

Supporting Information

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Energies

First column in a redox state data set is the energy given in Hartrees, whereas the second is in eV.

Extrapolated numbers are marked by the text 'crash' in the Hartrees column. For the DHAVHF with one linker the subfix indicates the position of the linker.

DHADHA with two S-phenyl

Table 1: Vacuum Energies with Thermal Hydrogens

ENERGY (vacuum) TO.S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2630.43246	-71577.73933	Crash	-71571.00559	-2629.789274	-71560.23733	-2630.430252	-71577.67923	-2630.48626	-71579.20331
2DHA_RS	-2630.431171	-71577.70424	Crash	-71571.00559	-2629.789841	-71560.25275	-2630.430251	-71577.67921	-2630.487073	-71579.22541
DHAVHF	-2630.422797	-71577.47639	-2630.170614	-71570.61412	-2629.794772	-71560.38693	-2630.455565	-71578.36804	-2630.493566	-71579.40211
VHVFHF	-2630.416906	-71577.31608	Crash	-71570.95117	-2629.815994	-71560.96442	-2630.448042	-71578.16333	-2630.488228	-71579.25683
2DHA_RR	-2630.432508	-71577.74062	-2630.164136	-71570.43784	-2629.805738	-71560.68534	-2630.476469	-71578.93687	-2630.49861	-71579.53935
2DHA_RS	-2630.432646	-71577.74439	-2630.164202	-71570.43966	-2629.805807	-71560.68723	-2630.476504	-71578.93782	-2630.498624	-71579.53974
DHAVHF	-2630.422778	-71577.47587	-2630.170792	-71570.61897	-2629.794998	-71560.3931	-2630.469318	-71578.74229	-2630.491197	-71579.33763
VHVFHF	-2630.415723	-71577.2839	Crash	-71570.81511	-2629.810825	-71560.82376	-2630.46074	-71578.50886	-2630.488675	-71579.26901
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

Table 2: Vacuum Energies without thermal hydrogens

ENERGY (vacuum) TO.S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2629.087402	-71541.13841	Crash	-71534.86885	-2628.535894	-71526.1311	-2629.277101	-71546.30039	Crash	-71544.93707
2DHA_RS	-2629.084672	-71541.06414	Crash	-71534.81443	-2628.536313	-71526.1425	-2629.279913	-71546.3769	Crash	-71544.93707
DHAVHF	-2629.078036	-71540.88354	Crash	-71534.51511	-2628.522899	-71525.7775	-2629.287641	-71546.58721	Crash	-71544.90986
VHVFHF	-2629.070902	-71540.68942	Crash	-71534.43347	-2628.52971	-71525.96285	-2629.289957	-71546.65021	Crash	-71544.7738
2DHA_RR	-2629.085947	-71541.09883	Crash	-71534.56953	-2628.506233	-71525.32401	-2629.265496	-71545.98461	Crash	-71544.90986
2DHA_RS	-2629.084752	-71541.06632	Crash	-71534.56953	-2628.50696	-71525.34379	-2629.26668	-71546.01683	Crash	-71544.90986
DHAVHF	-2629.078918	-71540.90756	Crash	-71534.62395	-2628.52318	-71525.78514	-2629.261068	-71545.86412	Crash	-71544.63775
VHVFHF	-2629.069715	-71540.65714	Crash	-71534.46068	-2628.528713	-71525.9357	-2629.262717	-71545.90899	Crash	-71544.47448
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

Table 3: Junction Energies

(junction) TO_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2629.090475	-71541.22203	Crash	-71535.08655	-2628.575116	-71527.19841	-2629.346206	-71548.18084	Crash	-71545.59014
2DHA_RS	-2629.085446	-71541.0852	Crash	-71534.89607	-2628.565211	-71526.92886	-2629.342507	-71548.08018	Crash	-71545.45409
DHAVHF	-2629.080417	-71540.94834	Crash	-71534.84164	-2628.569531	-71527.04643	-2629.33692	-71547.92815	Crash	-71545.29082
VHVFHF	-2629.071754	-71540.7126	Crash	-71534.48789	-2628.54967	-71526.50599	-2629.336798	-71547.92483	Crash	-71545.20918
PARA										
2DHA_RR	-2629.086339	-71541.10949	Crash	-71534.65116	-2628.535108	-71526.10972	-2629.328875	-71547.70923	Crash	-71545.42688
2DHA_RS	-2629.085985	-71541.09986	Crash	-71534.65116	-2628.532662	-71526.04316	-2629.325963	-71547.62999	Crash	-71545.42688
DHAVHF	-2629.08145	-71540.97645	Crash	-71534.95049	-2628.571735	-71527.1064	-2629.324939	-71547.60213	Crash	-71545.18197
VHVFHF	-2629.070109	-71540.66784	Crash	-71534.46068	-2628.54884	-71526.48338	-2629.322891	-71547.5464	Crash	-71545.01871
VHVFHF	-2629.069715	-71540.65714	Crash	-71534.46068	-2628.528713	-71525.9357	-2629.262717	-71545.90899	Crash	-71544.47448
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

DHADHA with one S-phenyl

Table 4: Vacuum Energies with Thermal Hydrogens

ENERGY (vacuum) ET_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2001.296699	-54458.07698	-2001.025858	-54450.70703	-2000.643344	-54440.29829	-2001.287109	-54457.81604	-2001.347464	-54459.45838
2DHA_RS	-2001.295364	-54458.04067	-2001.026191	-54450.71608	-2000.6429	-54440.28619	-2001.286633	-54457.80309	-2001.346261	-54459.42565
DHAVHF(DHA)	-2001.287376	-54457.82329	Crash	-54451.03743	-2000.636587	-54440.11442	-2001.293359	-54457.98611	-2001.353342	-54459.61833
DHAVHF(VHF)	-2001.285508	-54457.77246	-2001.034452	-54450.94087	-2000.647685	-54440.41642	-2001.317576	-54458.64508	-2001.357412	-54459.72908
VHVFHF	-2001.282961	-54457.70317	Crash	-54451.17349	-2000.664686	-54440.87904	-2001.311497	-54458.47965	-2001.353369	-54459.61906
PARA										
2DHA_RR	-2001.296742	-54458.07817	-2001.028188	-54450.77042	-2000.665467	-54440.90029	-2001.332285	-54459.04534	-2001.360729	-54459.81934
2DHA_RS	-2001.296827	-54458.08046	-2001.028156	-54450.76956	-2000.665493	-54440.90099	-2001.332285	-54459.04533	-2001.360483	-54459.81263
DHAVHF(DHA)	-2001.287348	-54457.82254	Crash	-54450.84695	-2000.636826	-54440.12093	-2001.329272	-54458.96336	-2001.355056	-54459.66497
DHAVHF(VHF)	-2001.286988	-54457.81275	-2001.034738	-54450.94868	-2000.649157	-54440.45647	-2001.325551	-54458.86209	-2001.354696	-54459.65516
VHVFHF	-2001.281849	-54457.67291	Crash	-54451.06464	-2000.659646	-54440.74189	-2001.316747	-54458.62251	-2001.353967	-54459.63534

Table 5: Vacuum Energies without thermal Hydrogens

ENERGY (vacuum) -uden H ET_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2000.666425	-54440.92635	-2000.361939	-54432.64088	-2000.037139	-54423.80259	-2000.736458	-54442.83206	-2000.733193	-54442.74321
2DHA_RS	-2000.665921	-54440.91265	-2000.361966	-54432.64159	-2000.036462	-54423.78418	-2000.735652	-54442.81011	-2000.73306	-54442.73958
DHAVHF(DHA)	-2000.656928	-54440.66793	-2000.347902	-54432.25891	-2000.039353	-54423.86284	-2000.747545	-54443.13376	-2000.728514	-54442.61587
DHAVHF(VHF)	-2000.655486	-54440.62868	-2000.359384	-54432.57134	-2000.021263	-54423.3706	-2000.740037	-54442.92943	-2000.755246	-54443.3433
VHVFHF	-2000.652958	-54440.55989	-2000.351592	-54432.3593	-2000.041562	-54423.92295	crash	54444.34343	-2000.75194	-54443.25334
PARA										
2DHA_RR	-2000.666342	-54440.9241	-2000.361122	-54432.61863	-2000.021527	-54423.37779	-2000.742511	-54442.99675	-2000.738543	-54442.88878
2DHA_RS	-2000.666409	-54440.92592	-2000.361121	-54432.61862	-2000.021601	-54423.3798	-2000.74261	-54442.99946	-2000.738696	-54442.89296
DHAVHF(DHA)	-2000.656737	-54440.66274	-2000.34734	-54432.2436	-2000.039494	-54423.86669	-2000.7392	-54442.90667	-2000.730608	-54442.67286
DHAVHF(VHF)	-2000.655989	-54440.64238	-2000.361727	-54432.63509	crash	-54421.5947	-2000.747821	-54443.14126	-2000.741034	-54442.95657
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

