Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences

Supplementary information for

Initial excited-state relaxation of the bilin chromophores of phytochromes: a computational study

Angela Strambi[a] and Bo Durbeej

Division of Computational Physics, IFM, Linköping University, SE-581 83 Linköping, Sweden
E-mail: bodur@ifm.liu.se; Fax: +46-(0)13-13 75 68; Tel: +46-(0)13-28 24 97

[a] Current address: Istituto Toscano Tumori, Via Fiorentina 1, I-53100 Siena, Italy

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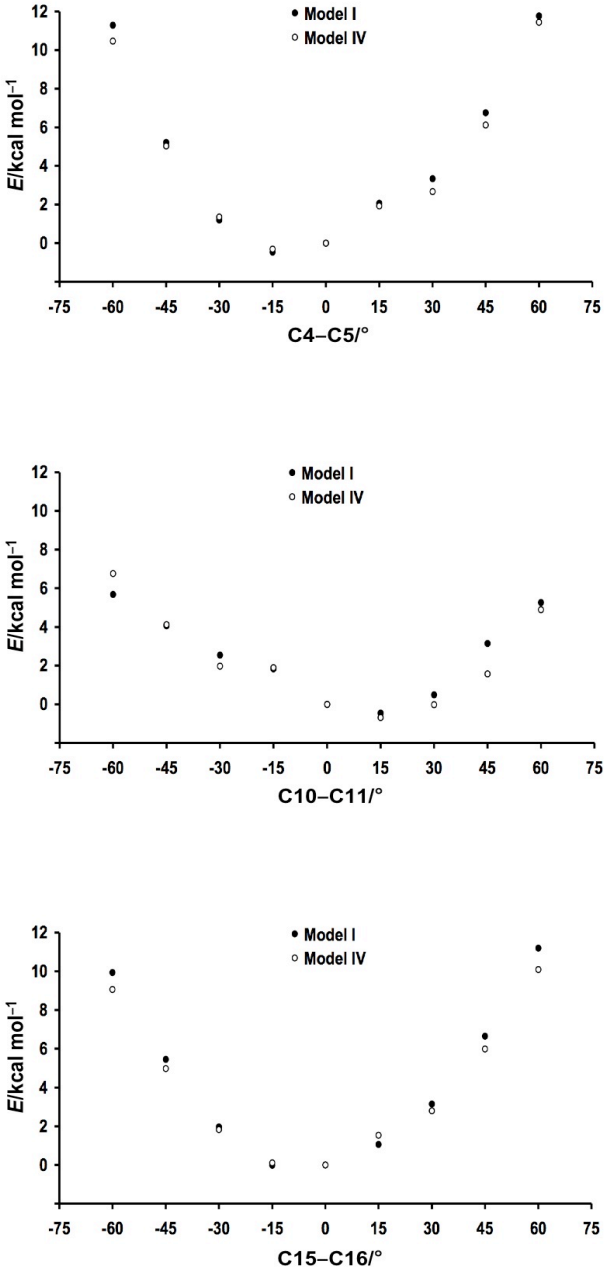
1. Figure S1



S_1 potential energy curves for up to ±60º torsional motion around the C4–C5, C10–C11 and C15–C16 bonds of two models (I and IV) of *ZsZsZa* BV computed at the TD-B3LYP/SVP//B3LYP/SVP level of theory. For each bond and model, energies (*E*) are given relative the structure at which the corresponding dihedral angle is 0º.

2. Table S1

Table S1 Calculated absorption maxima for different models of *ZsZsZa* BV and *ZsZsEa* BV[a]

	eV	nm
ZsZsZa BV		
Model I	1.87	663
Model II	1.83	678
Model III	1.86	667
Model IV	1.85	670
ZsZsEa BV		
Model I	1.87	663
Model II	1.78	697
Model III	1.87	663
Model IV	1.77	700

[a] All calculations performed at the B3LYP/SVP level of theory and using the PCM with the dielectric constant set to 4.

3. Table S2

Table S2 Effect of computational model on absolute differences in B3LYP/SVP ground-state and CIS/SVP excited-state bond lengths (Å) and dihedral angles (°) of *ZsZsZa* BV and *ZsZsEa* BV

	AB bridge				BC bridge				CD bridge			
	4–5		5–6		9–10		10–11		14–15		15–16	
	Bond	Angle	Bond	Angle	Bond	Angle	Bond	Angle	Bond	Angle	Bond	Angle
ZsZsZa BV												
Model I	0.00	0.7	0.02	2.3	0.01	0.4	0.01	4.2	0.01	0.4	0.01	0.5
Model II	0.00	1.0	0.02	2.7	0.01	0.1	0.00	3.5	0.01	3.9	0.01	1.4
Model III	0.01	0.7	0.02	2.3	0.01	1.3	0.01	4.2	0.01	0.5	0.01	0.5
Model IV	0.00	0.8	0.02	2.4	0.01	0.1	0.00	3.5	0.01	2.0	0.01	0.9
ZsZsEa BV												
Model I	0.00	0.9	0.02	3.4	0.01	1.1	0.01	5.6	0.01	3.0	0.01	1.8
Model II	0.00	0.7	0.01	0.9	0.01	1.1	0.00	2.5	0.01	1.7	0.01	0.2
Model III	0.00	0.8	0.02	3.1	0.01	1.3	0.01	6.2	0.01	2.4	0.01	1.8
Model IV	0.00	0.9	0.02	1.2	0.01	1.6	0.01	3.0	0.01	1.0	0.01	1.3

4. Cartesian coordinates of optimized structures

B3LYP/SVP S_0 structure of *ZsZsZs* DHBV

N	1.312827	-1.314377	0.852528
C	1.461013	-2.431155	0.068949
C	2.943542	-2.745614	-0.021205
C	3.630933	-1.633321	0.791547
C	2.496010	-0.786535	1.360812
C	0.431157	-3.130026	-0.489183
C	-0.959446	-2.764175	-0.406706
C	-2.065203	-3.682846	-0.667368
C	-3.212147	-2.984878	-0.427615
C	-2.803734	-1.634633	-0.073618
N	-1.412477	-1.553118	-0.059053
C	-3.650283	-0.559191	0.121860
C	-3.238699	0.795544	0.244419
C	-3.978115	1.980081	0.459947
C	-3.072793	3.045517	0.456338
C	-1.778531	2.519971	0.222742
N	-1.920169	1.163110	0.106940
C	-0.548698	3.243127	0.103086
C	0.674737	2.804544	-0.326286
C	1.905622	3.590476	-0.312961
C	2.930964	2.825788	-0.756673
C	2.401317	1.485547	-1.104830
N	1.031749	1.554589	-0.817890
O	2.973989	0.502211	-1.540576
H	3.982722	3.086678	-0.854316
O	2.565360	0.165352	2.099925
H	-1.962254	-4.724276	-0.970618
H	-4.241675	-3.332580	-0.509446
H	-3.298634	4.102705	0.583065
H	-5.056681	2.031586	0.596793
H	1.944740	4.620462	0.040898
H	-1.222618	0.417947	0.021974
H	-4.726044	-0.749246	0.134971
H	-0.599518	4.294792	0.393239
H	0.405771	0.805427	-1.085229
H	0.674522	-4.058504	-1.010040
H	3.257071	-2.741146	-1.075790
H	3.145993	-3.752908	0.376392
H	0.386181	-0.946597	1.064306
H	4.257168	-2.000342	1.618349
H	4.249070	-0.975252	0.163451

TD-B3LYP/SVP S_1 structure of *ZsZsZs* DHBV

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.383764
C	1.389412	0.000000	1.786216
C	2.176851	-0.041595	0.664100
C	1.310517	-0.017230	-0.514759
C	-1.117636	-0.065106	2.209414
C	-2.453041	-0.326479	1.819581
C	-3.638558	-0.252526	2.627689
C	-4.723071	-0.593305	1.842168
C	-4.235934	-0.898689	0.529608
N	-2.862619	-0.719633	0.571808
C	-4.906482	-1.268076	-0.635743
C	-4.298956	-1.532760	-1.888233
C	-5.010515	-1.677461	-3.139960
C	-4.052143	-1.805894	-4.116343
C	-2.777419	-1.780604	-3.438411
N	-2.942695	-1.613789	-2.093968
C	-1.511076	-1.925988	-4.086825
C	-0.299688	-2.172529	-3.471048
N	-0.158704	-2.435176	-2.147060
C	1.143594	-2.741283	-1.737425
C	1.986988	-2.785503	-3.007376
C	1.079974	-2.178468	-4.093766
O	1.459744	-2.963785	-0.591631
O	1.560253	-0.038266	-1.717573
H	3.262017	-0.093536	0.602182
H	-4.197616	-1.926452	-5.189727
H	-6.093741	-1.653879	-3.259653
H	-3.647073	0.045709	3.674654
H	-5.770313	-0.625858	2.138694
H	1.711130	-0.034853	2.826528
H	-2.317313	-0.981544	-0.251339
H	-5.996703	-1.317864	-0.585653
H	-0.944819	0.065589	3.279500
H	-0.789494	0.214739	-0.597588
H	-1.500612	-1.840762	-5.176475
H	1.366399	-1.128784	-4.280259
H	1.098602	-2.711420	-5.056267
H	-0.965423	-2.402120	-1.520696
H	2.244755	-3.840112	-3.208584
H	2.920443	-2.231359	-2.847563

