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Electronic Supplementary Information: Absorption Shifts of Diastereotopically Ligated Chlorophyll Dimers of Photosystem I

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Benchmark data

Table 1 Benchmarking vertical excitation energies (VEEs, in eV) and oscillator strengths (*f*) of a chlorophyll (Chl) monomer at the *ab initio* ADC(2) and CC2 levels as well as at the TDDFT level using different functionals and def2-SVP basis sets.

VEE	*f*	VEE	*f*	VEE	*f*
ADC(2)		RVS-ADC(2)		LT-SOS-ADC(2)	
1.99	0.281	2.04	0.293	1.96	0.236
2.11	0.047	2.17	0.048	2.34	0.039
3.01	0.755	3.07	0.772	3.25	1.115
3.11	1.031	3.18	1.010	3.46	1.148
3.25	0.057	3.30	0.073	3.52	0.018
3.32	0.000	3.37	0.000	3.61	0.299
3.37	0.017	3.42	0.018	3.87	0.009
3.63	0.147	3.70	0.148	3.91	0.106
CC2		RVS-CC2		LT-SOS-CC2	
2.18	0.237	2.21	0.249	2.04	0.207
2.31	0.050	2.35	0.051	2.37	0.026
3.22	0.765	3.26	0.781	3.38	0.951
3.32	0.960	3.36	0.968	3.57	1.166
3.38	0.088	3.42	0.078	3.60	0.007
3.43	0.024	3.47	0.032	3.69	0.143
3.54	0.015	3.56	0.016	3.99	0.090
3.76	0.151	3.81	0.150	4.03	0.006
ωB97X		CAM-B3LYP		BHLYP	
2.22	0.287	2.24	0.300	2.29	0.346
2.60	0.038	2.52	0.029	2.56	0.024
3.66	0.100	3.50	0.069	3.57	0.074
3.87	0.062	3.74	0.071	3.85	1.188
3.91	1.320	3.79	0.835	3.90	0.035
4.02	0.099	3.84	0.163	4.02	0.291
4.09	1.587	3.96	1.533	4.05	1.257
4.34	0.578	4.12	0.379	4.20	0.255

Coordinates of the chlorophyll monomer

The optimized Cartesian coordinates in Å.

```
82
Energy =
Mg   -0.1287395   -2.8898354    1.0006262
C    -1.9694253   -5.6285762   -0.1302548
C     0.6821028   -2.1436294   -2.2402726
C     1.5994561   -0.1725886    2.1389455
C    -0.9173051   -3.7723775    4.2947443
N    -0.6123816   -3.7726081   -0.9165186
C    -1.4056277   -4.8743514   -1.1596156
C    -1.5792318   -5.1099916   -2.6554502
C    -0.4769334   -4.1978686   -3.2649667
C    -0.1085764   -3.2887004   -2.0900827
C     0.7432063   -4.9839936   -3.7816759
C    -3.0105868   -4.7594574   -3.1288951
C    -3.2664644   -5.1424706   -4.5963375
C    -4.6450896   -4.7812968   -5.1261951
O    -4.8731306   -4.2780680   -6.2099596
O    -5.6215536   -5.1140949   -4.2383723
N     0.9430849   -1.4004336    0.1006261
C     1.1654567   -1.2523219   -1.2466209
C     1.9711977   -0.0654039   -1.4963829
C     2.2364000    0.5035375   -0.2447526
C     1.5763333   -0.3554715    0.7459718
C     2.3844799    0.4394183   -2.8444382
C     2.9783578    1.7116056    0.0928296
C     3.8701408    2.3919029   -0.6695772
N     0.2708626   -2.1116346    2.8921910
C     1.0059520   -0.9785035    3.1412953
C     1.0904831   -0.7370938    4.5787854
C     0.3802671   -1.7627969    5.1919864
C    -0.1269156   -2.6145199    4.1174978
C     1.8154068    0.4064509    5.2237783
C     0.1962772   -2.0083798    6.6659395
C     1.2204883   -2.9922222    7.2679681
N    -1.1856854   -4.3561056    1.9259485
C    -1.4250725   -4.6074148    3.2795805
C    -2.2423444   -5.8078081    3.4352497
C    -2.4744095   -6.2508828    2.1246259
C    -1.8139198   -5.3334181    1.2491448
C    -2.7172266   -6.4170313    4.7176231
C    -3.1371060   -7.2819450    1.3245913
O    -3.7933919   -8.2522306    1.6628981
C    -2.8406728   -6.8802151   -0.2103525
C    -2.2164635   -8.0569041   -0.9459927
O    -1.0353379   -8.1828279   -1.2224288
O    -3.1598254   -8.9851198   -1.2342738
C    -2.6736038  -10.2082953   -1.8071066
C    -6.9648866   -4.8321527   -4.6617934
H     0.9761812   -1.9104228   -3.2746798
H     2.1609325    0.6997814    2.5029000
H    -1.1644456   -4.0468595    5.3313046
H     1.5462896   -4.3032655   -4.1289842
H     0.4572513   -5.6375304   -4.6312043
H     1.1627496   -5.6290390   -2.9831525
H    -3.7547783   -5.2779226   -2.4922341
H    -3.1847471   -3.6711375   -2.9821142
H    -2.5387909   -4.6677662   -5.2830615
H    -3.1452655   -6.2430746   -4.7138627
H     2.3202246    1.5464127   -2.8909575
H     1.7461778    0.0316343   -3.6524679
H     3.4352735    0.1682913   -3.0889396
H     2.7822530    2.1121662    1.1032641
H     4.3495771    3.3041354   -0.2831388
H     4.1711351    2.0636500   -1.6743697
H     1.6780545    0.4090123    6.3225437
H     1.4603694    1.3875030    4.8431577
H     2.9087648    0.3644027    5.0299348
H    -0.8312436   -2.3870792    6.8574141
H     0.2581528   -1.0412778    7.2084781
H     1.0404760   -3.1425962    8.3524503
H     2.2564649   -2.6173125    7.1430674
H     1.1675801   -3.9827138    6.7722556
H    -1.8682089   -6.6958549    5.3771837
H    -3.3103593   -7.3283465    4.5159509
H    -3.3525828   -5.7122415    5.2952869
H    -3.8425643   -6.7007364   -0.6587640
H    -2.1491876  -10.0182064   -2.7652785
H    -3.5626300  -10.8422414   -1.9721582
H    -1.9672421  -10.7113309   -1.1166559
H    -7.6192220   -5.1388919   -3.8265939
H    -7.2172663   -5.4017878   -5.5788899
H    -7.0927108   -3.7525910   -4.8782982
H    -0.8815495   -3.5832778   -4.0982569
H    -1.3777445   -6.1773220   -2.8870519
```