Table 6: Junction Energies

(junction)	E0		E1		E2		Em2		Em1	
ET_S										
META										
2DHA_RR	-2000.666905	-54440.93941	-2000.370633	-54432.87744	-2000.06971	-54424.6889	-2000.780671	-54444.03515	-2000.761569	-54443.51536
2DHA_RS	-2000.666422	-54440.92627	-2000.370261	-54432.86731	-2000.069353	-54424.67919	-2000.779298	-54443.99777	-2000.761554	-54443.51494
DHAVHF(DHA)	-2000.658177	-54440.70192	-2000.365208	-54432.72981	-2000.097779	-54425.45271	-2000.791772	-54444.33723	-2000.756965	-54443.39008
DHAVHF(VHF)	-2000.65562	-54440.63234	-2000.36688	-54432.77532	-2000.050269	-54424.15989	-2000.77912	-54443.99294	-2000.770859	-54443.76814
VHVFHF	-2000.653632	-54440.57824	-2000.360752	-54432.60857	-2000.073975	-54424.80497	-2000.77753	-54443.94968	-2000.768012	-54443.69069
PARA										
2DHA_RR	-2000.666486	-54440.92802	-2000.369154	-54432.83721	-2000.051662	-54424.1978	-2000.786974	-54444.20666	-2000.765407	-54443.61979
2DHA_RS	-2000.66658	-54440.93059	-2000.369841	-54432.8559	-2000.052608	-54424.22354	-2000.787226	-54444.21351	-2000.765627	-54443.62577
DHAVHF(DHA)	-2000.664849	-54440.88348	-2000.364904	-54432.72155	-2000.082904	-54425.04794	-2000.81615	-54445.00057	-2000.769239	-54443.72406
DHAVHF(VHF)	-2000.656699	-54440.66169	-2000.371035	-54432.88837	-2000.057417	-54424.35439	-2000.78986	-54444.28519	-2000.763662	-54443.57231
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

DHADHA with two S

Table 7: Vacuum energies with thermal hydrogens

ENERGY (vacuum)	E0		E1		E2		Em2		Em1	
TO_S										
META										
2DHA_RR	-2168.564397	-59009.66457	-2168.286981	-59002.11569	-2167.890609	-58991.32985	-2168.561369	-59009.58218	-2168.620594	-59011.19374
2DHA_RS	-2168.564261	-59009.66086	-2168.287114	-59002.11929	-2167.891081	-58991.34269	-2168.561265	-59009.57934	-2168.62112	-59011.20806
DHAVHF	-2168.553638	-59009.37179	-2168.2951	-59002.3366	-2167.895758	-58991.46996	-2168.569919	-59009.81483	-2168.624846	-59011.30946
VHVFHF	-2168.550727	-59009.29258	crash	-59002.63322	-2167.919703	-58992.12155	-2168.571146	-59009.84822	-2168.617946	-59011.12171
PARA										
2DHA_RR	-2168.563517	-59009.64062	-2168.28946	-59002.18313	-2167.917422	-58992.05948	-2168.607405	-59010.83488	-2168.63203	-59011.50495
2DHA_RS	-2168.5636	-59009.64287	-2168.289453	-59002.18296	-2167.917455	-58992.06037	-2168.607442	-59010.83588	-2168.632053	-59011.50558
DHAVHF	-2168.553509	-59009.36828	-2168.294358	-59002.31643	-2167.899185	-58991.56322	-2168.600299	-59010.64151	-2168.624811	-59011.30851
VHVFHF	-2168.549801	-59009.26739	crash	-59002.46995	-2167.919695	-58992.12131	-2168.595264	-59010.50449	-2168.618552	-59011.13819
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

Table 8: Vacuum energies without thermal hydrogens

ENERGY (vacuum) U H	E0		E1		E2		Em2		Em1	
TO_S										
META										
2DHA_RR	-2167.210015	-58972.80993	crash	-58965.97946	-2166.589555	-58955.92634	-2167.398844	-58977.94824	-2167.37931	-58977.41668
2DHA_RS	-2167.209455	-58972.79469	crash	-58966.03389	-2166.592339	-58956.00211	-2167.397854	-58977.92131	-2167.380331	-58977.44447
DHAVHF	-2167.216825	-58972.99524	crash	-58966.16994	-2166.611034	-58956.51083	-2167.410732	-58978.27171	crash	-58977.0545
VHVFHF	-2167.231695	-58973.39986	crash	-58966.68696	-2166.64785	-58957.51264	-2167.457612	-58979.54741	crash	-58977.68037
PARA										
2DHA_RR	-2167.207171	-58972.73253	crash	-58965.8162	-2166.570236	-58955.40066	-2167.38709	-58977.62838	-2167.381041	-58977.46379
2DHA_RS	-2167.206767	-58972.72155	-2166.955673	-58965.88893	-2166.570427	-58955.40586	-2167.387454	-58977.63829	-2167.381197	-58977.46802
DHAVHF	-2167.217726	-58973.01976	crash	-58966.22437	-2166.612237	-58956.54356	-2167.399918	-58977.97745	crash	-58976.94566
VHVFHF	-2167.22888	-58973.32329	-2166.989903	-58966.82039	-2166.647501	-58957.50315	-2167.413174	-58978.33817	crash	-58977.19056
VHVFHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHVFHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

Table 9: Junction energies

(junction) TO_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-2167.211624	-58972.85371	crash	-58966.33321	-2166.644024	-58957.40852	-2167.467429	-58979.81454	-2167.397535	-58977.91262
2DHA_RS	-2167.209529	-58972.79672	crash	-58966.25158	-2166.63691	-58957.21496	-2167.467142	-58979.80672	-2167.399249	-58977.95927
DHAVHF	-2167.218598	-58973.04348	-2167.057773	-58968.66721	-2166.688183	-58958.61015	-2167.468739	-58979.85016	crash	-58977.92527
VHFVHF	-2167.23211	-58973.41118	crash	-58966.79581	-2166.675849	-58958.27452	-2167.507555	-58980.9064	crash	-58978.11575
PARA										
2DHA_RR	-2167.208208	-58972.76076	crash	-58965.78898	-2166.606803	-58956.39569	-2167.450406	-58979.3513	crash	-58977.27219
2DHA_RS	-2167.206482	-58972.71381	crash	-58965.95225	-2166.604413	-58956.33066	-2167.450992	-58979.36726	-2167.398886	-58977.94939
DHAVHF	-2167.222689	-58973.1548	crash	ikk muligt	-2166.960399	-58966.01754	-2167.46181	-58979.66162	crash	ikk muligt
VHFVHF	-2167.229091	-58973.32901	crash	-58966.87744	-2166.674516	-58958.23826	-2167.464174	-58979.72595	crash	-58977.59873
VHFVHF	-2167.22888	-58973.32329	-2166.989903	-58966.82039	-2166.647501	-58957.50315	-2167.413174	-58978.33817	crash	-58977.19056
VHFVHF	-2000.652305	-54440.54212	-2000.357323	-54432.51525	-2000.065793	-54424.58232	-2000.789703	-54444.28091	-2000.766859	-54443.65931
VHFVHF	-2000.651798	-54440.52833	-2000.349206	-54432.29438	-2000.038385	-54423.83652	-2000.738329	-54442.88297	-2000.750969	-54443.22691