B3LYP/SVP S_0 structure of *ZsZsZa* BV

C	-3.753204	1.137114	-0.094592
C	-3.057506	-0.139515	-0.025713
N	-4.018908	-1.118179	0.026693
C	-5.315287	-0.565924	-0.033063
C	-5.101980	0.930815	-0.087899
C	-1.683981	-0.280087	-0.015199
C	-0.923493	-1.469603	0.133322
C	-1.264932	-2.816562	0.481162
C	-0.110323	-3.574251	0.454622
C	0.986009	-2.721703	0.119497
N	0.435269	-1.451365	-0.046303
C	2.335008	-3.053836	0.017483
C	3.437404	-2.191182	-0.112607
C	4.789692	-2.507039	-0.401813
C	5.520244	-1.320985	-0.422755
C	4.631240	-0.257285	-0.138404
N	3.376919	-0.805833	0.013159
C	4.894787	1.141317	0.035682
C	3.936179	2.119118	0.074949
C	4.086170	3.515254	0.483302
C	2.876364	4.122751	0.447111
C	1.867783	3.149380	-0.046425
N	2.580842	1.932884	-0.200190
O	0.690070	3.274903	-0.290542
O	-6.330138	-1.214117	-0.045349
C	-6.154220	1.922616	-0.126527
C	-7.474960	1.652328	-0.119167
H	6.582099	-1.207800	-0.631884
H	5.163667	-3.509564	-0.603262
H	-2.250830	-3.172267	0.768374
H	-0.017270	-4.632474	0.693954
H	-3.233378	2.094247	-0.127087
H	0.905379	-0.678877	-0.499218
H	2.655798	-0.321542	0.539266
H	2.565972	-4.121038	0.049828
H	-1.121746	0.650807	-0.134141
H	-3.873008	-2.117168	-0.044137
H	-5.815830	2.963599	-0.164727
H	-8.204934	2.464701	-0.151716
H	-7.849540	0.627535	-0.082491
H	5.935997	1.437216	0.174380
H	5.033417	3.944000	0.810151
H	2.274537	1.286926	-0.920587
H	2.625403	5.146547	0.719109

TD-B3LYP/SVP S_1 structure of *ZsZsZa* BV

C	0.011435	0.014710	-0.000528
C	0.005881	0.008303	1.450868
N	1.334319	0.000791	1.845600
C	2.202293	0.040201	0.726396
C	1.303851	0.009000	-0.442838
C	-1.075930	-0.050063	2.326696
C	-0.968565	-0.362829	3.699762
C	-1.952212	-0.300530	4.747256
C	-1.384437	-0.781944	5.904648
C	-0.021368	-1.162390	5.622787
N	0.186789	-0.849988	4.272258
C	0.944917	-1.720833	6.435612
C	2.303111	-1.977302	6.041646
C	3.237403	-2.907987	6.531174
C	4.396454	-2.823748	5.733335
C	4.185355	-1.827996	4.762375
N	2.904447	-1.349407	4.962864
C	4.942564	-1.323228	3.647474
C	6.274134	-1.501995	3.359698
N	7.253129	-2.128223	4.105962
C	8.495326	-2.095805	3.458033
C	8.232936	-1.391499	2.146442
C	6.902083	-1.046637	2.133761
C	9.209811	-1.135564	1.121578
C	10.519206	-1.492341	1.189116
O	9.525041	-2.544335	3.902628
O	3.415745	0.080399	0.828041
H	-2.963007	0.083701	4.622318
H	-1.852022	-0.848849	6.885825
H	5.268299	-3.469114	5.812933
H	3.059391	-3.605697	7.347247
H	6.351483	-0.537787	1.341374
H	2.600937	-0.450915	4.608199
H	0.883696	-1.335190	3.714497
H	0.645928	-2.036892	7.436910
H	4.390871	-0.740696	2.900676
H	7.159302	-2.468346	5.055386
H	8.841860	-0.610816	0.233115
H	11.197733	-1.261092	0.364338
H	10.920029	-2.011618	2.062312
H	-2.074672	0.118844	1.921187
H	-0.893556	-0.024564	-0.605998
H	1.638864	0.395567	2.727478
H	1.663001	-0.024299	-1.469815

B3LYP/SVP S_0 structure of *ZsZsEa* BV

C	-4.062828	-0.935712	0.053452
C	-2.938665	-0.017076	-0.067452
N	-3.469123	1.245665	-0.184927
C	-4.870383	1.228715	-0.137386
C	-5.233449	-0.235207	0.014788
C	-1.574665	-0.237251	-0.086880
C	-0.866529	-1.457005	0.067639
C	-1.238501	-2.809438	0.369664
C	-0.094912	-3.581143	0.365981
C	1.027889	-2.737095	0.088842
N	0.495964	-1.458341	-0.069967
C	2.376462	-3.071991	0.024601
C	3.474722	-2.193536	-0.073566
C	4.835975	-2.469570	-0.354194
C	5.534405	-1.260522	-0.362432
C	4.614051	-0.225368	-0.080591
N	3.377344	-0.813475	0.063759
C	4.810524	1.186975	0.092680
C	3.800083	2.111706	0.097847
N	2.463495	1.842216	-0.219682
C	1.671117	3.006842	-0.072286
C	2.600595	4.039578	0.449826
C	3.847299	3.511253	0.514407
O	0.489187	3.053872	-0.336500
O	-5.577215	2.202053	-0.208447
C	-6.580065	-0.756812	0.092215
C	-7.701974	-0.010638	0.046217
H	-2.243362	-3.158193	0.586337
H	6.593695	-1.118025	-0.566721
H	5.240548	-3.458540	-0.563233
H	-0.026415	-4.647219	0.577285
H	-3.972747	-2.015118	0.138763
H	0.993749	-0.675815	-0.471278
H	2.643171	-0.351650	0.591315
H	2.610779	-4.138420	0.054552
H	4.754388	3.999090	0.871147
H	2.232177	1.201797	-0.972988
H	5.830907	1.535914	0.260559
H	2.277895	5.042815	0.722717
H	-0.952335	0.653103	-0.231890
H	-2.934290	2.104422	-0.272965
H	-6.658511	-1.844504	0.195940
H	-7.662113	1.075523	-0.056529
H	-8.683986	-0.485275	0.112052

TD-B3LYP/SVP S_1 structure of *ZsZsEa* BV

C	2.721453	3.736303	0.684938
C	3.053938	2.416653	0.185154
N	1.866199	1.867374	-0.280292
C	0.791385	2.775190	-0.132462
C	1.378984	3.949493	0.529344
C	4.273604	1.742363	0.215282
C	4.417140	0.347778	0.029901
C	5.594877	-0.461934	-0.117676
C	5.207624	-1.783649	-0.181757
C	3.772031	-1.845375	-0.076009
N	3.343722	-0.516014	0.011526
C	2.906164	-2.929283	-0.038517
C	1.479305	-2.814470	-0.004726
C	0.482876	-3.671226	0.519712
C	-0.750764	-3.007227	0.443384
C	-0.534902	-1.742591	-0.151865
N	0.823717	-1.665551	-0.405501
C	-1.306583	-0.573241	-0.423922
C	-2.656439	-0.317457	-0.263360
C	-3.766009	-1.191107	0.048386
C	-4.922801	-0.450977	0.086752
C	-4.540175	0.990287	-0.197948
N	-3.163646	0.956713	-0.419615
O	-5.235708	1.977922	-0.230518
C	-6.258292	-0.928164	0.337610
C	-7.365942	-0.148415	0.367098
O	-0.345784	2.521833	-0.505822
H	-1.697892	-3.378559	0.826327
H	6.609245	-0.072248	-0.182527
H	5.854214	-2.649666	-0.314623
H	0.668261	-4.646872	0.965241
H	-3.685419	-2.267075	0.189928
H	1.216326	-1.012194	-1.071703
H	2.460168	-0.265349	0.445164
H	3.340183	-3.928537	0.030547
H	3.442960	4.400983	1.159100
H	1.846498	1.185414	-1.029679
H	5.171508	2.317736	0.446720
H	0.796779	4.817156	0.834584
H	-0.730054	0.301214	-0.745142
H	-2.588549	1.788290	-0.550942
H	-6.354140	-2.005148	0.514250
H	-7.306212	0.928118	0.193739
H	-8.346204	-0.588283	0.566788