Coordinates of the α-chlorophyll monomer

The optimized Cartesian coordinates in Å.

```
94
Energy =
C    -4.2428400    6.1872084   -2.0769653
C    -3.1279783    5.8147143   -1.1573177
N    -2.1815861    6.7256299   -0.6952510
C    -2.7466047    4.6058046   -0.5967242
C    -1.2886298    6.0679570    0.1014797
N    -1.6131456    4.7792504    0.1773928
Mg   -0.1793328    3.2036068    0.6627256
C     2.0647108    5.5343226   -0.6069276
C    -0.7239293    2.0812921   -2.5496414
C    -1.8404390    0.4839222    1.9393292
C     0.8347821    4.0733443    3.9129039
N     0.6646775    3.6907002   -1.3152651
C     1.4715648    4.7622349   -1.6033926
C     1.6315720    4.9454844   -3.1070935
C     0.4482572    4.0996725   -3.6506582
C     0.1165289    3.1977599   -2.4580586
C    -0.7736047    4.9683791   -4.0085146
C     3.0206951    4.4553864   -3.5717113
C     3.3118550    4.8051068   -5.0381129
C     4.6366650    4.2799898   -5.5616687
O     4.8175429    3.7772824   -6.6546206
O     5.6301342    4.4548041   -4.6476603
N    -1.0978861    1.5419738   -0.1643090
C    -1.2467160    1.2756883   -1.5022202
C    -2.0387667    0.0658331   -1.6882012
C    -2.3718751   -0.3894656   -0.4078219
C    -1.7589379    0.5560635    0.5367004
C    -2.3489348   -0.5740042   -3.0062984
C    -3.1234582   -1.5730691   -0.0126875
```