DHADHA with one S

Table 10: Vacuum energies with thermal hydrogens

ENERGY (vacuum) ET_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-1770.363115	-48174.05177	-1770.089265	-48166.59996	-1769.692713	-48155.80922	-1770.35302	-48173.77707	-1770.417908	-48175.54279
2DHA_RS	-1770.361995	-48174.0213	-1770.085705	-48166.50308	-1769.692041	-48155.79092	-1770.352056	-48173.75086	-1770.412993	-48175.40904
DHAVHF(DHA)	-1770.352823	-48173.77173	-1770.088731	-48166.5854	-1769.686027	-48155.62728	-1770.359482	-48173.95294	-1770.419616	-48175.58926
DHAVHF(VHF)	-1770.352461	-48173.76187	-1770.094946	-48166.75454	-1769.696739	-48155.91877	-1770.365071	-48174.10502	-1770.42218	-48175.65903
VHFVHF	-1770.349833	-48173.69037	crash	-48167.05533	-1769.716214	-48156.4487	-1770.363062	-48174.05035	-1770.416463	-48175.50347
PARA										
2DHA_RR	-1770.362216	-48174.02733	-1770.09119	-48166.65232	-1769.720731	-48156.57162	-1770.390922	-48174.80845	-1770.427456	-48175.80261
2DHA_RS	-1770.362336	-48174.0306	-1770.091167	-48166.65171	-1769.720741	-48156.57189	-1770.397548	-48174.98875	-1770.427477	-48175.80318
DHAVHF(DHA)	-1770.352694	-48173.76823	-1770.088892	-48166.58978	-1769.687857	-48155.67708	-1770.39491	-48174.91698	-1770.421718	-48175.64646
DHAVHF(VHF)	-1770.352327	-48173.75822	-1770.095333	-48166.76505	-1769.699079	-48155.98244	-1770.390551	-48174.79834	-1770.421102	-48175.6297
VHFVHF	-1770.349028	-48173.66846	crash	-48166.83764	-1769.710634	-48156.29686	-1770.386499	-48174.68811	-1770.417222	-48175.52411

Table 11: Vacuum energies without thermal hydrogens

ENERGY (vacuum) - U_H ET_S META	E0		E1		E2		Em2		Em1	
2DHA_RR	-1769.731276	-48156.85855	-1769.404958	-48147.979	-1769.059694	-48138.58388	-1769.768299	-48157.86602	-1769.80652	-48158.90605
2DHA_RS	-1769.730108	-48156.82679	-1769.412525	-48148.1849	-1769.061715	-48138.63888	-1769.790029	-48158.45731	-1769.80074	-48158.74878
DHAVHF(DHA)	-1769.720953	-48156.57767	-1769.397798	-48147.78415	-1769.059317	-48138.57361	-1769.800478	-48158.74166	-1769.795092	-48158.59509
DHAVHF(VHF)	-1769.722582	-48156.622	-1769.439638	-48148.92268	-1769.077583	-48139.07067	-1769.792078	-48158.51307	-1769.836316	-48159.71685
VHFVHF	-1769.719878	-48156.54841	-1769.427486	-48148.59202	-1769.099102	-48139.65623	-1769.810092	-48159.00325	-1769.833216	-48159.63249
PARA										
2DHA_RR	-1769.730208	-48156.8295	-1769.410952	-48148.1421	-1769.083705	-48139.23726	-1769.782266	-48158.24607	-1769.808755	-48158.96687
2DHA_RS	-1769.730352	-48156.83342	-1769.41086	-48148.13961	-1769.083721	-48139.23768	-1769.789186	-48158.43437	-1769.808806	-48158.96828
DHAVHF(DHA)	-1769.720735	-48156.57172	-1769.396652	-48147.75297	-1769.05853	-48138.5522	-1769.786819	-48158.36998	-1769.801456	-48158.76826
DHAVHF(VHF)	-1769.722509	-48156.62	-1769.440975	-48148.95908	-1769.078934	-48139.10744	-1769.809866	-48158.99712	-1769.826825	-48159.45858
VHFVHF	-1769.718394	-48156.50803	-1769.423763	-48148.49071	-1769.097737	-48139.61908	-1769.808491	-48158.95968	-1769.832842	-48159.62232

Table 12: Junction energies

(junction)	E0		E1		E2		Em2		Em1	
ET_S										
META										
2DHA_RR	-1769.732425	-48156.88984	-1769.422273	-48148.45016	-1769.11433	-48140.07062	-1769.829824	-48159.5402	-1769.832258	-48159.60642
2DHA_RS	-1769.730024	-48156.82451	-1769.421222	-48148.42155	-1769.096885	-48139.59589	-1769.837132	-48159.73905	-1769.828465	-48159.50321
DHAVHF(DHA)	-1769.720712	-48156.5711	-1769.426525	-48148.56587	-1769.107248	-48139.87788	-1769.848511	-48160.0487	-1769.822786	-48159.34867
DHAVHF(VHF)	-1769.722804	-48156.62802	-1769.450184	-48149.20967	-1769.110832	-48139.97541	-1769.835963	-48159.70724	-1769.851807	-48160.13837
VHFFVHF	-1769.720243	-48156.55833	-1769.436813	-48148.8458	-1769.13107	-48140.52613	-1769.848773	-48160.05583	-1769.849207	-48160.06763
PARA										
2DHA_RR	-1769.730644	-48156.84135	-1769.420716	-48148.4078	-1769.116363	-48140.12593	-1769.831924	-48159.59733	-1769.833351	-48159.63616
2DHA_RS	-1769.730687	-48156.84254	-1769.420593	-48148.40444	-1769.117918	-48140.16824	-1769.838534	-48159.7772	-1769.833363	-48159.63651
DHAVHF(DHA)	-1769.724821	-48156.68292	-1769.425595	-48148.54056	-1769.143766	-48140.8716	-1769.84594	-48159.97872	-1769.826115	-48159.43927
DHAVHF(VHF)	-1769.723509	-48156.6472	-1769.456059	-48149.36953	-1769.125372	-48140.37107	-1769.853943	-48160.1965	-1769.844918	-48159.95091
VHFFVHF	-1769.71906	-48156.52615	-1769.433214	-48148.74788	-1769.129889	-48140.49398	-1769.861818	-48160.41079	-1769.848912	-48160.0596
VHFFVHF	-1769.718394	-48156.50803	-1769.423763	-48148.49071	-1769.097737	-48139.61908	-1769.808491	-48158.95968	-1769.832842	-48159.62232

DHADHA with no linkers

Table 13: Vacuum energy

ENERGY	E0		E1		E2		Em2		Em1	
(vacuum)										
NUL_S										
META										
2DHA_RR	-1372.161071	-37338.41827	-1371.876638	-37330.67845	-1371.468763	-37319.5796	-1372.112178	-37337.08783	-1372.198002	-37339.42323
2DHA_RS	-1372.160807	-37338.4111	-1371.8759	-37330.65839	-1371.468523	-37319.57309	-1372.111071	-37337.0577	-1372.198018	-37339.42366
DHAVHF	-1372.1517	-37338.16327	crash	-37331.09648	-1371.464655	-37319.46783	-1372.123271	-37337.3897	-1372.206455	-37339.65324
VHFFVHF	-1372.149045	-37338.09105	-1371.879256	-37330.74969	-1371.486442	-37320.06069	-1372.140088	-37337.84731	-1372.203741	-37339.5794
PARA										
2DHA_RR	-1372.161101	-37338.4191	-1371.883403	-37330.86253	-1371.48681	-37320.0707	-1372.141094	-37337.87467	-1372.210668	-37339.7679
2DHA_RS	-1372.161204	-37338.42191	-1371.882762	-37330.84511	-1371.485382	-37320.03185	-1372.139942	-37337.84334	-1372.210139	-37339.7535
DHAVHF	-1372.151612	-37338.16089	crash	-37330.98764	-1371.463877	-37319.44666	-1372.136307	-37337.74441	-1372.206115	-37339.64399
VHFFVHF	-1372.147866	-37338.05895	-1371.875698	-37330.65289	-1371.485678	-37320.0399	-1372.137275	-37337.77076	-1372.201378	-37339.51508
VHFFVHF	-1769.71906	-48156.52615	-1769.433214	-48148.74788	-1769.129889	-48140.49398	-1769.861818	-48160.41079	-1769.848912	-48160.0596
VHFFVHF	-1769.718394	-48156.50803	-1769.423763	-48148.49071	-1769.097737	-48139.61908	-1769.808491	-48158.95968	-1769.832842	-48159.62232