B3LYP/SVP S_0 structure of *ZaZsEa* BV

N	6.534599	-0.534442	-0.007782
C	5.381580	-1.274234	-0.040755
C	5.794166	-2.684232	-0.137670
C	7.140100	-2.750788	-0.162976
C	7.682734	-1.361289	-0.104041
C	4.075754	-0.848499	0.005971
C	3.594969	0.484403	0.177864
C	4.241820	1.690884	0.566193
C	3.303589	2.711971	0.531667
C	2.051431	2.158204	0.153986
N	2.271843	0.793885	-0.026316
C	0.832430	2.833136	0.011073
C	-0.460655	2.330952	-0.133367
C	-1.634368	3.055793	-0.488993
C	-2.698009	2.174143	-0.538742
C	-2.217844	0.879045	-0.178308
N	-0.863883	1.004506	0.020435
C	-2.856406	-0.384000	-0.024912
C	-4.208507	-0.657616	-0.000266
N	-4.703802	-1.941048	0.077231
C	-6.105529	-1.962624	0.088945
C	-6.512838	-0.505754	0.038105
C	-5.364720	0.230019	-0.015570
C	-7.875049	-0.018883	0.061088
C	-8.973779	-0.797410	0.118819
O	-6.780336	-2.960787	0.133831
O	8.817147	-0.961600	-0.135636
H	-3.713889	2.412491	-0.837309
H	5.275468	1.786191	0.887898
H	3.463541	3.756632	0.793571
H	-1.653969	4.118431	-0.725916
H	-5.308751	1.314871	-0.026502
H	-0.319027	0.301447	0.506570
H	1.643028	0.180262	-0.531888
H	0.906404	3.923315	0.014800
H	5.082055	-3.508479	-0.164387
H	7.780950	-3.628759	-0.220473
H	6.606748	0.473408	-0.067604
H	3.322673	-1.632462	-0.106272
H	-2.186480	-1.242210	0.088065
H	-4.153161	-2.792317	0.079057
H	-7.985858	1.070410	0.026280
H	-8.901222	-1.886146	0.154367
H	-9.969514	-0.347617	0.130543

TD-B3LYP/SVP S_1 structure of *ZaZsEa* BV

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.389200
C	1.388910	0.000000	1.799454
C	2.196628	-0.014177	0.682940
C	1.289523	-0.026797	-0.526330
C	-1.139911	0.032954	2.160063
C	-1.245031	-0.073085	3.593590
C	-0.402308	-0.592882	4.585582
C	-1.036184	-0.413217	5.833474
C	-2.276527	0.197339	5.602876
N	-2.397497	0.363128	4.234483
C	-3.282149	0.605027	6.554366
C	-4.629133	0.752729	6.322709
C	-5.634299	1.288939	7.210852
C	-6.846778	1.249865	6.572501
C	-6.660323	0.663911	5.266544
N	-5.308067	0.420855	5.142837
C	-7.562182	0.368687	4.228385
C	-8.953814	0.420077	4.242661
C	-9.800205	0.183561	3.073110
C	-11.101013	0.312074	3.432591
C	-11.157085	0.625305	4.883678
N	-9.790952	0.691768	5.286015
O	-12.092597	0.790904	5.625700
C	3.633830	0.000662	0.652631
C	4.384895	-0.012151	-0.481954
O	1.573000	-0.047649	-1.702532
H	0.544284	-1.099513	4.416940
H	-7.782879	1.640907	6.963252
H	-5.424708	1.691590	8.200769
H	-0.662565	-0.725953	6.806466
H	1.724263	0.046403	2.833301
H	-3.063178	0.999114	3.807032
H	-4.925173	-0.205949	4.443317
H	-2.936569	0.796044	7.572610
H	-9.398607	-0.041559	2.085262
H	-9.536984	0.784206	6.261821
H	-7.126578	0.043316	3.279705
H	-11.992852	0.212278	2.816482
H	-2.087974	0.148112	1.622098
H	-0.821562	-0.030830	-0.593361
H	4.135200	0.021602	1.626635
H	3.915981	-0.035080	-1.468391
H	5.476215	0.000632	-0.422556

B3LYP/SVP S_0 structure of *ZsZsZa* PCB

C	3.757293	1.095392	-0.054160
C	3.061687	-0.195283	-0.104597
N	4.029662	-1.162308	-0.198921
C	5.320163	-0.588467	-0.190556
C	5.095186	0.897866	-0.115536
C	1.694223	-0.344449	-0.067260
C	0.937671	-1.545083	-0.195593
C	1.275709	-2.874705	-0.586779
C	0.132384	-3.654302	-0.501980
C	-0.948769	-2.826077	-0.091095
N	-0.411129	-1.546863	0.059552
C	-2.293337	-3.168163	0.081665
C	-3.391822	-2.314483	0.229903
C	-4.727711	-2.631342	0.585440
C	-5.472599	-1.456955	0.587479
C	-4.615822	-0.390822	0.218414
N	-3.354041	-0.923903	0.045948
C	-4.942479	0.989462	0.008986
C	-4.055541	2.026764	-0.063543
C	-4.357098	3.476505	-0.399462
C	-2.974239	4.145551	-0.551771
C	-1.971652	3.112693	-0.054226
N	-2.700852	1.936553	0.168346
O	-0.783215	3.201596	0.120100
O	6.351998	-1.209033	-0.233354
C	6.226710	1.870887	-0.103433
C	7.059565	1.817134	1.190986
H	-6.525801	-1.347970	0.838135
H	-5.078505	-3.628656	0.846597
H	2.246549	-3.208353	-0.943688
H	0.041212	-4.708948	-0.757250
H	3.227952	2.046619	0.001846
H	-0.852727	-0.818710	0.606753
H	-2.687211	-0.499815	-0.592233
H	-2.516040	-4.237771	0.088017
H	1.127395	0.580615	0.072807
H	3.894936	-2.163440	-0.136863
H	-6.003198	1.224274	-0.094428
H	-4.937044	3.925487	0.424243
H	-4.980508	3.550635	-1.302058
H	-2.264810	1.151067	0.637233
H	-2.730286	4.390823	-1.598109
H	-2.856918	5.073800	0.025537
H	7.885608	2.542016	1.137426
H	6.445491	2.065380	2.070680
H	7.493919	0.817678	1.340142
H	5.831517	2.886496	-0.261672
H	6.885597	1.641183	-0.958862

TD-B3LYP/SVP S_1 structure of *ZsZsZa* PCB

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.516517
N	1.308394	0.000000	1.924437
C	2.264599	-0.059085	0.905784
C	1.487086	-0.138741	-0.401114
C	-1.093971	0.024353	2.361600
C	-1.055183	-0.077753	3.775727
C	-2.071928	0.224093	4.734506
C	-1.574490	-0.024527	5.999402
C	-0.221710	-0.500020	5.869885
N	0.065822	-0.480233	4.489958
C	0.683692	-0.917094	6.827641
C	2.051566	-1.285268	6.547821
C	2.908320	-2.188563	7.202662
C	4.132501	-2.210924	6.505769
C	4.038836	-1.314818	5.422139
N	2.752068	-0.788540	5.459814
C	4.911693	-0.963983	4.344239
C	6.269096	-1.206285	4.227974
N	7.114806	-1.745385	5.163856
C	8.436734	-1.808294	4.670071
C	8.361405	-1.284775	3.257429
C	7.063446	-0.927443	3.042606
C	9.509832	-1.184727	2.296062
C	10.884899	-1.646569	2.784753
O	9.380233	-2.202726	5.311844
O	3.455445	-0.052330	1.112172
H	-3.055859	0.619030	4.484692
H	-2.084626	0.133489	6.948468
H	4.970256	-2.871624	6.718538
H	2.639751	-2.794093	8.066410
H	6.630515	-0.513142	2.130842
H	2.516273	0.098735	5.027437
H	0.703297	-1.179189	4.115749
H	0.329768	-1.023368	7.854860
H	4.459583	-0.463854	3.480372
H	6.900589	-1.931824	6.136696
H	-2.076907	0.154114	1.903620
H	-0.441824	0.941109	-0.370493
H	-0.630996	-0.813673	-0.390662
H	1.593978	0.138887	2.887234
H	1.714776	-1.100786	-0.888261
H	1.841132	0.649676	-1.082194
H	11.621683	-1.516111	1.977718
H	11.225064	-1.070126	3.657035
H	10.881412	-2.706719	3.077087
H	9.229905	-1.749504	1.386425
H	9.568573	-0.132493	1.958167

B3LYP/SVP S_0 structure of *ZsZsEa* PCB

C	4.129706	-0.754067	-0.228267
C	2.966123	0.126943	-0.067499
N	3.458208	1.404265	0.054759
C	4.859185	1.426807	-0.037032
C	5.264043	-0.014746	-0.212853
C	1.619311	-0.154840	-0.018302
C	0.966482	-1.409621	-0.190910
C	1.391417	-2.710032	-0.600582
C	0.297058	-3.557562	-0.552724
C	-0.842719	-2.805402	-0.147288
N	-0.383277	-1.500968	0.040294
C	-2.168731	-3.220810	-0.010454
C	-3.308351	-2.419164	0.143328
C	-4.633848	-2.792663	0.475868
C	-5.421650	-1.644014	0.501372
C	-4.600858	-0.539924	0.171226
N	-3.319716	-1.024640	-0.004220
C	-4.961519	0.839422	-0.002056
C	-4.095897	1.895489	-0.018867
N	-2.743458	1.817971	0.245226
C	-2.023156	3.000766	0.054403
C	-3.026613	4.033915	-0.441133
C	-4.406782	3.351212	-0.318318
O	-0.835845	3.096944	0.245121
O	5.551476	2.412310	0.016267
C	6.694142	-0.426059	-0.313999
C	7.472410	-0.240729	1.002262
H	2.391638	-2.977930	-0.926523
H	-6.480206	-1.580645	0.745131
H	-4.951946	-3.807824	0.708537
H	0.276435	-4.611041	-0.827691
H	4.070866	-1.835430	-0.320444
H	-0.879442	-0.811880	0.590499
H	-2.665328	-0.560673	-0.627326
H	-2.339802	-4.299454	-0.038828
H	-4.993896	3.774559	0.513962
H	-2.924922	4.954713	0.150877
H	-5.024267	3.447130	-1.222727
H	-2.312897	1.027463	0.710335
H	-6.024756	1.052486	-0.124848
H	-2.770351	4.296272	-1.480472
H	0.956763	0.698158	0.166556
H	2.899749	2.245358	0.157677
H	8.522033	-0.540172	0.863824
H	7.459000	0.811077	1.323575
H	7.045956	-0.857607	1.808573
H	7.170806	0.189945	-1.096374
H	6.748691	-1.474459	-0.646889