C	-4.0305074	-2.2625754	-0.7482075
N	-0.4619532	2.4221723	2.5966218
C	-1.2394154	1.3356937	2.8995221
C	-1.3365357	1.1725718	4.3502323
C	-0.5793423	2.1926829	4.9094309
C	-0.0308661	2.9638133	3.7917622
C	-2.1155248	0.1002600	5.0492592
C	-0.3942418	2.5190445	6.3646295
C	-1.3631634	3.6125749	6.8572520
N	1.2275911	4.4348526	1.5208181
C	1.4375917	4.7852463	2.8537059
C	2.3097455	5.9546525	2.9377638
C	2.5945028	6.2849814	1.6034599
C	1.9155436	5.3227910	0.7889220
C	2.7800161	6.6455016	4.1786501
C	3.2542505	7.2571848	0.7314459
O	3.9308250	8.2410101	0.9926991
C	2.8965378	6.8081281	-0.7617374
C	2.1047484	7.8847096	-1.4825058
O	2.3195165	8.3139116	-2.6005507
O	1.0495780	8.3084495	-0.7195452
C	0.2375037	9.3244820	-1.3182583
C	6.9296581	3.9964450	-5.0529223
H	-4.8985238	6.9727130	-1.6443376
H	-4.8716660	5.3004022	-2.2801936
H	-3.8652481	6.5619522	-3.0525257
H	-3.1978584	3.6158168	-0.7226958
H	-0.4088779	6.5429392	0.5503779
H	-1.0264787	1.8015250	-3.5705109
H	-2.4351696	-0.3458683	2.3471014
H	1.0733943	4.4086993	4.9329291
H	-1.6414311	4.3443835	-4.3027802
H	-0.5376480	5.6605518	-4.8424287
H	-1.0803052	5.5725355	-3.1288195
H	3.8063209	4.9075179	-2.9348772
H	3.0880882	3.3571947	-3.4121123
H	2.5308948	4.4207997	-5.7229000
H	3.3234012	5.9124848	-5.1498594
H	-2.3700285	-1.6791459	-2.9136453
H	-1.5950393	-0.3124346	-3.7749588
H	-3.3422643	-0.2646121	-3.4004122
H	-2.9227632	-1.9374140	1.0110991
H	-4.5215322	-3.1575476	-0.3375199
H	-4.3304662	-1.9506016	-1.7594614
H	-1.9647730	0.1340895	6.1458950
H	-1.8211409	-0.9130580	4.7025618
H	-3.2067060	0.1985487	4.8624161
H	0.6531325	2.8419731	6.5486997
H	-0.5330194	1.6007639	6.9736387
H	-1.1991132	3.8486294	7.9290983
H	-2.4165371	3.2894326	6.7305569
H	-1.2340154	4.5471770	6.2737846
H	1.9314519	6.9454293	4.8288152
H	3.3598373	7.5507369	3.9171232
H	3.4309628	5.9834281	4.7888733
H	3.8344082	6.6742963	-1.3377148
H	-0.4809388	9.6425747	-0.5393107
H	-0.2931933	8.9328547	-2.2127800
H	0.8503084	10.1900130	-1.6411175
H	7.6027174	4.1912625	-4.1990180
H	7.2792565	4.5418548	-5.9533310
H	6.9105637	2.9135625	-5.2920674
H	1.5300726	6.0143109	-3.3905581
H	0.7407636	3.4967681	-4.5365151
H	-2.1498359	7.7209345	-0.9181035

Coordinates of the β-chlorophyll monomer

The optimized Cartesian coordinates in Å.

94
Energy =

C	1.4205058	-4.5690882	1.2013596
C	1.1686427	-3.3684248	2.0530334
N	-0.0461340	-3.1198052	2.6865997
C	1.9725579	-2.2966494	2.4104999
C	0.0546566	-1.9483004	3.3816720
N	1.2696785	-1.4343639	3.2295732
H	2.4546093	-4.5382965	0.8106140
H	0.7325851	-4.6141222	0.3301674
H	-0.8730495	-3.7165377	2.6419980
H	3.0105810	-2.0863944	2.1291078
H	-0.7520580	-1.4959551	3.9705208
Mg	1.9210588	0.4852126	3.9769291
C	3.6750078	1.0526099	1.0040203
C	-0.8319200	1.9839745	2.5623733
C	0.3565174	0.3828828	7.0311159
C	4.9649929	-0.3218805	5.5469353
N	1.5080842	1.4237568	2.0322093
C	2.3355723	1.4443598	0.9350051
C	1.6145456	1.9716005	-0.2956566
C	0.2437893	2.4331606	0.2723038
C	0.2809029	1.9166730	1.7125862
C	0.0468420	3.9572379	0.1963860
C	1.5046445	0.9422893	-1.4378710
C	0.9621252	1.5581127	-2.7480476
C	1.9553184	2.5829501	-3.2609352
O	2.9958918	2.3066159	-3.8334861
O	1.5900914	3.8461047	-2.9295595
N	0.0758609	1.1014701	4.6864291
C	-0.9460699	1.6161641	3.9295926
C	-2.1552878	1.7322357	4.7365544
C	-1.8260759	1.2612554	6.0139042
C	-0.4064402	0.8843240	5.9597039
C	-3.4608696	2.3045146	4.2774436
C	-2.6523846	1.1701021	7.2105727
C	-4.0060948	1.1374470	7.2924880
N	2.5591921	0.1037619	5.9526723
C	1.7324967	0.0455577	7.0449559
C	2.4828676	-0.3900821	8.2228692
C	3.7903767	-0.5893665	7.8019871
C	3.8197846	-0.2671734	6.3740206
C	1.9132951	-0.5514050	9.5998999
C	4.9834246	-0.9729627	8.6322248
C	5.8126008	0.2433364	9.0898946
N	3.9049874	0.4194776	3.4592305
C	5.0274824	0.0038655	4.1759498
C	6.1985085	-0.0341772	3.3036372
C	5.7189858	0.3681940	2.0486112
C	4.3196634	0.6326705	2.1997616
C	7.5967268	-0.4129866	3.6776455
C	6.1076829	0.5957894	0.6606372
O	7.1953028	0.5135969	0.1146717
C	4.7292794	0.9669222	-0.0987863
C	4.9089052	2.1747221	-0.9991044

