340	-0.10288
B	-3.56827	-0.00175	-0.07068
B	0.35889	-1.71023	0.23640
B	4.52271	-0.52075	-0.31083
B	5.21228	-1.97467	-0.10017
B	3.42978	2.38431	0.52327
B	5.75404	0.80648	-0.12084
B	6.16116	-0.74005	-0.22510

da-QP-2 ($C_1 - {}^2A$)

B	0.62977	0.73378	-0.13257
B	2.08464	-2.44084	0.00645
B	3.24349	2.03482	0.00592
B	-1.53316	2.56931	0.03101
B	-2.70400	0.99366	-0.01423
B	-1.14661	-2.20098	-0.02159
B	2.97506	-0.96284	-0.20212
B	-1.98635	-0.54006	-0.18477

B	-3.65166	-0.58816	0.18086
B	3.68278	-2.44498	0.10833
B	-3.09058	2.66839	0.06203
B	-5.31445	-1.06570	0.27062
B	-4.29781	-2.19464	-0.00017
B	-5.17253	0.44654	0.27378
B	-2.73565	-2.15081	-0.06649
B	-0.27794	-0.68958	-0.18035
B	1.33315	-0.80905	-0.17611
B	2.30125	0.57544	-0.41053
B	1.64493	2.20841	-0.16277
B	-1.00065	0.87001	-0.35893
B	-4.31169	1.76045	0.14282
B	0.02616	2.32150	-0.08487
B	3.87606	0.40903	0.09513
B	4.84022	1.69188	0.25275
B	0.43819	-2.27982	-0.11629
B	4.68597	-1.17364	0.27860
B	5.46143	0.25789	0.40348

da-DR-3 (C_s – ²A')

B	-1.61659	2.59833	0.99560
B	-2.76200	1.51480	0.84430
B	-3.32729	-0.00002	0.42607
B	-2.76197	-1.51482	0.84429
B	-1.61654	-2.59833	0.99560
B	-0.11049	-3.21601	0.95377
B	1.47344	-3.05016	0.80764
B	2.85413	-2.22570	0.62647
B	3.61007	-0.80730	0.52333
B	3.61010	0.80735	0.52332
B	2.85408	2.22572	0.62647
B	1.47341	3.05021	0.80764
B	-0.11054	3.21598	0.95377
B	-1.05203	3.28748	-0.48148
B	-2.48370	2.53769	-0.46743
B	-3.58731	1.35664	-0.68529
B	-3.58729	-1.35669	-0.68528
B	-2.48367	-2.53774	-0.46742
B	-1.05198	-3.28747	-0.48148
B	0.55380	-3.36728	-0.60525
B	2.05891	-2.78374	-0.77681
B	3.10095	-1.56143	-0.92448
B	3.52414	0.00002	-0.97733
B	3.10092	1.56146	-0.92449
B	2.05887	2.78377	-0.77680

B	0.55375	3.36728	-0.60525
B	-4.27516	-0.00003	-1.06946

da-QP-4 ($C_s - {}^2A'$)

B	4.19775	-0.80819	-0.71203
B	-1.27583	2.90945	-0.15860
B	-3.07970	-0.00001	0.31366
B	0.19495	0.00000	1.06877
B	1.13431	-1.42558	0.66181
B	-2.14027	-1.48337	0.13842
B	-3.75908	-1.46062	-0.46305
B	0.40322	-2.80335	-0.02051
B	3.50138	-2.17260	-0.65275
B	1.98909	2.57376	-0.32443
B	1.85286	0.00002	1.31126
B	2.74149	0.98145	0.24463
B	-2.85372	2.82118	-0.47247
B	1.13429	1.42559	0.66183
B	1.98909	-2.57373	-0.32442
B	-1.27583	-2.90943	-0.15853
B	-2.85370	-2.82117	-0.47244
B	-4.43350	-0.00002	-0.62238
B	-1.42676	-0.00002	0.74433
B	-0.49223	-1.42102	0.35110
B	2.74148	-0.98138	0.24455
B	-0.49225	1.42102	0.35111
B	-2.14028	1.48338	0.13844
B	3.50136	2.17257	-0.65277
B	-3.75905	1.46057	-0.46305
B	4.19770	0.80813	-0.71200
B	0.40322	2.80337	-0.02049