TD-B3LYP/SVP S_1 structure of *ZsZsEa* PCB

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.517151
N	1.313566	0.000000	1.920002
C	2.262851	-0.104464	0.902526
C	1.480148	-0.208374	-0.398964
C	-1.085725	0.022234	2.368432
C	-1.043680	-0.091630	3.789795
C	-2.037461	0.208525	4.754800
C	-1.522291	-0.070067	6.021193
C	-0.196836	-0.563677	5.863978
N	0.080014	-0.523674	4.490445
C	0.727334	-1.038280	6.816547
C	2.083303	-1.321550	6.544940
C	3.037768	-2.093636	7.270170
C	4.227579	-2.112571	6.546970
C	4.049025	-1.337904	5.364209
N	2.731273	-0.898666	5.387705
C	4.844110	-1.021832	4.235374
C	6.191718	-1.263123	3.999947
C	7.246531	-1.776573	4.866069
C	8.415155	-1.826576	4.170698
C	8.130173	-1.330516	2.778113
N	6.763142	-0.996214	2.780888
O	8.874971	-1.227609	1.833288
C	9.781760	-2.242146	4.597689
C	10.775305	-1.065718	4.684925
O	3.456617	-0.121071	1.104977
H	5.122964	-2.671926	6.806806
H	-3.016438	0.627868	4.527293
H	-2.020903	0.078764	6.977547
H	2.833103	-2.618304	8.202093
H	7.103818	-2.045575	5.910799
H	2.447007	-0.049259	4.912064
H	0.708118	-1.219974	4.096106
H	0.362007	-1.227391	7.827175
H	-0.388501	0.965898	-0.367672
H	1.860409	0.534369	-1.116099
H	-0.670426	-0.777459	-0.396957
H	1.600801	0.164280	2.877978
H	-2.071915	0.148001	1.916040
H	1.670152	-1.199786	-0.842645
H	4.309006	-0.549494	3.402173
H	6.261297	-0.668400	1.959312
H	11.768877	-1.434528	4.982275
H	10.876698	-0.562630	3.711692
H	10.449580	-0.322928	5.430129
H	10.163459	-2.970936	3.860444
H	9.717774	-2.761468	5.567188

B3LYP/SVP S_0 structure of *ZaZsEa* PCB

N	6.506838	-0.458766	0.039173
C	5.379700	-1.222730	-0.023052
C	5.810846	-2.674715	-0.161600
C	7.344402	-2.653481	-0.044180
C	7.722321	-1.179243	0.000336
C	4.074104	-0.803326	0.009744
C	3.582039	0.525483	0.189563
C	4.210112	1.737229	0.602367
C	3.265399	2.750168	0.556593
C	2.023962	2.190683	0.149931
N	2.262701	0.826902	-0.037326
C	0.804959	2.853585	-0.006955
C	-0.482520	2.339886	-0.189896
C	-1.652718	3.052740	-0.567626
C	-2.705980	2.156659	-0.652795
C	-2.219522	0.867472	-0.293157
N	-0.872652	1.007321	-0.058934
C	-2.843744	-0.410503	-0.166659
C	-4.187620	-0.703342	-0.158892
N	-4.673780	-1.990242	-0.102310
C	-6.077221	-2.013593	-0.110300
C	-6.492371	-0.566206	-0.147211
C	-5.361797	0.178708	-0.176671
C	-7.926107	-0.154485	-0.121309
C	-8.619577	-0.453796	1.220825
O	-6.762802	-3.005685	-0.090951
O	8.803789	-0.663064	0.008956
H	-3.716759	2.385499	-0.975324
H	5.234492	1.844638	0.949318
H	3.411882	3.793611	0.831126
H	-1.680146	4.117170	-0.795412
H	-5.310688	1.264237	-0.179312
H	-0.332167	0.306834	0.435576
H	1.649930	0.212709	-0.561243
H	0.866861	3.944303	0.017018
H	5.474174	-3.062090	-1.137019
H	7.866238	-3.133971	-0.884332
H	5.325323	-3.292430	0.608635
H	6.525216	0.555883	0.036630
H	3.324278	-1.587161	-0.125635
H	7.714603	-3.133492	0.875369
H	-2.161038	-1.259920	-0.061738
H	-4.116296	-2.836857	-0.107700
H	-9.675541	-0.148115	1.175172
H	-8.586872	-1.528980	1.449934
H	-8.142051	0.094288	2.047965
H	-8.000927	0.918082	-0.360094
H	-8.452156	-0.703905	-0.921521

TD-B3LYP/SVP S_1 structure of *ZaZsEa* PCB

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.360769
C	1.444625	0.000000	1.829989
C	2.284427	0.116783	0.545355
C	1.282690	0.036305	-0.598824
C	-1.095100	-0.014773	2.201183
C	-2.475671	0.053209	1.861883
C	-3.164839	0.345856	0.647770
C	-4.528551	0.242203	0.880456
C	-4.723523	-0.096592	2.255473
N	-3.449607	-0.168009	2.819070
C	-5.925198	-0.319084	2.934715
C	-6.102397	-0.447169	4.361253
C	-7.211280	-0.978499	5.069250
C	-6.944897	-0.875135	6.432530
C	-5.673215	-0.260514	6.594827
N	-5.173496	-0.053028	5.312719
C	-4.903875	0.102838	7.730048
C	-5.295033	0.145918	9.064556
N	-4.413850	0.414225	10.083599
C	-5.054579	0.401526	11.338245
C	-6.501464	0.117464	11.033810
C	-6.600563	-0.027545	9.680475
C	-7.611100	0.033878	12.042120
C	-7.246523	0.250931	13.513085
O	-4.492254	0.590786	12.391156
O	1.464733	0.011020	-1.783353
H	-7.573265	-1.248021	7.236565
H	-2.710350	0.662742	-0.288322
H	-5.332178	0.427037	0.169457
H	-8.088833	-1.424579	4.604645
H	-7.517818	-0.205434	9.123694
H	-4.430412	0.609476	5.115691
H	-3.259536	-0.648645	3.692456
H	-6.826931	-0.413301	2.327164
H	1.618936	0.825175	2.538239
H	-0.825384	-0.092609	-0.585008
H	-0.860496	-0.089062	3.267400
H	3.033431	-0.679968	0.424908
H	-3.865521	0.387342	7.526136
H	-3.413825	0.556207	9.991018
H	-8.390037	0.760146	11.741243
H	2.825188	1.073678	0.466530
H	1.651380	-0.933731	2.380310
H	-8.152676	0.159995	14.131103
H	-6.514017	-0.488658	13.867242
H	-6.812612	1.246417	13.685386
H	-8.094546	-0.954190	11.922343

B3LYP/SVP S_0 structure of *ZaZsZa* PΦB

N	5.331373	0.419788	0.021789
C	4.311182	-0.503665	0.005642
C	4.937211	-1.817352	-0.054363
C	6.294675	-1.685705	-0.077370
C	6.591019	-0.203641	-0.057351
C	2.953830	-0.274556	0.041707
C	2.281881	0.973484	0.187737
C	2.741230	2.271251	0.554689
C	1.663364	3.141037	0.499112
C	0.507328	2.401653	0.130787
N	0.927939	1.081202	-0.022742
C	-0.796450	2.885425	-0.024871
C	-2.000453	2.193331	-0.163133
C	-3.265023	2.725484	-0.536567
C	-4.184685	1.690114	-0.570527
C	-3.517132	0.490170	-0.183681
N	-2.201124	0.822452	0.016158
C	-3.971803	-0.851513	-0.005658
C	-5.265732	-1.304371	0.052553
N	-6.412887	-0.569528	0.023466
C	-7.608493	-1.321598	0.087078
C	-7.191820	-2.785787	0.113281
C	-5.655476	-2.768208	0.186761
O	-8.702469	-0.833196	0.108406
C	7.291224	-2.735126	-0.117413
C	8.624054	-2.538318	-0.137714
O	7.641856	0.385153	-0.105750
H	-5.219175	1.774888	-0.892874
H	-3.443520	3.767519	-0.797198
H	3.747278	2.523837	0.878721
H	1.666268	4.202520	0.741664
H	4.370097	-2.747725	-0.056425
H	0.398540	0.372958	-0.518289
H	-1.559710	0.217633	0.516285
H	-0.885663	3.974389	-0.038943
H	2.326107	-1.163532	-0.057594
H	5.237544	1.422609	-0.077822
H	6.896137	-3.756759	-0.131402
H	9.307990	-3.389896	-0.168636
H	9.053514	-1.534748	-0.125521
H	-3.199795	-1.617302	0.106308
H	-5.280056	-3.157943	1.146939
H	-5.176911	-3.364076	-0.604850
H	-6.457531	0.444286	0.034412
H	-7.576360	-3.271869	-0.797088
H	-7.676555	-3.282494	0.966207