O	4.4458459	3.2917376	-0.8067295
O	5.6900021	1.8468069	-2.0445279
C	6.0350110	2.9061131	-2.9540955
C	2.5814397	4.8673664	-3.1686175
H	1.3042580	-5.5156336	1.7712887
H	-1.7443800	2.3918007	2.1019229
H	-0.1726001	0.2605438	7.9872967
H	5.9051827	-0.6433079	6.0199643
H	0.0939722	4.2938260	-0.8585263
H	0.8500609	4.4765244	0.7582105
H	-0.9261412	4.2666797	0.6290792
H	2.5013136	0.5047898	-1.6533371
H	0.8505418	0.1025040	-1.1185374
H	0.8601407	0.7700210	-3.5195271
H	-0.0265160	2.0310152	-2.5858420
H	-3.3306495	2.9825742	3.4112544
H	-3.9467382	2.8822690	5.0906658
H	-4.1821267	1.5152832	3.9704681
H	-2.0933502	1.1151344	8.1620167
H	-4.6549361	1.1438902	6.4051607
H	-4.5061542	1.0786215	8.2714679
H	1.0389411	-1.2369427	9.6063449
H	1.5612139	0.4184825	10.0121509
H	2.6616475	-0.9586525	10.3073457
H	5.6331834	-1.6682028	8.0574596
H	4.6476975	-1.5472569	9.5219903
H	6.1751797	0.8256858	8.2184681
H	6.6936326	-0.0673837	9.6887838
H	5.1974572	0.9272012	9.7091904
H	8.2590645	-0.3566426	2.7933050
H	7.6452849	-1.4441011	4.0882251
H	8.0043569	0.2610645	4.4611080
H	4.5633417	0.0974680	-0.7735854
H	6.8573323	2.5111530	-3.5771577
H	6.3676719	3.8073987	-2.4006912
H	5.1579151	3.1520942	-3.5833578
H	2.0984200	5.8240415	-2.9023159
H	2.8911219	4.8719142	-4.2329107
H	3.4639133	4.6828074	-2.5230606
H	2.1905438	2.8440921	-0.6649708
H	-0.5942572	1.9403399	-0.2697950

Coordinates of the A76-A79 dimer

The optimized Cartesian coordinates in Å.

188
Energy =

C	2.1093980	6.0935360	-2.7466280
C	2.5414571	4.7911173	-3.3417165
N	3.8728751	4.3866080	-3.4108327
C	1.8325541	3.7409056	-3.9042159
C	3.9248640	3.1500473	-3.9872493
N	2.6996729	2.7336006	-4.2941836
H	4.6763224	4.9277501	-3.0892940
H	0.7490294	3.6289279	-4.0172785
H	4.8441878	2.5697685	-4.1237483
Mg	2.1594010	0.6035310	-4.1316300
C	4.5825376	0.5723839	-1.5914239
C	-0.1345243	1.6798466	-1.7217526
C	-0.4440337	-0.1700253	-6.2335861
C	4.2515010	-1.5180038	-6.0141488
N	2.2405674	1.0984262	-1.9569138
C	3.3581885	1.0859065	-1.1674209
C	3.0779657	1.6593283	0.2131007
C	1.5260031	1.7013361	0.2371242
C	1.1689718	1.5271205	-1.2399915
C	0.9367658	0.5426971	1.0598755
C	3.8071845	3.0057651	0.4341671
C	4.0785104	3.3102381	1.9241564
C	2.7675714	3.4279853	2.6768748
O	1.9688462	4.3285579	2.4275380
O	2.4059338	2.5019347	3.5862437
N	0.0861392	0.8281015	-4.0380024
C	-0.6503139	1.3320709	-2.9962163
C	-2.0672956	1.3600269	-3.3432928
C	-2.1689726	0.8159279	-4.6252132
C	-0.7968042	0.4911117	-5.0441386
C	-3.1562874	1.8940094	-2.4676772
C	-3.3665539	0.5738565	-5.4250939
C	-4.5957081	0.2564898	-4.9501858
N	1.9701368	-0.5589449	-5.8691995
C	0.8227642	-0.6803409	-6.6113727
C	1.0735523	-1.4938945	-7.8001051
C	2.4046570	-1.8797619	-7.7376562
C	2.9479355	-1.2966838	-6.5099257
C	0.0494479	-1.8507713	-8.8348290
C	3.1399127	-2.8084561	-8.6629973
C	3.0840880	-4.2763354	-8.1954573
N	4.0653088	-0.1837234	-3.9588198
C	4.7791158	-1.0486422	-4.7921156
C	6.0375033	-1.4382300	-4.1628045
C	6.0305822	-0.7888720	-2.9168281
C	4.8073590	-0.0483317	-2.8477333
C	7.0692639	-2.3709994	-4.7140329
C	6.7341688	-0.6682268	-1.6398727
O	7.7872339	-1.1511207	-1.2531500
C	5.8182947	0.2877504	-0.7326104
C	5.4251340	-0.3557299	0.5857459
O	5.6090270	0.1149616	1.6991552
O	4.7453800	-1.5069735	0.3681387
C	4.1337354	-2.1145704	1.5153737
C	3.2666388	1.4227549	4.0134856
C	-1.6765980	4.2085270	0.6513750
C	-1.5673892	3.1554306	1.7170521
N	-0.5530157	3.1545040	2.6670313
C	-2.3431967	2.0408848	2.0274852
C	-0.7278332	2.0793046	3.4819657
N	-1.8085950	1.3854369	3.1262896
H	0.2803603	3.7795626	2.6919068
H	-3.2499897	1.6717095	1.5348474
H	-0.0484374	1.8216599	4.3014201
Mg	-2.3585970	-0.5174710	4.1023710
C	-3.8804788	-1.2364469	1.0772718
C	0.4554748	-2.2176880	2.9985353
C	-0.8909651	0.0627135	7.1217907
C	-5.4436018	0.5220918	5.3836377
N	-1.8227678	-1.6517812	2.2779466
C	-2.5686478	-1.7142179	1.1280600
C	-1.8014621	-2.3814902	-0.0106839
C	-0.5028288	-2.8721340	0.7012660
C	-0.6048582	-2.2232674	2.0831841
C	-0.3878956	-4.4038869	0.7782783
C	-1.5602792	-1.4483693	-1.2169587
C	-1.1109249	-2.1691197	-2.5008009