Table 14: Junction energies

(junction)	E0		E1		E2		Em2		Em1	
NUL_S										
META										
2DHA_RR	-1372.16158	-37338.43214	crash	-37331.58629	-1371.505984	-37320.59244	-1372.13969	-37337.83646	-1372.20448	-37339.59949
2DHA_RS	-1372.161112	-37338.41941	-1371.886639	-37330.95059	-1371.505548	-37320.58057	-1372.137986	-37337.7901	-1372.204346	-37339.59586
DHAVHF	-1372.152519	-37338.18558	crash	-37331.39581	-1371.503502	-37320.52491	-1372.148044	-37338.0638	-1372.212097	-37339.80677
VHFFVHF	-1372.150005	-37338.11717	-1371.889833	-37331.03751	-1371.52436	-37321.09247	-1372.162541	-37338.45829	-1372.208167	-37339.69982
PARA										
2DHA_RR	-1372.16144	-37338.42833	-1371.89268	-37331.11499	-1371.518997	-37320.94654	-1372.162583	-37338.45943	-1372.214965	-37339.88481
2DHA_RS	-1372.161535	-37338.43091	-1371.891967	-37331.09559	-1371.517311	-37320.90066	-1372.161244	-37338.42299	-1372.214382	-37339.86894
DHAVHF	-1372.152879	-37338.19535	-1371.890776	-37331.06318	-1371.501983	-37320.48357	-1372.16441	-37338.50914	-1372.214202	-37339.86406
VHFFVHF	-1372.148868	-37338.08622	-1371.888542	-37331.0024	-1371.523966	-37321.08176	-1372.159751	-37338.38236	-1372.205737	-37339.63369
VHFFVHF	-1372.147866	-37338.05895	-1371.875698	-37330.65289	-1371.485678	-37320.0399	-1372.137275	-37337.77076	-1372.201378	-37339.51508
VHFFVHF	-1769.71906	-48156.52615	-1769.433214	-48148.74788	-1769.129889	-48140.49398	-1769.861818	-48160.41079	-1769.848912	-48160.0596
VHFFVHF	-1769.718394	-48156.50803	-1769.423763	-48148.49071	-1769.097737	-48139.61908	-1769.808491	-48158.95968	-1769.832842	-48159.62232

Stereo Chemistry Energies

DHADHA with two S-phenyl

RR versus RS

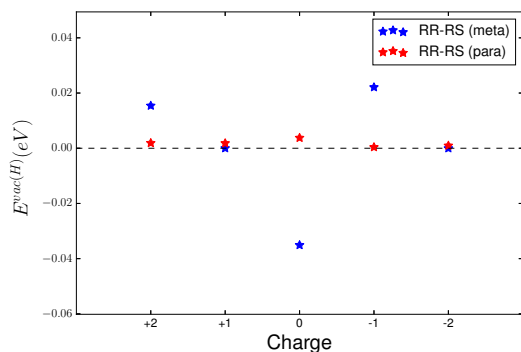


Figure 1: Vacuum energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

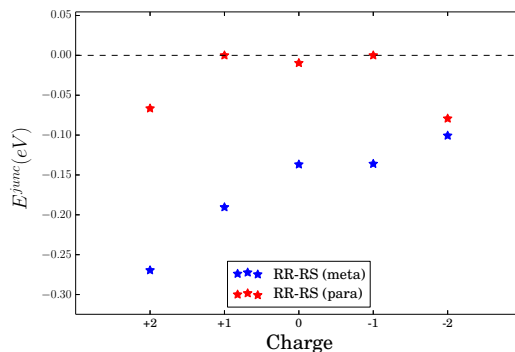


Figure 3: Junction energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

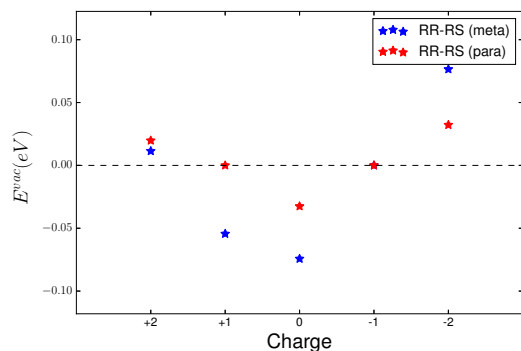


Figure 2: Vacuum energy difference (no H at linker S) between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

Meta versus Para

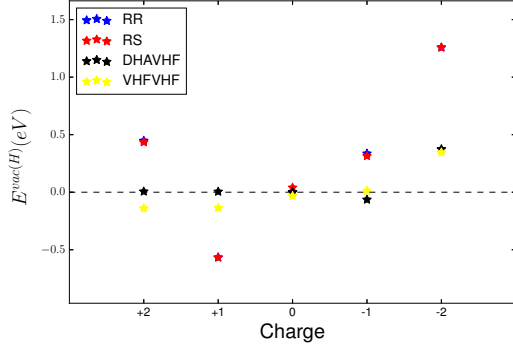


Figure 4: Vacuum energy difference between the para and meta configurations.

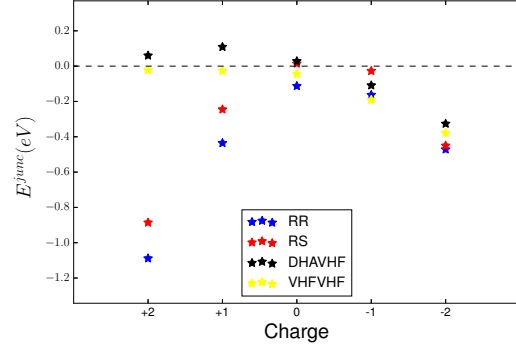


Figure 6: Junction energy difference between the para and meta configurations.

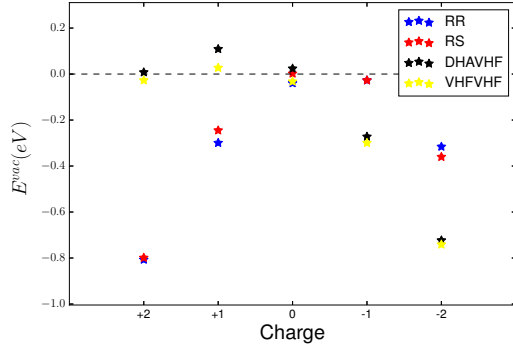


Figure 5: Vacuum energy difference (no H at S linker) between the para and meta configurations.

DHADHA with one S-phenyl

RS versus RR - Significance of linker position

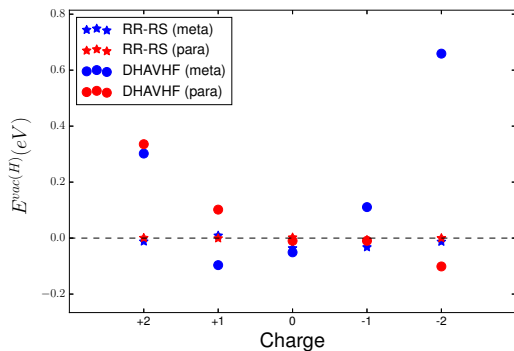


Figure 7: Vacuum energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

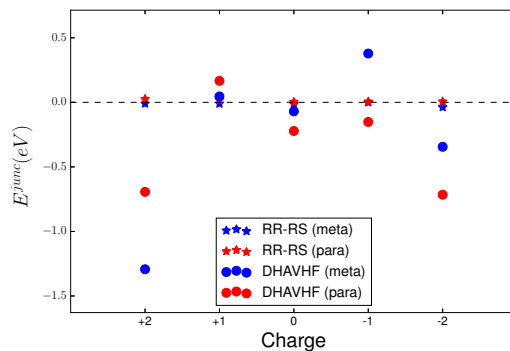


Figure 9: Junction energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

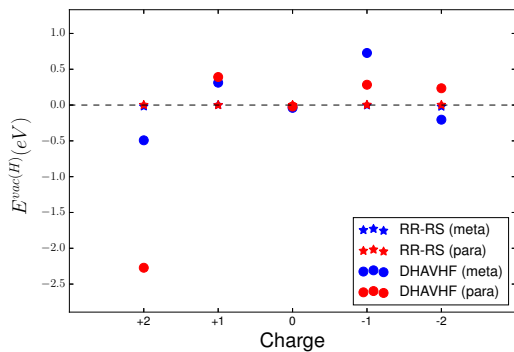


Figure 8: Vacuum energy difference (no H at linker S) between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