TD-B3LYP/SVP S_1 structure of *ZaZsZa* PΦB

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.519443
N	1.296298	0.000000	1.937911
C	2.259790	-0.041104	0.903691
C	1.480211	-0.127717	-0.402076
C	-1.137987	0.016685	2.298748
C	-1.245602	-0.046579	3.713544
C	-0.298472	-0.341190	4.746421
C	-0.933396	-0.236240	5.968069
C	-2.309451	0.106967	5.735672
N	-2.452212	0.176696	4.345798
C	-3.311270	0.320330	6.667537
C	-4.711787	0.505196	6.404828
C	-5.689419	1.118616	7.209295
C	-6.924504	1.019997	6.541097
C	-6.712484	0.338864	5.329800
N	-5.349750	0.072244	5.255318
C	-7.587138	-0.046344	4.261020
C	-8.965300	-0.091421	4.262930
N	-9.828845	0.158826	5.315186
C	-11.167406	0.001753	4.936537
C	-11.117063	-0.351778	3.470335
C	-9.786298	-0.408525	3.116022
C	-12.256107	-0.592359	2.625404
C	-13.552384	-0.529962	3.030860
O	-12.120815	0.125621	5.670866
O	3.443548	-0.014574	1.093008
H	0.732050	-0.656335	4.598586
H	-0.502993	-0.420886	6.951060
H	-7.862445	1.458730	6.874278
H	-5.498594	1.608817	8.161964
H	-9.383003	-0.636159	2.128872
H	-4.956914	-0.626906	4.633412
H	-3.228984	0.647692	3.894162
H	-3.003710	0.371985	7.713779
H	-7.113341	-0.348976	3.322543
H	-9.564999	0.295801	6.283457
H	-12.033367	-0.843571	1.582094
H	-14.362566	-0.726783	2.323996
H	-13.810165	-0.285005	4.063930
H	-2.078004	0.095126	1.744323
H	-0.451081	0.937990	-0.366223
H	-0.626194	-0.819976	-0.384847
H	1.599278	0.094254	2.902591
H	1.716474	-1.090401	-0.883362
H	1.830415	0.661239	-1.083931

B3LYP/SVP S_0 structure of *ZaZsEa* PΦB

N	4.768826	-1.949705	-0.054573
C	4.275407	-0.663317	0.014024
C	5.434499	0.221085	0.005133
C	6.579795	-0.518321	-0.053236
C	6.169139	-1.974236	-0.081891
C	2.926714	-0.384061	0.050786
C	2.295686	0.886266	0.198196
C	2.781755	2.175802	0.559155
C	1.722403	3.066204	0.501393
C	0.548887	2.349722	0.139740
N	0.943233	1.020452	-0.009062
C	-0.743916	2.858790	-0.015120
C	-1.962726	2.191482	-0.156202
C	-3.213830	2.748988	-0.534612
C	-4.154835	1.732063	-0.572284
C	-3.513830	0.519590	-0.182748
N	-2.191845	0.825062	0.022697
C	-3.996743	-0.813247	-0.006970
C	-5.299762	-1.237753	0.049825
C	-5.723159	-2.692718	0.180769
C	-7.259208	-2.675001	0.100503
C	-7.642431	-1.201565	0.080753
N	-6.430512	-0.476836	0.021762
O	-8.725483	-0.689003	0.102965
C	7.943229	-0.034625	-0.098736
C	9.039789	-0.815337	-0.160167
O	6.842419	-2.974515	-0.122789
H	3.797075	2.406917	0.865577
H	-5.185859	1.837563	-0.899611
H	-3.369943	3.794233	-0.796672
H	1.747951	4.128812	0.737744
H	5.380422	1.306229	0.002989
H	0.397798	0.321865	-0.500798
H	-1.566330	0.208565	0.528534
H	-0.811264	3.949347	-0.028096
H	-5.361738	-3.091390	1.142668
H	-7.759188	-3.165779	0.947985
H	-5.254744	-3.299105	-0.608838
H	-6.451726	0.537669	0.036633
H	-3.241253	-1.595567	0.103423
H	-7.650156	-3.146684	-0.814744
H	2.250762	-1.239647	-0.046072
H	4.216854	-2.799723	-0.038303
H	8.056180	1.054893	-0.078573
H	8.964527	-1.904244	-0.181461
H	10.036047	-0.367489	-0.189421

TD-B3LYP/SVP S_1 structure of *ZaZsEa* PΦB

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.361787
C	1.445795	0.000000	1.829045
C	2.284334	0.114106	0.543357
C	1.280349	0.035927	-0.599493
C	-1.091452	-0.015418	2.205343
C	-2.471754	0.047632	1.874504
C	-3.167695	0.316407	0.653546
C	-4.525817	0.218270	0.890388
C	-4.721337	-0.093437	2.277843
N	-3.441494	-0.153486	2.837074
C	-5.915066	-0.292215	2.956448
C	-6.088552	-0.435452	4.382001
C	-7.162516	-1.012929	5.089038
C	-6.894652	-0.888857	6.461466
C	-5.663479	-0.220178	6.610293
N	-5.175785	0.003953	5.325848
C	-4.896408	0.182420	7.748501
C	-5.318064	0.316326	9.059869
N	-4.460169	0.590746	10.113941
C	-5.139638	0.687482	11.329787
C	-6.592310	0.476630	10.974072
C	-6.650863	0.256890	9.615243
C	-7.695754	0.522373	11.897216
C	-7.583671	0.745824	13.231452
O	-4.626825	0.900750	12.405116
O	1.462497	0.011339	-1.784404
H	-7.496337	-1.295699	7.270255
H	-2.715329	0.609099	-0.291271
H	-5.331397	0.387881	0.177750
H	-8.019126	-1.504006	4.631201
H	-7.554971	0.110197	9.028318
H	-4.460508	0.694549	5.121676
H	-3.248195	-0.606387	3.724123
H	-6.819826	-0.365052	2.350141
H	1.621197	0.827011	2.534882
H	-0.825114	-0.089145	-0.585138
H	-0.851809	-0.087101	3.270477
H	3.030387	-0.685251	0.422085
H	-3.842084	0.410570	7.553519
H	-3.450220	0.659168	10.056673
H	-8.688725	0.359424	11.462813
H	-6.609528	0.909734	13.697841
H	-8.473939	0.765418	13.865458
H	2.827884	1.069218	0.463333
H	1.653165	-0.932569	2.380908

B3LYP/SVP S_0 structure of *ZsZsEa* PΦB

N	2.653553	1.840542	-0.219088
C	3.998164	1.939072	0.077288
C	4.277942	3.398622	0.388469
C	2.884181	4.057915	0.481825
C	1.909738	3.010383	-0.040895
C	4.880949	0.897341	0.078025
C	4.547606	-0.487297	-0.108046
C	5.394394	-1.576552	-0.420288
C	4.625052	-2.738219	-0.417949
C	3.285849	-2.387453	-0.118049
N	3.270419	-0.993538	0.033615
C	2.155684	-3.208152	0.004605
C	0.820277	-2.814436	0.107942
C	-0.317597	-3.587262	0.479873
C	-1.426758	-2.758728	0.500413
C	-1.012840	-1.449371	0.106634
N	0.344715	-1.517141	-0.087495
C	-1.683729	-0.208013	-0.078225
C	-3.039411	0.045377	-0.069353
N	-3.549229	1.318515	-0.194570
C	-4.949609	1.326895	-0.155548
C	-5.339795	-0.129359	-0.009003
C	-4.183017	-0.851401	0.039963
C	-6.696877	-0.627647	0.051197
C	-7.805114	0.137213	-0.005199
O	-5.638877	2.313525	-0.230761
O	0.725993	3.088642	-0.260075
H	-2.430776	-3.043765	0.799260
H	6.457589	-1.495261	-0.637045
H	4.965614	-3.747249	-0.645368
H	-0.286417	-4.641134	0.752346
H	-4.113320	-1.933150	0.115706
H	0.843319	-0.819314	-0.624356
H	2.593401	-0.542701	0.642008
H	2.343498	-4.283940	0.034656
H	4.876726	3.834696	-0.428844
H	2.780902	4.979450	-0.108801
H	4.873067	3.501599	1.307005
H	2.247364	1.045085	-0.697490
H	5.937226	1.127487	0.227306
H	2.599538	4.311607	1.515934
H	-1.034143	0.659803	-0.237887
H	-3.001685	2.169394	-0.272070
H	-6.794917	-1.714218	0.151027
H	-7.744878	1.222757	-0.104433
H	-8.795787	-0.320677	0.048434