C	0.2447814	-2.8351145	-2.4111757
O	0.4584668	-4.0306980	-2.5068417
O	1.2324073	-1.9201857	-2.1780022
N	-0.5256920	-1.0111311	4.9258507
C	0.5190862	-1.6392510	4.2952179
C	1.7018649	-1.6071513	5.1442859
C	1.3384830	-0.9111009	6.3069425
C	-0.0840925	-0.5767291	6.1579491
C	3.0207318	-2.2468595	4.8374654
C	2.1526667	-0.5583069	7.4614167
C	3.5054960	-0.4727038	7.5293736
N	-3.0685066	0.1180048	5.9634780
C	-2.2751611	0.3581703	7.0549996
C	-3.0677098	0.9641502	8.1258978
C	-4.3601928	1.0885321	7.6345510
C	-4.3408820	0.5515675	6.2710343
C	-2.5431758	1.3447817	9.4775943
C	-5.5783818	1.6027445	8.3498056
C	-6.4760185	0.4772911	8.9004214
N	-4.3083214	-0.5203889	3.4775258
C	-5.4418417	0.0454061	4.0547822
C	-6.5228319	0.1249573	3.0705341
C	-5.9653948	-0.3811354	1.8865080
C	-4.6134554	-0.7500351	2.1921834
C	-7.9040428	0.6559172	3.2896049
C	-6.2154394	-0.6285605	0.4660832
O	-7.2245225	-0.4980882	-0.2094118
C	-4.7961531	-1.0777251	-0.1316341
C	-4.8925188	-2.2825100	-1.0418879
O	-4.9596495	-3.4433823	-0.6852965
O	-4.8642569	-1.8982168	-2.3495003
C	-4.9454790	-2.9609096	-3.3135149
C	2.5584271	-2.4559901	-2.0012191
H	-0.1698178	0.5429010	1.0420677
H	1.2453508	0.5999336	2.1206542
H	1.2815515	-0.4277194	0.6514374
H	3.2183856	3.8291780	-0.0239397
H	4.7845061	2.9811587	-0.0889751
H	4.5839185	4.2924983	2.0187457
H	4.7535937	2.5346317	2.3327286
H	-3.5008079	1.1385739	-1.7282820
H	-4.0421643	2.1908855	-3.0624904
H	-2.8138781	2.7728651	-1.8859540
H	-5.4434178	0.1138698	-5.6383587
H	-4.7868155	0.0875172	-3.8791191
H	0.4951198	-2.4236989	-9.6711317
H	-0.4311573	-0.9468299	-9.2651657
H	-0.7643426	-2.4733609	-8.4046829
H	2.7124218	-2.7292599	-9.6851725
H	4.1994237	-2.4872851	-8.7587799
H	2.0349544	-4.6310367	-8.1394898
H	3.5211125	-4.3855179	-7.1819981
H	3.6395325	-4.9441020	-8.8857186
H	7.5170068	-1.9752428	-5.6507985
H	6.6308408	-3.3601575	-4.9646370
H	7.8812089	-2.5260192	-3.9793040
H	3.6747043	-3.0523287	1.1554081
H	3.3463149	-1.4512801	1.9301230
H	4.8818279	-2.3224229	2.3046822
H	2.6240785	0.7591661	4.6212768
H	4.0923569	1.8136034	4.6412117
H	3.6891589	0.8548312	3.1613977
H	-0.3254603	-4.8344704	-0.2407085
H	-1.2689380	-4.8345819	1.2962429
H	0.5180688	-4.7107460	1.3407176
H	-2.4941438	-0.9096510	-1.4677617
H	-0.8192010	-0.6723328	-0.9461646
H	-1.8373231	-2.9570824	-2.7761830
H	-1.0700439	-1.4323174	-3.3282102
H	2.9174707	-3.0579483	4.0900187
H	3.4704500	-2.6844764	5.7525323
H	3.7643508	-1.5228820	4.4359087
H	4.0030329	-0.1927968	8.4703290
H	4.1567537	-0.6556931	6.6625260
H	-1.6860180	2.0476471	9.4032148
H	-2.1803232	0.4572471	10.0392007
H	-3.3212064	1.8320405	10.0968881
H	-6.1715299	2.2464609	7.6639834
H	-5.2655727	2.2669971	9.1830614
H	-6.8259768	-0.1860353	8.0837722
H	-7.3674782	0.8866088	9.4191964
H	-5.9163982	-0.1543640	9.6197019
H	-8.4896093	0.6075380	2.3524466
H	-7.8839915	1.7109666	3.6369215
H	-8.4436016	0.0747873	4.0675789
H	-4.1663468	-3.7253662	-3.1189822
H	-4.7868348	-2.4858277	-4.2984054
H	-5.9381664	-3.4527629	-3.2702754
H	3.1459332	-1.6761942	-1.4899722
H	3.0149871	-2.6818682	-2.9858236
H	2.5235908	-3.3853848	-1.3991915
H	-1.7338199	5.2273326	1.0878574
H	-0.8063116	4.1884255	-0.0392773
H	-2.5903983	4.0424557	0.0511422
H	2.3812171	6.1664386	-1.6716770
H	2.5610661	6.9632648	-3.2693067
H	1.0102071	6.1901393	-2.8205978
H	-4.4883102	-0.2128593	-0.7608125
H	3.4359747	0.9556648	0.9893266
H	6.4166679	1.1858543	-0.4739223
H	4.9028700	-2.1719795	-6.6132413
H	-1.2694617	-0.3866991	-6.9274296
H	-3.2373512	0.6520744	-6.5201808
H	-0.8736217	2.0062733	-0.9766531
H	1.1417650	2.6632943	0.6273414
H	1.5895438	-0.3149467	8.3802999
H	-0.3907594	0.3469568	8.0591186
H	1.3737672	-2.7098484	2.6466638
H	-6.3887968	0.9456778	5.7554653
H	0.3958343	-2.4742122	0.1836501
H	-2.3971102	-3.2529340	-0.3612083