Meta versus Para

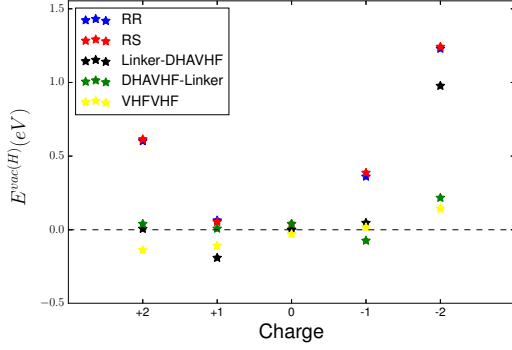


Figure 10: Vacuum energy difference between the para and meta configurations.

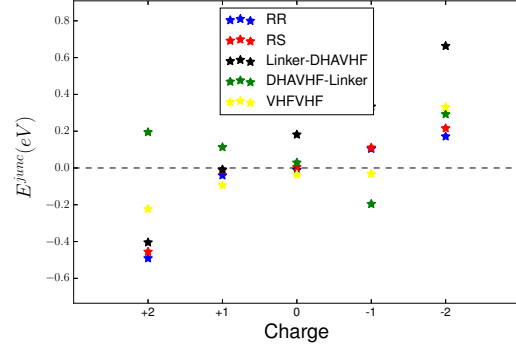


Figure 12: Junction energy difference between the para and meta configurations.

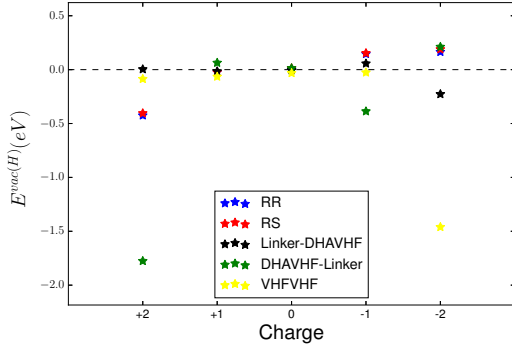


Figure 11: Vacuum energy difference (no H at S linker) between the para and meta configurations.

DHADHA with two S

RR versus RS

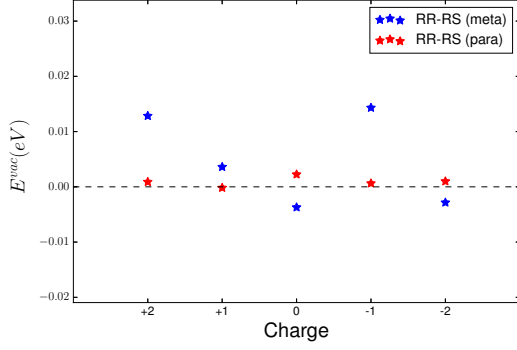


Figure 13: Vacuum energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

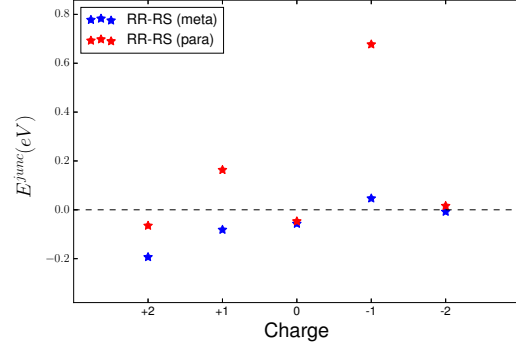


Figure 15: Junction energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

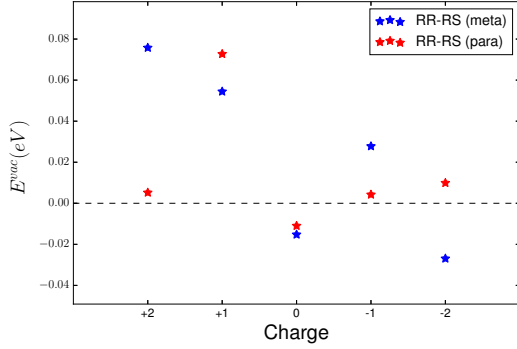


Figure 14: Vacuum energy difference (no H at linker S) between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

Meta versus Para

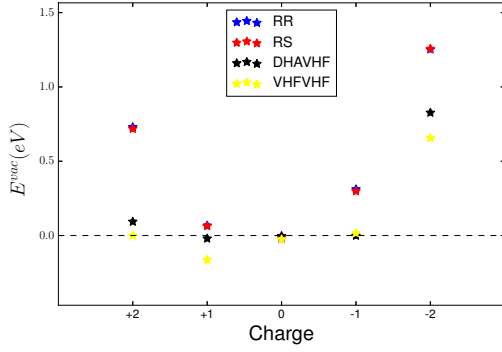


Figure 16: Vacuum energy difference between the para and meta configurations.

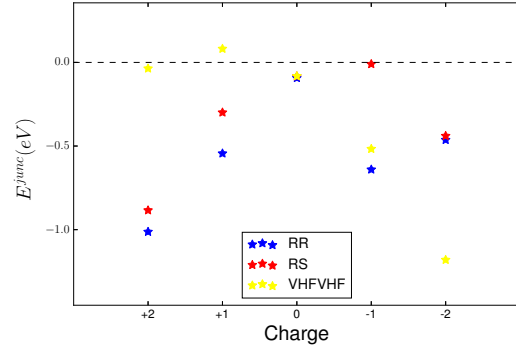


Figure 18: Junction energy difference between the para and meta configurations.

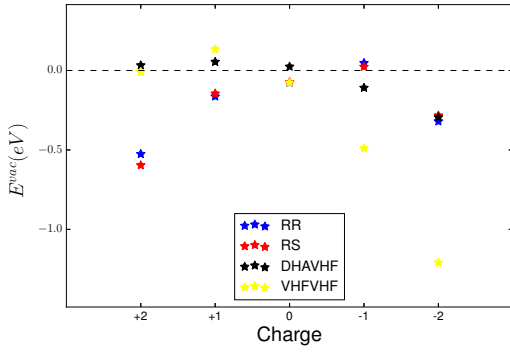


Figure 17: Vacuum energy difference (no H at S linker) between the para and meta configurations.

DHADHA with one S

RR versus RS - and Linker Position

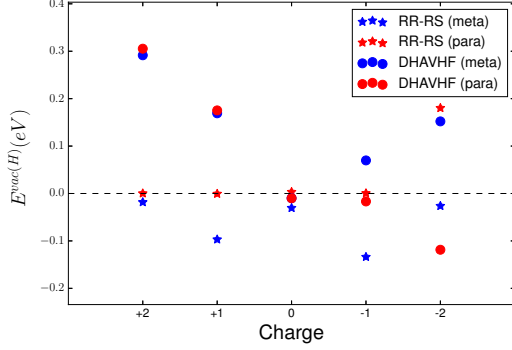


Figure 19: Vacuum energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

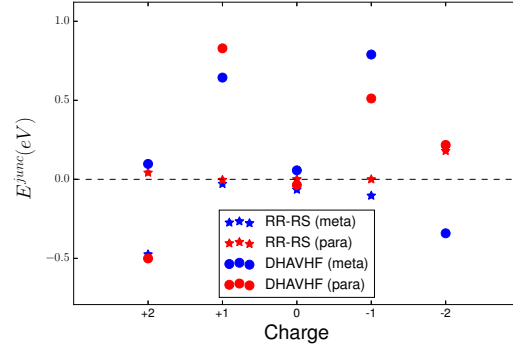


Figure 21: Junction energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

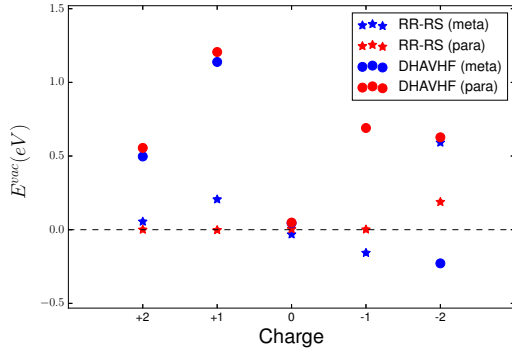


Figure 20: Vacuum energy difference (no H at linker S) between the diastereoisomers DHADHA(RR) and DHADHA(RS) and the two different linked DHAVHF, the Linker-DHA(S)-VHF and DHA(S)-VHF-Linker, both in para and meta configurations.