TD-B3LYP/SVP S_1 structure of *ZsZsEa* PΦB

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.445360
N	1.322547	0.000000	1.852582
C	2.197214	0.028032	0.765750
C	1.298434	0.009133	-0.453177
C	-1.041189	-0.019980	2.355707
C	-2.448791	0.112101	2.151151
C	-3.283806	0.495758	1.080932
C	-4.610059	0.528310	1.546788
C	-4.604479	0.179592	2.914952
N	-3.280069	-0.051764	3.253133
C	-5.663308	0.128802	3.880602
C	-5.479021	0.268541	5.251501
C	-6.399777	0.134093	6.342417
C	-5.728747	0.426165	7.519939
C	-4.376609	0.746222	7.204679
N	-4.240678	0.607519	5.829744
C	-3.306917	1.117602	8.065981
C	-1.967606	1.140872	7.734887
N	-1.440999	0.679991	6.551250
C	-0.068003	0.855539	6.386626
C	0.424338	1.562535	7.641772
C	-0.806608	1.637916	8.575694
O	0.536403	0.498715	5.399045
O	3.404388	0.061594	0.835183
C	1.746143	-0.006513	-1.822652
C	3.043119	0.000030	-2.215736
H	-2.951367	0.783984	0.086597
H	-6.135836	0.391176	8.529485
H	-7.439056	-0.174783	6.240795
H	-5.490882	0.826211	0.980692
H	-0.895776	-0.039508	-0.616801
H	-3.025796	-0.639883	4.039442
H	-3.605079	1.202240	5.304144
H	-6.683780	0.016970	3.509866
H	-0.688389	0.990576	9.461906
H	1.273644	1.005209	8.064548
H	-1.000615	2.652979	8.954976
H	-1.979497	0.155814	5.871812
H	-3.574362	1.399854	9.086553
H	0.810763	2.554966	7.356913
H	-0.726048	-0.100817	3.402919
H	1.633277	0.058577	2.818858
H	0.955481	-0.024144	-2.581393
H	3.856199	0.017065	-1.486648
H	3.298721	-0.011958	-3.278511

B3LYP/SVP S_0 structure of *ZaEaZs* PΦB

C	-6.657347	0.705953	-0.390454
C	-5.240563	0.736776	-0.076362
N	-4.879427	-0.557475	0.278338
C	-6.009137	-1.406318	0.288186
C	-7.147513	-0.557307	-0.217149
C	-4.413602	1.831628	-0.147581
C	-2.993112	1.856459	-0.011182
C	-2.158690	2.993443	0.187023
C	-0.844009	2.562572	0.231969
C	-0.828865	1.150431	0.048903
N	-2.166386	0.769911	-0.077452
C	0.196708	0.198026	-0.018842
C	1.580334	0.357238	0.076606
C	2.423222	1.486431	0.296398
C	3.736468	1.056844	0.304782
C	3.748654	-0.358766	0.086265
N	2.445455	-0.732400	-0.037681
C	4.805608	-1.316883	0.023349
C	6.156395	-1.090841	-0.048399
C	7.206626	-2.191019	-0.050965
C	8.559271	-1.458876	-0.040493
C	8.216696	0.017541	-0.183392
N	6.806703	0.103688	-0.146494
O	8.939148	0.966712	-0.301372
O	-5.989018	-2.554991	0.656377
C	-8.497444	-1.025259	-0.454041
C	-8.927793	-2.286763	-0.257633
H	4.600841	1.685537	0.501143
H	2.088544	2.508283	0.450802
H	-2.520532	4.013306	0.301150
H	0.027670	3.191267	0.389714
H	-7.206906	1.575057	-0.751314
H	-2.466542	-0.147967	-0.387177
H	2.146611	-1.683673	-0.220110
H	-0.141325	-0.833835	-0.171131
H	-4.890221	2.795893	-0.331760
H	-4.091579	-0.785658	0.875450
H	-9.198474	-0.266926	-0.819338
H	-9.967845	-2.553442	-0.460294
H	-8.259621	-3.068292	0.109149
H	4.506546	-2.368375	0.028149
H	7.077410	-2.813959	-0.950918
H	7.065641	-2.854644	0.815192
H	6.359366	1.007153	-0.259861
H	9.118113	-1.595114	0.898735
H	9.235405	-1.752296	-0.856519

TD-B3LYP/SVP S_1 structure of *ZaEaZs* PΦB

N	-4.879820	-0.525050	0.327886
C	-5.233490	0.770527	-0.046097
C	-6.638968	0.750253	-0.357535
C	-7.139502	-0.521064	-0.168923
C	-6.007181	-1.369215	0.342351
C	-4.388633	1.859690	-0.161275
C	-2.966407	1.871772	-0.066780
C	-2.097330	2.972741	0.080889
C	-0.784479	2.493746	0.105588
C	-0.830661	1.081565	-0.047264
N	-2.167294	0.739897	-0.125461
C	0.173899	0.076719	-0.149422
C	1.548528	0.236063	0.023659
C	2.353819	1.353374	0.429991
C	3.678414	0.951878	0.441596
C	3.739749	-0.419679	0.043769
N	2.442387	-0.808839	-0.181955
C	4.818420	-1.337577	-0.099431
C	6.170699	-1.074257	-0.101236
N	6.779830	0.143190	-0.052820
C	8.193504	0.105745	-0.056024
C	8.581069	-1.366829	-0.051608
C	7.254371	-2.135948	-0.182466
O	8.885794	1.084869	-0.057133
C	-8.488116	-0.972315	-0.399089
C	-8.935171	-2.235343	-0.184983
O	-5.998849	-2.519583	0.717374
H	4.516182	1.563768	0.767950
H	1.978140	2.327955	0.727480
H	-2.417114	4.008807	0.176831
H	0.114322	3.096488	0.192331
H	-7.187165	1.617171	-0.727404
H	-2.500222	-0.173439	-0.414180
H	2.177142	-1.727415	-0.518501
H	-0.176809	-0.932429	-0.389261
H	-4.863789	2.824545	-0.352580
H	-4.085134	-0.750600	0.917711
H	-9.185011	-0.214583	-0.774935
H	-9.978483	-2.493460	-0.384300
H	-8.270276	-3.016120	0.190925
H	4.548362	-2.389814	-0.228312
H	7.174313	-2.667916	-1.145662
H	7.110894	-2.891599	0.605405
H	6.300468	1.037659	-0.092316
H	9.115180	-1.581487	0.888189
H	9.292511	-1.555280	-0.869127

B3LYP/SVP S_0 structure of *ZsZsZa* BV + Cl^-

N	-3.733393	2.003032	-0.190441
C	-4.903358	1.302556	-0.116317
C	-6.001762	2.277630	-0.269284
C	-5.473811	3.505527	-0.426768
C	-3.985139	3.378358	-0.363845
C	-5.158353	-0.046755	0.007622
C	-4.337138	-1.215903	0.022406
C	-4.874805	-2.537198	-0.122013
C	-3.819499	-3.417848	-0.135868
C	-2.610447	-2.662307	0.005220
N	-2.982563	-1.325171	0.105517
C	-1.341724	-3.246800	-0.029876
C	-0.024278	-2.763450	-0.006632
C	1.149610	-3.570880	-0.121471
C	2.251207	-2.735399	-0.070902
C	1.765228	-1.398976	0.081921
N	0.407688	-1.461992	0.108377
C	2.421415	-0.135892	0.241632
C	3.750388	0.155072	0.086108
C	4.359082	1.452996	0.335119
C	5.699037	1.395709	0.085037
C	6.002924	-0.005246	-0.376597
N	4.778765	-0.680023	-0.320550
O	7.048634	-0.501177	-0.737879
C	6.673582	2.462234	0.220790
C	7.989870	2.356225	-0.038966
O	-3.145924	4.244527	-0.441855
H	-5.934129	-2.762295	-0.228127
H	-3.856514	-4.499437	-0.255692
H	3.292516	-3.046414	-0.091425
H	1.148983	-4.654901	-0.224137
H	3.791042	2.314199	0.686497
Cl	-1.175913	0.952797	1.038367
H	-1.387577	-4.335066	-0.125087
H	1.770314	0.697609	0.519623
H	4.677593	-1.618122	-0.683891
H	6.268513	3.420583	0.565810
H	8.651492	3.216208	0.091803
H	8.424078	1.416402	-0.385198
H	-6.223232	-0.289805	0.011511
H	-7.052540	1.988228	-0.267606
H	-5.978405	4.457868	-0.578715
H	-0.181005	-0.618056	0.301767
H	-2.347108	-0.540416	0.407006
H	-2.780854	1.660228	0.077272

TD-B3LYP/SVP S_1 structure of *ZsZsZa* BV + Cl^-

N	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.383490
C	1.380610	0.000000	1.798008
C	2.198472	-0.006911	0.692458
C	1.303529	-0.026664	-0.514652
C	-1.086897	0.006123	2.242628
C	-2.471551	0.059834	1.939796
C	-3.223084	0.170774	0.730501
C	-4.567786	0.141739	1.070403
C	-4.660173	0.029192	2.494568
N	-3.383621	-0.006575	2.970313
C	-5.867079	0.002597	3.249561
C	-6.135102	0.085621	4.615808
C	-7.472285	0.180774	5.156255
C	-7.371451	0.330767	6.514113
C	-5.971511	0.341454	6.858489
N	-5.260778	0.178207	5.692910
C	-5.506197	0.574188	8.170666
C	-4.251480	0.857516	8.715939
N	-3.022056	0.905382	8.134694
C	-2.038838	1.296316	9.079628
C	-2.781850	1.527692	10.347119
C	-4.088323	1.253839	10.119627
O	-0.855799	1.404230	8.844865
C	3.643242	-0.002639	0.664527
C	4.408973	-0.015792	-0.448263
O	1.576505	-0.062933	-1.697173
Cl	-2.370662	-0.797601	5.723763
H	-8.179224	0.460934	7.232583
H	-8.377702	0.164527	4.551409
H	-2.824638	0.281537	-0.275364
H	-5.419735	0.217725	0.396678
H	1.688304	0.014233	2.843787
H	-6.766529	-0.027852	2.630134
H	-0.847017	-0.054576	3.309327
H	-0.807782	-0.092667	-0.601318
H	4.128766	0.011643	1.647753
H	5.499409	-0.011852	-0.370417
H	3.959904	-0.031512	-1.443651
H	-6.315862	0.629090	8.902343
H	-4.922589	1.323780	10.818051
H	-2.299154	1.861940	11.263891
H	-3.079839	-0.200989	3.951354
H	-4.250753	-0.116761	5.678923
H	-2.745514	0.477038	7.218682