Coordinates of the B49-B52 dimer

The optimized Cartesian coordinates in Å.

188
Energy =

C	-1.8803295	-6.3691382	-2.4552193
C	-2.3231553	-5.1185896	-3.1449108
N	-3.6609546	-4.7589964	-3.3028898
C	-1.6150626	-4.0740459	-3.7173599
C	-3.7159644	-3.5475572	-3.9315494
N	-2.4878236	-3.1113335	-4.1950307
H	-2.2590635	-7.2848420	-2.9569371

H	−2.2227852	−6.3989816	−1.3984366
H	−4.4661189	−5.3048172	−2.9936965
H	−0.5308583	−3.9340237	−3.7799871
H	−4.6421500	−2.9998037	−4.1393176
Mg	−1.9713294	−0.9771297	−4.1762188
C	−4.4101368	−0.7422878	−1.6580392
C	0.2919086	−1.9220580	−1.6818084
C	0.6493435	−0.1868697	−6.2404482
C	−4.1458741	0.7769191	−6.3128545
N	−2.0674226	−1.2903789	−1.9695678
C	−3.2027949	−1.2576107	−1.1980637
C	−2.9653441	−1.9100435	0.1542486
C	−1.4223154	−1.8787928	0.2420056
C	−1.0186151	−1.7397337	−1.2271991
C	−0.9440966	−0.6581038	1.0458243
C	−3.6022638	−3.3199755	0.1696539
C	−3.2283322	−4.1728827	1.3991903
C	−3.2376203	−3.4170573	2.7162810
O	−2.3628033	−3.5056033	3.5740646
O	−4.3029221	−2.6174628	2.8311726
N	0.1036181	−1.1346844	−4.0225184
C	0.8362138	−1.5894956	−2.9508802
C	2.2608198	−1.5469035	−3.2595889
C	2.3698864	−1.0041392	−4.5426872
C	1.0000260	−0.7572358	−5.0054382
C	3.3748298	−1.9028384	−2.3253495
C	3.5698544	−0.6344563	−5.2831283
C	4.7972915	−1.1986504	−5.1854533
N	−1.7981568	0.0404663	−5.9970505
C	−0.6343420	0.1879967	−6.7078458
C	−0.9042607	0.8479859	−7.9839964
C	−2.2688055	1.1013992	−8.0141362
C	−2.8100596	0.6122245	−6.7456615
C	0.1298090	1.1921781	−9.0130513
C	−3.0506125	1.8291581	−9.0718024
C	−3.1999123	3.3348969	−8.7763360
N	−3.8757793	−0.1848437	−4.0738342
C	−4.6590239	0.4499965	−5.0393449
C	−5.9788975	0.7641401	−4.4949857
C	−5.9345713	0.3150623	−3.1649789
C	−4.6330112	−0.2461251	−2.9675284
C	−7.1042731	1.4521861	−5.2015851
C	−6.6802897	0.2273999	−1.9060255
O	−7.8250747	0.5542259	−1.6295681
C	−5.6724239	−0.4256123	−0.8498092
C	−5.3089260	0.5482756	0.2671358
O	−5.2587451	0.2830325	1.4592962
O	−4.9632668	1.7489562	−0.2489684
C	−4.4416129	2.7125242	0.6770547
C	−4.3291434	−1.7048775	3.9540040
C	1.5186696	−4.2901388	1.2237797
C	1.3491054	−3.1638086	2.1837073
N	0.2908903	−3.0725649	3.0775984
C	2.1061883	−2.0212843	2.4066975
C	0.4192204	−1.9138171	3.7770173
N	1.5133332	−1.2599391	3.3949574