Meta versus Para

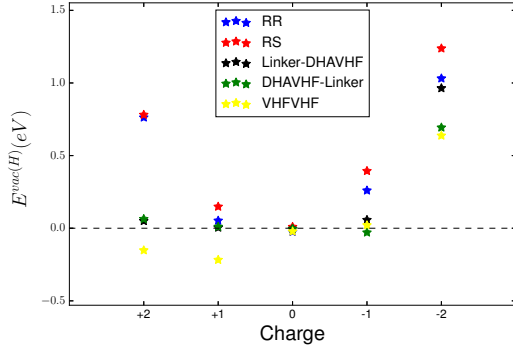


Figure 22: Vacuum energy difference between the para and meta configurations.

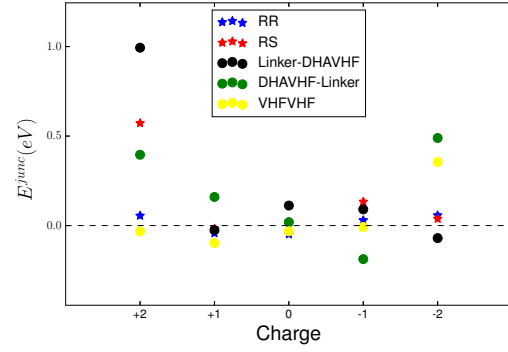


Figure 24: Junction energy difference between the para and meta configurations.

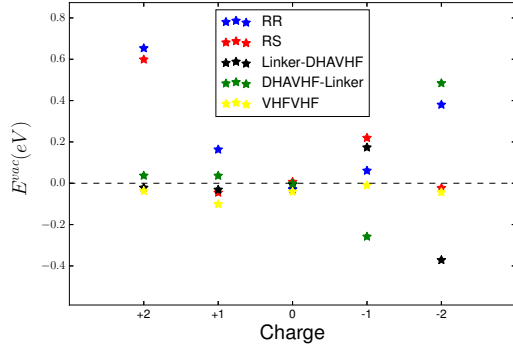


Figure 23: Vacuum energy difference (no H at S linker) between the para and meta configurations.

DHADHA with no linkers

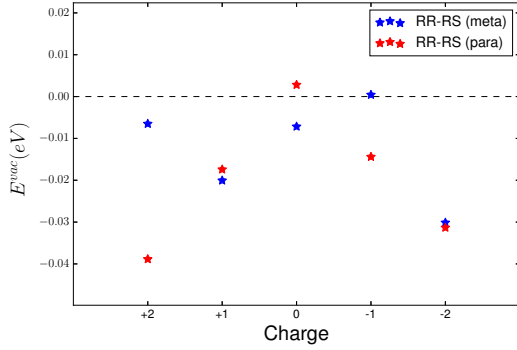


Figure 25: Vacuum energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

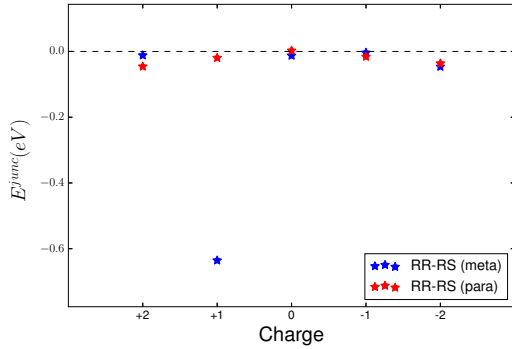


Figure 26: Junction energy difference between the diastereoisomers DHADHA(RR) and DHADHA(RS), both in para and meta configurations.

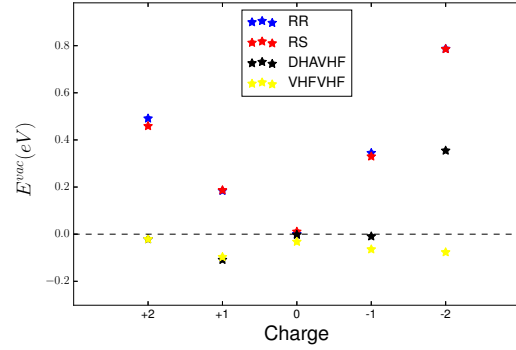


Figure 27: Vacuum energy difference between the para and meta configurations.

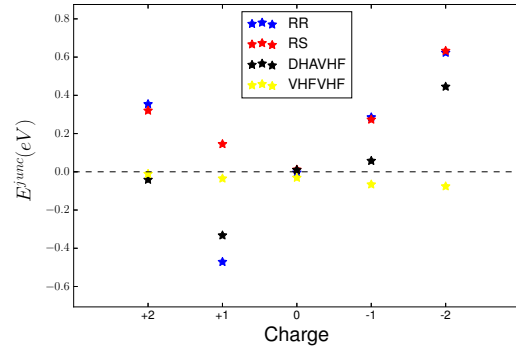


Figure 28: Junction energy difference between the para and meta configurations.

Switching Step Energies

DHADHA with two S-phenyl

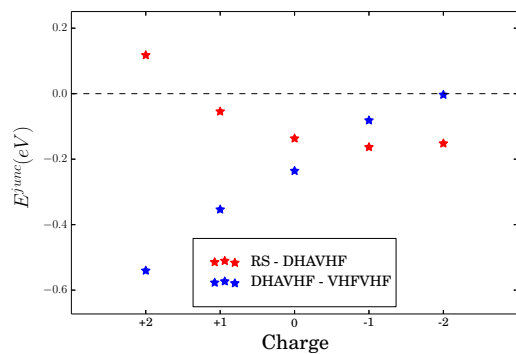


Figure 29: The meta conformation.

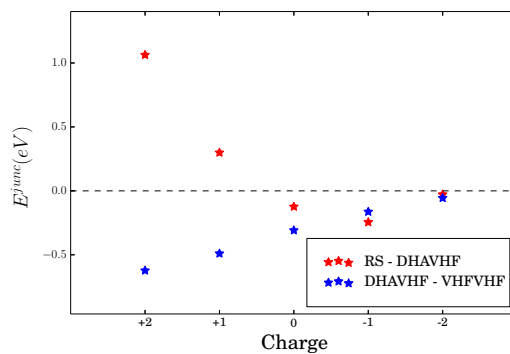


Figure 30: The para conformation.

DHADHA with one S-phenyl

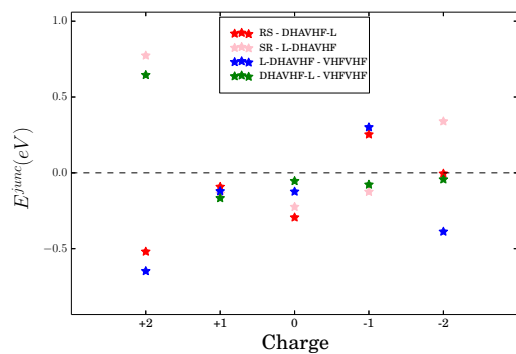


Figure 31: The meta conformation.