B3LYP/SVP S_0 structure of *ZsZsZa* PCB + Cl^-

N	4.809316	-0.810247	0.023804
C	3.743817	0.070284	0.116977
C	4.334466	1.401595	0.261967
C	5.686507	1.308926	0.257697
C	6.034791	-0.142317	0.122444
C	2.403230	-0.193057	0.080399
C	1.742298	-1.454055	-0.099023
C	2.211807	-2.769050	-0.392794
C	1.105532	-3.603520	-0.433748
C	-0.053574	-2.812511	-0.180698
N	0.387240	-1.522339	0.005891
C	-1.375940	-3.294437	-0.168813
C	-2.635986	-2.712402	-0.054248
C	-3.857038	-3.455566	-0.166724
C	-4.904507	-2.572039	-0.076135
C	-4.353613	-1.255584	0.087238
N	-2.999861	-1.374882	0.107966
C	-5.169272	-0.082375	0.144160
C	-4.918299	1.263756	0.020099
N	-3.741825	1.936786	-0.109593
C	-3.891922	3.306897	-0.368351
C	-5.390832	3.581691	-0.484717
C	-6.054834	2.280170	-0.023417
O	-2.986927	4.089837	-0.492761
C	6.736844	2.368325	0.357663
C	7.528796	2.562772	-0.946420
O	7.126997	-0.671150	0.106455
Cl	-1.166555	0.868595	1.063676
H	-5.968805	-2.788584	-0.143211
H	-3.906253	-4.532293	-0.321770
H	3.239932	-3.063618	-0.586215
H	1.094694	-4.672451	-0.640916
H	3.730198	2.304767	0.349220
H	-1.428170	-4.376879	-0.314723
H	1.739959	0.664280	0.223090
H	4.752750	-1.819290	0.016295
H	6.268130	3.317255	0.664495
H	-6.233399	-0.324129	0.202852
H	-6.869296	1.936851	-0.677357
H	-5.612599	3.824388	-1.536860
H	-0.186779	-0.697351	0.296961
H	-2.351231	-0.604225	0.409961
H	-2.787246	1.557546	0.115674
H	-5.650369	4.467400	0.111886
H	-6.477353	2.379002	0.991008
H	8.305309	3.332999	-0.816460
H	8.023878	1.626027	-1.243059
H	6.868798	2.880145	-1.769400
H	7.441010	2.082303	1.158679

TD-B3LYP/SVP S_1 structure of *ZsZsZa* PCB + Cl^-

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.523351
N	1.292860	0.000000	1.950949
C	2.236889	-0.124565	0.919288
C	1.457031	-0.287254	-0.385038
C	-1.176298	-0.025897	2.250374
C	-1.502124	-0.135068	3.636843
C	-2.813478	-0.443905	4.105147
C	-2.754009	-0.565893	5.482219
C	-1.402338	-0.321997	5.886654
N	-0.676273	-0.058836	4.735871
C	-0.961892	-0.412900	7.228175
C	0.301353	-0.328235	7.837377
C	0.584534	-0.622417	9.218444
C	1.939607	-0.459620	9.423919
C	2.521518	-0.042108	8.178360
N	1.501629	0.004051	7.260263
C	3.841773	0.288206	7.786162
C	4.978887	0.403746	8.569396
N	5.087909	0.306043	9.941006
C	6.416425	0.506595	10.362054
C	7.198556	0.715138	9.108542
C	6.318769	0.658552	8.067012
C	8.677103	0.933001	9.118341
C	9.476493	-0.313716	9.540182
O	6.785701	0.508189	11.520400
O	3.431122	-0.123159	1.074533
Cl	2.051249	1.295426	4.566675
H	-3.680568	-0.590598	3.463098
H	-3.563613	-0.821510	6.164006
H	2.473796	-0.652262	10.351366
H	-0.158186	-0.948431	9.945151
H	6.538361	0.771517	7.004878
H	-1.766904	-0.658283	7.924946
H	3.976010	0.491313	6.719122
H	4.323565	0.246535	10.600829
H	9.001153	1.272890	8.120875
H	-2.069442	-0.042061	1.619400
H	-0.719608	-0.730597	-0.399343
H	1.607706	-1.317462	-0.748934
H	1.654478	0.375728	6.297791
H	0.275867	0.384852	4.704556
H	1.619926	0.243235	2.921419
H	1.872011	0.386568	-1.148545
H	-0.323665	0.993943	-0.357137
H	10.556027	-0.093052	9.558450
H	9.178990	-0.643892	10.547204
H	9.310759	-1.148556	8.840431
H	8.903628	1.750290	9.826521

B3LYP/SVP S_0 structure of *ZaZsZa* PΦB + Cl^-

C	5.693777	-2.620590	-0.091926
C	5.295936	-1.154953	-0.007788
N	6.446613	-0.435628	0.241531
C	7.625178	-1.182493	0.257229
C	7.232255	-2.616100	-0.087588
C	4.024067	-0.689010	-0.136181
C	3.561906	0.670556	-0.089675
C	4.236420	1.937116	-0.072612
C	3.266476	2.919608	-0.050084
C	1.985245	2.280315	-0.056251
N	2.230956	0.919345	-0.082039
C	0.754804	2.940361	-0.047588
C	-0.573442	2.487595	-0.067622
C	-1.730568	3.327387	-0.074241
C	-2.849494	2.515277	-0.104358
C	-2.390243	1.159975	-0.113302
N	-1.032488	1.188188	-0.094379
C	-3.066921	-0.102441	-0.162198
C	-4.407897	-0.352499	-0.050720
N	-5.443516	0.538785	0.185543
C	-6.680637	-0.109322	0.252697
C	-6.376993	-1.560575	-0.010116
C	-5.026246	-1.664157	-0.171010
C	-7.361647	-2.625102	-0.068527
C	-8.688118	-2.474959	0.101848
O	-7.736725	0.439954	0.485293
O	8.718479	-0.731691	0.489969
H	5.309737	2.105177	-0.115790
H	3.420154	3.997668	-0.041352
H	-3.882164	2.850358	-0.157872
H	-1.706224	4.416056	-0.068652
H	-4.454420	-2.569093	-0.375585
Cl	0.388110	-1.511626	-0.189839
H	1.535340	0.124289	-0.102409
H	0.843169	4.029810	-0.024422
H	-2.414018	-0.971355	-0.290841
H	-5.347064	1.514809	0.430504
H	-6.954834	-3.622919	-0.270038
H	-9.355948	-3.337932	0.040322
H	-9.124750	-1.495333	0.305382
H	3.234683	-1.435052	-0.272143
H	5.256655	-3.092876	-0.983262
H	5.284820	-3.155167	0.781284
H	6.472153	0.554938	0.454784
H	7.687492	-3.304490	0.638616
H	7.665061	-2.858283	-1.071897
H	-0.475856	0.290186	-0.105975

TD-B3LYP/SVP S_1 structure of *ZaZsZa* PΦB + Cl^-

C	4.965002	-0.166055	-1.682070
C	4.378626	-0.033914	-0.372857
N	5.420249	0.197634	0.505893
C	6.656578	0.246408	-0.159324
C	6.332064	-0.014853	-1.599412
C	3.020676	-0.130914	-0.091858
C	2.368730	-0.081244	1.160805
C	2.844836	-0.051075	2.520914
C	1.744794	-0.037221	3.347023
C	0.560653	-0.056602	2.521654
N	0.997815	-0.086829	1.217018
C	-0.755498	-0.045004	3.000941
C	-2.003885	-0.071658	2.327533
C	-3.290773	-0.065105	2.953864
C	-4.254726	-0.102754	1.953141
C	-3.569470	-0.129583	0.702754
N	-2.226402	-0.116551	0.974852
C	-3.991222	-0.181258	-0.665733
C	-5.253982	-0.039691	-1.179288
C	-5.613944	-0.138423	-2.651055
C	-7.151920	-0.071121	-2.688079
C	-7.572586	0.281032	-1.263572
N	-6.409639	0.237851	-0.487865
O	-8.669233	0.540706	-0.836031
O	7.719628	0.466428	0.386592
C	7.294501	-0.084019	-2.674593
C	8.630608	0.075464	-2.552520
Cl	-0.420328	-0.204411	-1.478746
H	-5.330346	-0.151708	2.111050
H	-3.457242	-0.048845	4.030086
H	3.883544	-0.082585	2.841122
H	1.735214	-0.021830	4.435938
H	4.378045	-0.368576	-2.577917
H	-1.528051	-0.135156	0.185046
H	-0.837435	-0.013286	4.089800
H	2.357585	-0.248980	-0.955787
H	5.339643	0.436712	1.485225
H	6.870042	-0.284563	-3.665954
H	9.279444	0.005895	-3.429740
H	9.089785	0.277370	-1.582453
H	-3.179668	-0.325402	-1.388698
H	-5.203431	-1.059106	-3.092796
H	-5.151280	0.701681	-3.197262
H	-6.446956	0.456722	0.502556
H	-7.556253	0.679794	-3.382711
H	-7.618872	-1.033991	-2.953834
H	0.432987	-0.110056	0.327619