H	2.4390841	−4.1410157	0.6284268
H	0.6712851	−4.3583775	0.5055509
H	−0.5561653	−3.6606009	3.1617260
H	3.0337597	−1.6981480	1.9202078
H	−0.2971304	−1.5749315	4.5344155
Mg	1.9806694	0.7148598	4.0557789
C	3.6762633	1.1874216	1.0770644
C	−0.7646884	2.2923268	2.6644440
C	0.3046698	0.2719276	6.9880669
C	4.9924339	−0.0903887	5.6372629
N	1.5617408	1.7014043	2.1330228
C	2.3700227	1.6820178	1.0211622
C	1.6701306	2.2884644	−0.1890120
C	0.3659323	2.8692056	0.4299940
C	0.3655834	2.2789195	1.8382689
C	0.3364199	4.4067254	0.4298766
C	1.3962004	1.2828203	−1.3237861
C	0.7628457	1.9197719	−2.5834519
C	1.7848643	2.7553608	−3.3168878
O	2.5498849	2.3356669	−4.1720590
O	1.8073866	4.0324519	−2.8560442
N	0.0896920	1.2340576	4.7269643
C	−0.9285297	1.7418891	3.9632499
C	−2.1989601	1.6062746	4.6646211
C	−1.9103783	0.9760000	5.8833547
C	−0.4497996	0.7924965	5.9168155
C	−3.5179942	2.1049743	4.1576979
C	−2.8138660	0.5528332	6.9446527
C	−4.1450253	0.3037609	6.8552277
N	2.5743565	0.2792816	6.0193040
C	1.7085864	0.0779586	7.0614169
C	2.4426705	−0.3943785	8.2370317
C	3.7749264	−0.4855909	7.8567796
C	3.8357266	−0.0679540	6.4531061
C	1.8304137	−0.6937644	9.5719362
C	4.9591987	−0.8684390	8.6996071
C	5.7735738	0.3476461	9.1839511
N	3.9649229	0.7293469	3.5645735
C	5.0645175	0.2407746	4.2659602
C	6.1976042	0.0560965	3.3599377
C	5.7048037	0.4146855	2.0955877
C	4.3410291	0.8164934	2.2792344
C	7.5673686	−0.4313606	3.7126294
C	6.0332058	0.4703096	0.6727437
O	7.0772243	0.2496664	0.0806610
C	4.6405307	0.8394870	−0.0513091
C	4.8356900	1.8089761	−1.1937150
O	4.6254764	3.0131344	−1.1702976
O	5.3156923	1.1418245	−2.2664692
C	5.6685766	1.9299027	−3.4185098
C	2.8910877	4.8591570	−3.3262685
H	−0.7756934	−6.4194003	−2.4513503
H	1.0099979	−2.2546332	−0.9183918
H	1.4854800	0.0386510	−6.9174590
H	−4.8374222	1.2683156	−7.0136676
H	0.1590191	−0.5884829	1.0844400
H	−1.3138829	−0.6924757	2.0890090
H	−1.3313800	0.2753471	0.5916746
H	−3.3030979	−3.8695522	−0.7482978
H	−4.7029402	−3.1950337	0.1255763
H	−2.2186585	−4.6181144	1.3009775
H	−3.9369459	−5.0239875	1.4954214
H	4.2256753	−1.1998710	−2.4522964
H	3.7685345	−2.9264628	−2.5085736
H	3.0482735	−1.8662755	−1.2660107
H	3.4438672	0.2138862	−5.9772483
H	5.0028227	−2.0603545	−4.5338633
H	5.6394237	−0.8177952	−5.7834219