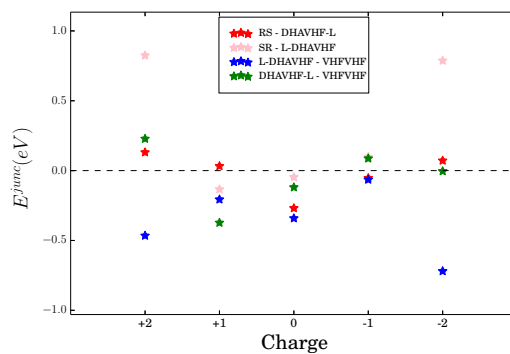


Figure 32: The para conformation.

DHADHA with two S

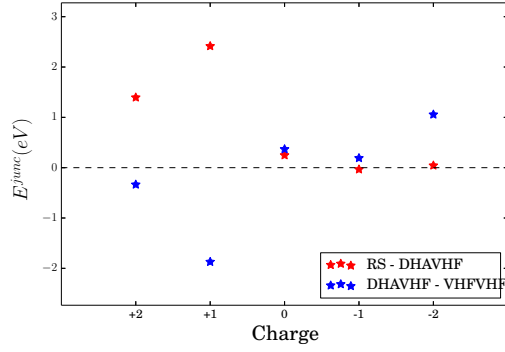


Figure 33: The meta conformation.

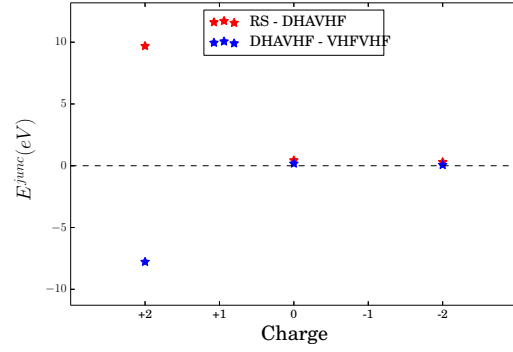


Figure 34: The para conformation.

DHADHA with one S

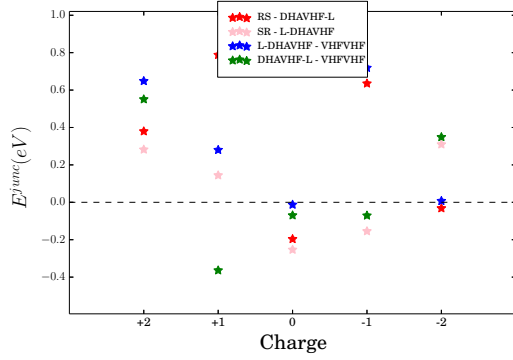


Figure 35: The meta conformation.

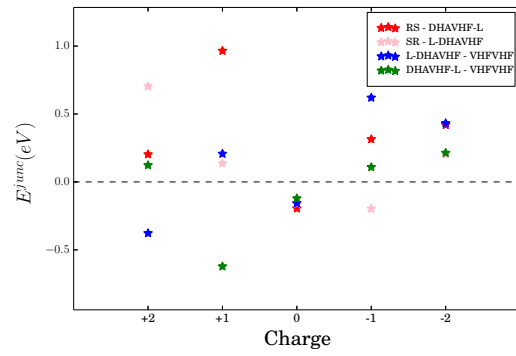


Figure 36: The para conformation.

DHADHA with no linkers

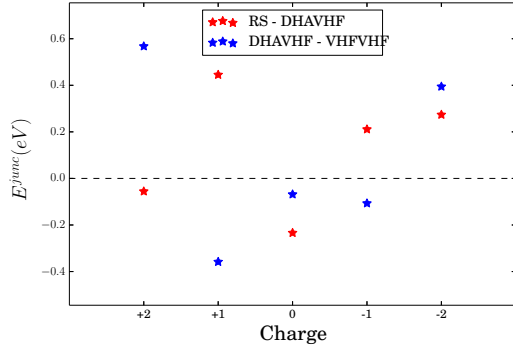


Figure 37: The meta conformation.

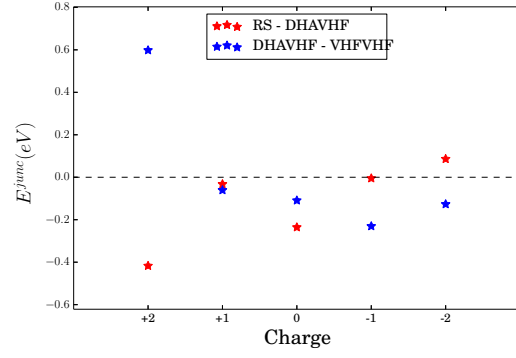


Figure 38: The para conformation.

Addition Energies

DHADHA with two S-phenyl

Table 15: Two sulphur-phenyl linker group

Junction	E0	E1	Em1
<i>META</i>			
2DHA_RR	1.767	1.753	1.777
2DHA_RS	1.820	1.778	1.743
DHAVHF	1.764	1.689	1.705
VHFVHF	1.728	1.757	1.781
<i>PARA</i>			
2DHA_RR	2.141	2.083	2.035
2DHA_RS	2.122	2.159	2.124
DHAVHF	1.820	1.818	1.785
VHFVHF	1.856	1.770	1.823
Vacuum with H	E0	E1	E2
<i>META</i>			
2DHA_RR	5.270	4.035	2.988
2DHA_RS	5.177	4.054	3.067
DHAVHF	4.937	3.365	2.960
VHFVHF	4.424	3.622	3.034
<i>PARA</i>			
2DHA_RR	5.504	2.450	2.401
2DHA_RS	5.509	2.448	2.397
DHAVHF	4.995	3.369	2.457
VHFVHF	4.484	3.523	2.745
Vacuum without H	E0	E1	Em1
<i>META</i>			
2DHA_RR	2.471	2.468	2.435
2DHA_RS	2.377	2.422	2.433
DHAVHF	2.342	2.369	2.349
VHFVHF	2.172	2.215	2.208
<i>PARA</i>			
2DHA_RR	2.718	2.716	2.736
2DHA_RS	2.653	2.729	2.737
DHAVHF	2.553	2.555	2.504
VHFVHF	2.379	2.329	2.383

Table 16: Two sulphur-phenyl linker groups

Diff	E0	uden H	E1	Uden H	E2	Uden H
<i>META</i>						
2DHA_RR	66.462	28.472	56.559	28.991	40.516	27.016
2DHA_RS	64.843	23.415	56.142	26.593	43.183	28.371
DHAVHF	64.262	24.674	49.820	28.730	42.389	27.409
VHVVHF	60.939	20.421	51.483	20.656	41.305	19.340
<i>PARA</i>						
2DHA_RR	61.102	21.239	14.965	23.308	15.250	25.628
2DHA_RS	61.490	20.035	11.782	20.874	11.403	22.388
DHAVHF	63.556	28.706	46.033	28.846	27.339	28.694
VHVVHF	58.599	21.975	49.748	23.980	33.589	23.487

DHADHA with one S-phenyl

Table 17: One sulphur-phenyl linker group.

Junction	E0	E1	Em1
<i>META</i>			
2DHA_RR	5.486	0.127	2.056
2DHA_RS	5.470	0.129	2.106
DHAVHF(DHA)	5.284	-0.695	1.741
DHAVHF(VHF)	4.721	0.758	2.911
VHFFVHF	4.857	-0.166	2.853
<i>PARA</i>			
2DHA_RR	5.399	0.549	2.105
2DHA_RS	5.380	0.558	2.107
DHAVHF(DHA)	5.321	-0.488	1.564
DHAVHF(VHF)	4.863	0.761	2.198
VHFFVHF	4.910	-0.094	2.496
Vacuum with H	E0	E1	Em1
<i>META</i>			
2DHA_RR	5.989	3.039	3.024
2DHA_RS	5.940	3.105	3.008
DHAVHF(DHA)	4.991	4.137	3.427
DHAVHF(VHF)	4.875	3.693	3.041
VHFFVHF	4.614	3.765	3.055
<i>PARA</i>			
2DHA_RR	5.567	2.562	2.515
2DHA_RS	5.579	2.558	2.499
DHAVHF(DHA)	5.133	3.750	2.544
DHAVHF(VHF)	5.022	3.628	2.635
VHFFVHF	4.646	3.714	2.975
Vacuum without H	E0	E1	Em1
<i>META</i>			
2DHA_RR	6.469	0.553	1.728
2DHA_RS	6.444	0.586	1.756
DHAVHF(DHA)	6.461	-0.013	1.430
DHAVHF(VHF)	5.343	1.143	3.128
VHFFVHF	5.507	0.236	
<i>PARA</i>			
2DHA_RR	6.341	0.935	1.857
2DHA_RS	6.340	0.932	1.861
DHAVHF(DHA)	6.409	-0.042	1.776
DHAVHF(VHF)	5.693	3.033	2.130
VHFFVHF	5.535	0.224	3.043

Table 18: One sulphur-phenyl linker group.