PBE0/SVP S_0 structure of *ZaZsZa* PΦB

N	5.294702	0.417076	0.017690
C	4.289708	-0.513196	0.016557
C	4.925370	-1.817710	-0.039929
C	6.276706	-1.669206	-0.075145
C	6.553253	-0.189384	-0.069660
C	2.934998	-0.297007	0.061586
C	2.264548	0.948802	0.207648
C	2.724797	2.236276	0.591029
C	1.653497	3.108042	0.527357
C	0.505699	2.375071	0.139883
N	0.921882	1.061897	-0.018292
C	-0.792192	2.860997	-0.026975
C	-1.990439	2.169044	-0.175409
C	-3.246250	2.698227	-0.565319
C	-4.160624	1.663763	-0.606454
C	-3.495015	0.472338	-0.205220
N	-2.189862	0.806309	0.007663
C	-3.950497	-0.865045	-0.026892
C	-5.245838	-1.302054	0.042304
N	-6.377114	-0.553904	0.031956
C	-7.574759	-1.287477	0.105401
C	-7.178642	-2.748518	0.112681
C	-5.651425	-2.752586	0.172183
O	-8.659250	-0.787792	0.146250
C	7.285114	-2.701819	-0.115132
C	8.610410	-2.478745	-0.146907
O	7.593992	0.407724	-0.133887
H	-5.189714	1.742994	-0.948089
H	-3.421896	3.738677	-0.834430
H	3.726451	2.480494	0.935620
H	1.655134	4.167385	0.779424
H	4.368858	-2.754390	-0.029541
H	0.397293	0.360307	-0.526060
H	-1.554328	0.206242	0.518676
H	-0.880821	3.949977	-0.041452
H	2.312173	-1.189819	-0.030730
H	5.186807	1.416105	-0.093662
H	6.907993	-3.729947	-0.118616
H	9.310967	-3.316422	-0.176919
H	9.017396	-1.465294	-0.145226
H	-3.184311	-1.637303	0.076638
H	-5.271960	-3.149928	1.127093
H	-5.185903	-3.350635	-0.624793
H	-6.405670	0.459153	0.055118
H	-7.579037	-3.217879	-0.799024
H	-7.665137	-3.247683	0.962422

TD-PBE0/SVP S_1 structure of *ZaZsZa* PΦB

C	4.737546	-1.797422	-0.220920
C	4.176398	-0.482281	-0.064217
N	5.224314	0.387982	0.109084
C	6.452389	-0.272853	0.051193
C	6.105729	-1.721921	-0.144432
C	2.826392	-0.189656	-0.084835
C	2.198763	1.063515	0.144837
C	2.658448	2.279631	0.689631
C	1.601815	3.190613	0.672274
C	0.476996	2.539788	0.126622
N	0.860536	1.246006	-0.149774
C	-0.825344	3.058302	-0.120651
C	-1.994122	2.321200	-0.253367
C	-3.286244	2.769898	-0.663717
C	-4.146725	1.691604	-0.632660
C	-3.421634	0.550841	-0.182049
N	-2.123468	0.961468	-0.005058
C	-3.798371	-0.794350	0.057576
C	-5.064891	-1.328769	0.115331
C	-5.365009	-2.795906	0.307488
C	-6.886033	-2.908623	0.203555
C	-7.388071	-1.483612	0.108181
N	-6.244623	-0.667194	0.036134
O	-8.507241	-1.064581	0.086843
O	7.529027	0.260873	0.135953
C	7.050178	-2.799164	-0.239316
C	8.392998	-2.655223	-0.161759
H	-5.182837	1.705887	-0.963572
H	-3.513811	3.784760	-0.985112
H	3.640887	2.457475	1.121379
H	1.611275	4.212281	1.046511
H	4.139217	-2.697935	-0.358439
H	0.351346	0.645408	-0.788029
H	-1.450283	0.434678	0.539310
H	-0.919176	4.143952	-0.179600
H	2.173200	-1.034453	-0.319945
H	5.166956	1.397545	0.120311
H	6.623460	-3.797392	-0.385622
H	9.047742	-3.526018	-0.244156
H	8.848947	-1.672788	-0.017675
H	-2.985550	-1.506564	0.225088
H	-4.988739	-3.118553	1.292442
H	-4.831201	-3.398811	-0.442527
H	-6.346740	0.341266	0.001741
H	-7.221164	-3.452333	-0.693371
H	-7.362370	-3.400250	1.063598

B3LYP/TZVP S_0 structure of *ZaZsZa* PΦB

N	5.319574	0.430849	0.037333
C	4.307110	-0.501272	0.023059
C	4.943726	-1.804030	-0.034418
C	6.292061	-1.665750	-0.075335
C	6.580679	-0.186009	-0.071748
C	2.957048	-0.284473	0.066028
C	2.281340	0.954758	0.211328
C	2.724490	2.246043	0.589572
C	1.648064	3.107314	0.525984
C	0.503762	2.372988	0.141136
N	0.927659	1.052500	-0.007909
C	-0.791554	2.853697	-0.025467
C	-1.988176	2.167423	-0.175177
C	-3.240122	2.697813	-0.564447
C	-4.160627	1.671959	-0.607603
C	-3.511103	0.474584	-0.210836
N	-2.193535	0.795637	-0.001866
C	-3.972586	-0.858694	-0.034964
C	-5.261800	-1.295655	0.036566
N	-6.400969	-0.549793	0.026506
C	-7.600636	-1.289489	0.107964
C	-7.201974	-2.755176	0.118518
C	-5.664919	-2.754125	0.168248
O	-8.688756	-0.789720	0.151472
C	7.286183	-2.710528	-0.116804
C	8.611403	-2.519605	-0.145612
O	7.624805	0.408738	-0.151647
H	-5.178293	1.760827	-0.947562
H	-3.410049	3.729175	-0.830923
H	3.714009	2.499485	0.929243
H	1.645424	4.156821	0.775146
H	4.388909	-2.730207	-0.022174
H	0.421796	0.361571	-0.540069
H	-1.579586	0.204294	0.536356
H	-0.879223	3.933533	-0.038948
H	2.339086	-1.169661	-0.027828
H	5.216197	1.421257	-0.110553
H	6.893727	-3.722915	-0.123344
H	9.284281	-3.366529	-0.176256
H	9.048133	-1.530550	-0.140980
H	-3.212010	-1.624834	0.061759
H	-5.287835	-3.150419	1.113152
H	-5.215120	-3.344532	-0.630135
H	-6.434657	0.458557	0.051925
H	-7.597107	-3.226293	-0.782613
H	-7.669387	-3.246726	0.970784

TD-B3LYP/TZVP S_1 structure of *ZaZsZa* PΦB

C	4.797959	-1.784606	-0.212774
C	4.217738	-0.477634	-0.052824
N	5.268379	0.405051	0.126038
C	6.504934	-0.246189	0.050463
C	6.164735	-1.698894	-0.146156
C	2.874963	-0.203637	-0.066300
C	2.228988	1.047601	0.165743
C	2.655194	2.252569	0.728693
C	1.577733	3.151845	0.708828
C	0.481031	2.500848	0.138621
N	0.881081	1.207542	-0.144657
C	-0.827826	3.014172	-0.143189
C	-1.987766	2.289979	-0.274145
C	-3.278088	2.744249	-0.697797
C	-4.149065	1.683647	-0.660453
C	-3.449539	0.532366	-0.193044
N	-2.135704	0.920562	-0.019179
C	-3.848829	-0.800868	0.051602
C	-5.117869	-1.315870	0.114098
C	-5.438702	-2.785787	0.312217
C	-6.971772	-2.879907	0.213490
C	-7.453739	-1.442290	0.114227
N	-6.295375	-0.638452	0.034715
O	-8.570315	-1.005512	0.095497
O	7.583701	0.294572	0.124446
C	7.104147	-2.775236	-0.252990
C	8.448048	-2.645933	-0.185972
H	-5.172923	1.709128	-0.995447
H	-3.490023	3.747504	-1.032540
H	3.618063	2.441318	1.173870
H	1.571472	4.159862	1.090845
H	4.214080	-2.683777	-0.346406
H	0.402700	0.622348	-0.813659
H	-1.493617	0.406112	0.565178
H	-0.908736	4.088117	-0.248990
H	2.232584	-1.049847	-0.285560
H	5.203886	1.410232	0.122991
H	6.676078	-3.762682	-0.400479
H	9.085197	-3.516182	-0.277643
H	8.918739	-1.682503	-0.041983
H	-3.051447	-1.517125	0.219748
H	-5.073122	-3.110535	1.289762
H	-4.928119	-3.392556	-0.437010
H	-6.386957	0.366827	0.004791
H	-7.307668	-3.418563	-0.674440
H	-7.439596	-3.355631	1.074990