H	-0.3270805	1.6256515	-9.9239189
H	0.7150643	0.3002490	-9.3216021
H	0.8591528	1.9346112	-8.6235519
H	-2.5554119	1.6937232	-10.0568667
H	-4.0567051	1.3688596	-9.1790810
H	-2.2060196	3.8224061	-8.7118053
H	-3.7106385	3.4990720	-7.8056452
H	-3.7862930	3.8479257	-9.5662374
H	-7.4217458	0.8943584	-6.1084431
H	-6.8094952	2.4685749	-5.5399448
H	-7.9771559	1.5508583	-4.5293394
H	-6.1539821	-1.2999815	-0.3685029
H	-4.2704983	3.6350391	0.0949114
H	-3.4869017	2.3490922	1.1091018
H	-5.1543177	2.8994389	1.5046660
H	-5.1764457	-1.0294346	3.7520404
H	-3.3842373	-1.1266660	4.0061645
H	-4.4611217	-2.2560239	4.9052995
H	1.6001334	-5.2715601	1.7373061
H	-1.6626172	2.7448952	2.2187005
H	-0.2598668	-0.0023090	7.8913796
H	5.9215611	-0.4490935	6.1057265
H	0.4058394	4.7857727	-0.6099711
H	1.1980890	4.8101423	1.0002219
H	-0.5924349	4.7968540	0.8942678
H	2.3292626	0.7660885	-1.6302449
H	0.7175177	0.4911604	-0.9529456
H	0.4229884	1.1213199	-3.2674713
H	-0.1096840	2.5443843	-2.3067453
H	-3.3892706	3.0374801	3.5709596
H	-4.2080982	2.3327598	4.9940944
H	-4.0303738	1.3779457	3.4888328
H	-2.3410562	0.3977482	7.9312561
H	-4.7011868	0.3927260	5.9106935
H	-4.7184214	-0.0101549	7.7406441
H	1.0270622	-1.4577477	9.4936824
H	1.3680214	0.2111086	10.0211158
H	2.5812329	-1.0729950	10.2920181
H	5.6230121	-1.5503698	8.1239470
H	4.6167655	-1.4575658	9.5767836
H	6.1437069	0.9441302	8.3254113
H	6.6490680	0.0340620	9.7894128
H	5.1462778	1.0190612	9.8046816
H	8.1976700	-0.4991333	2.8060333
H	7.5338980	-1.4319032	4.1938617
H	8.0672758	0.2510457	4.4329805
H	4.3438060	-0.1250211	-0.5167133
H	6.1960474	1.2383406	-4.0984772
H	6.3295050	2.7699794	-3.1246058
H	4.7529759	2.3169105	-3.9060129
H	2.6595331	5.8845077	-2.9867739
H	2.9651432	4.8207781	-4.4314015
H	3.8393430	4.5073286	-2.8727533
H	-3.4269389	-1.3208165	0.9694537
H	2.3130411	3.0995087	-0.5865463
H	-0.5286046	2.5000407	-0.1191083
H	-0.9995573	-2.7969629	0.6930036

Coordinates of P_A-P_B

The optimized Cartesian coordinates in Å.

Energy =

C	4.3571000	-6.3628200	-1.4971300
C	3.1749106	-5.8613748	-0.7091325
N	2.0992619	-6.6741212	-0.3539082
C	2.8559920	-4.6228224	-0.1593048
C	1.2098486	-5.9398706	0.3708636
N	1.6394646	-4.6855038	0.5080440
Mg	0.0771000	-3.1028100	1.0018700
C	-2.1440008	-5.5116425	-0.1386338
C	0.6389636	-2.1622897	-2.2622574
C	1.6631414	-0.2471279	2.1159089
C	-0.9619406	-3.7536726	4.2939603
N	-0.7345789	-3.7180969	-0.9461094
C	-1.5329125	-4.8067460	-1.1713609
C	-1.6556192	-5.1098807	-2.6578319
C	-0.5106652	-4.2445583	-3.2570442
C	-0.1841103	-3.2839901	-2.1093562
C	0.7297552	-5.0819889	-3.6199870
C	-3.0609140	-4.7515073	-3.1801285
C	-3.2910187	-5.1675352	-4.6404705
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