Diff	E0	no H	E1	no H	Em1	no H
<i>META</i>						
2DHA_RR	8.392	15.190	95.841	77.104	32.000	-18.990
2DHA_RS	7.901	15.112	116.799	77.973	29.981	-19.895
DHAVHF(DHA)	-5.873	18.219	79.463	-5261.945	49.201	-21.744
DHAVHF(VHF)	3.154	11.633	104.411	33.670	4.263	6.952
VHFVHF	-5.276	11.801		170.442	6.606	
<i>PARA</i>						
2DHA_RR	3.010	14.852	78.196	41.351	16.312	-13.367
2DHA_RS	3.571	15.153	113.021	40.132	15.685	-13.271
DHAVHF(DHA)	-3.666	16.971	79.035	-1056.199	38.520	11.949
DHAVHF(VHF)	3.165	14.586	102.529	74.921	16.609	-3.204
VHFVHF	-5.679	11.304		141.955	16.122	17.976

DHADHA with two S

Table 19: Two S linkers

Junction	E0	E1	Em1
<i>META</i>			
2DHA_RR	1.462	2.404	3.157
2DHA_RS	1.383	2.491	3.315
DHAVHF	-0.506	5.681	2.957
VHFVHF	1.911	1.906	1.914
<i>PARA</i>			
2DHA_RR	2.460	2.422	2.432
2DHA_RS	1.526	2.860	3.818
DHAVHF			
VHFVHF	2.182	2.188	2.143
Vacuum with H	E0	E1	Em1
<i>META</i>			
2DHA_RR	6.020	3.237	3.141
2DHA_RS	5.994	3.235	3.176
DHAVHF	5.098	3.831	3.432
VHFVHF	4.830	3.852	3.103
<i>PARA</i>			
2DHA_RR	5.593	2.666	2.534
2DHA_RS	5.597	2.663	2.532
DHAVHF	5.112	3.701	2.607
VHFVHF	4.927	3.551	2.505
Vacuum without H	E0	E1	Em1
<i>META</i>			
2DHA_RR	2.224	3.223	4.075
2DHA_RS	2.111	3.271	4.173
DHAVHF	2.766	2.834	2.842
VHFVHF	2.432	2.461	2.413
<i>PARA</i>			
2DHA_RR	2.185	3.499	4.567
2DHA_RS	2.086	3.650	4.576
DHAVHF	2.870	2.885	2.894
VHFVHF	2.636	2.814	2.720

Table 20: Two S-linker

Diff	E0	no H	E1	no H	Em1	no H
<i>META</i>						
2DHA_RR	66.462	28.472	56.559	28.991	40.516	27.016
2DHA_RS	64.843	23.415	56.142	26.593	43.183	28.371
DHAVHF	64.262	24.674	49.820	28.730	42.389	27.409
VHfVHF	60.939	20.421	51.483	20.656	41.305	19.340
<i>PARA</i>						
2DHA_RR	61.102	21.239	14.965	23.308	15.250	25.628
2DHA_RS	61.490	20.035	11.782	20.874	11.403	22.388
DHAVHF	63.556	28.706	46.033	28.846	27.339	28.694
VHfVHF	58.599	21.975	49.748	23.980	33.589	23.487

DHADHA with one S

Table 21: One sulphur linker.

Junction	E0	E1	Em1
<i>META</i>			
2DHA_RR	5.723	-0.060	2.783
2DHA_RS	5.724	0.423	2.443
DHAVHF(DHA)	5.228	0.683	2.078
DHAVHF(VHF)	3.908	1.816	3.941
VHFVHF	4.203	0.607	3.521
<i>PARA</i>			
2DHA_RR	5.639	-0.152	2.834
2DHA_RS	5.644	-0.202	2.653
DHAVHF(DHA)	5.386	-0.473	2.217
DHAVHF(VHF)	3.974	1.721	3.058
VHFVHF	4.245	0.476	3.182
Vacuum with H	E0	E1	Em1
<i>META</i>			
2DHA_RR	5.961	3.339	3.257
2DHA_RS	6.130	3.194	3.046
DHAVHF(DHA)	5.369	3.772	3.454
DHAVHF(VHF)	5.110	3.828	3.451
VHFVHF	4.822	3.972	3.266
<i>PARA</i>			
2DHA_RR	5.600	2.706	2.769
2DHA_RS	5.606	2.701	2.587
DHAVHF(DHA)	5.300	3.734	2.608
DHAVHF(VHF)	5.122	3.789	2.703
VHFVHF	4.975	3.710	2.692
Vacuum without H	E0	E1	Em1
<i>META</i>			
2DHA_RR	6.832	0.516	3.088
2DHA_RS	6.720	0.904	2.213
DHAVHF(DHA)	6.776	0.417	1.871
DHAVHF(VHF)	4.604	2.153	4.299
VHFVHF	4.872	0.979	3.713
<i>PARA</i>			
2DHA_RR	6.550	0.217	2.858
2DHA_RS	6.559	0.208	2.669
DHAVHF(DHA)	6.622	0.382	2.595
DHAVHF(VHF)	4.822	2.191	3.300
VHFVHF	4.903	0.854	3.777

Table 22: One sulphur linker.

Diff	E0	no H	E1	no H	Em1	no H
<i>META</i>						
2DHA_RR	3.988	16.232	101.801	111.662	14.552	9.870
2DHA_RS	6.626	14.816	86.766	53.248	19.799	-10.364
DHAVHF(DHA)	2.629	22.852	81.898	-63.723	39.848	-11.048
DHAVHF(VHF)	23.525	15.126	52.568	15.645	-14.207	8.308
VHfVHF	12.831	13.732	84.713	38.009	-7.803	5.176
<i>PARA</i>						
2DHA_RR	-0.697	13.913	105.606	169.760	-2.318	0.859
2DHA_RS	-0.675	13.948	107.475	197.016	-2.562	0.580
DHAVHF(DHA)	-1.619	18.667	112.677	223.917	14.986	14.564
DHAVHF(VHF)	22.409	17.593	54.590	21.451	-13.144	7.331
VHfVHF	14.680	13.424	87.180	44.325	-18.227	15.745

DHADHA with no linkers**Table 23: No linkers**

Junction	E0	E1	Em1
<i>META</i>			
2DHA_RR	5.679	4.148	2.930
2DHA_RS	6.292	2.901	2.982
DHAVHF	5.169	4.081	3.364
VHfVHF	5.497	2.865	2.824
<i>PARA</i>			
2DHA_RR	5.857	2.855	2.882
2DHA_RS	5.897	2.860	2.884
DHAVHF	5.463	3.447	3.024
VHfVHF	5.536	2.837	2.799
<i>Vacuum</i>	E0	E1	Em1
<i>META</i>			
2DHA_RR	6.735	3.359	3.340
2DHA_RS	6.740	3.333	3.379
DHAVHF	5.577	4.562	3.754
VHfVHF	5.853	3.348	3.220
<i>PARA</i>			
2DHA_RR	6.208	3.235	3.242
2DHA_RS	6.245	3.236	3.242
DHAVHF	5.690	4.368	3.383
VHfVHF	5.950	3.207	3.200

Table 24: No linkers

Diff	E0	E1	Em1
<i>META</i>			
2DHA_RR	15.685	-23.488	12.274
2DHA_RS	6.644	12.944	11.730
DHAVHF	7.321	10.538	10.373
VHFVHF	6.082	14.406	12.305
<i>PARA</i>			
2DHA_RR	5.653	11.751	11.109
2DHA_RS	5.571	11.644	11.036
DHAVHF	3.984	21.070	10.614
VHFVHF	6.951	11.542	12.550