

Electronic Supporting Information

Heteroatom-vacancy centres in *molecular* nanodiamonds: A computational study of organic molecules possessing triplet ground states through σ -overlap

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Table S1. Absolute energies obtained via calculations at CAM-B3LYP-D3(BJ)/Def2-QZVPP level of theory.

Molecule	Distortion	Energy (in Hartrees)	Expectation value of total spin-squared operator ($\langle S^2 \rangle$)
NV ⁻ Singlet	Acute	-1333.7757381	-
	Obtuse	-1333.7574228	-
NV ⁻ Triplet	Undistorted	-1333.7960768	2.0259
OV Singlet	Acute	-1354.1386294	-
	Obtuse	-1354.1225869	-
OV Triplet	Undistorted	-1354.1634571	2.0241
SV Singlet	Acute	-1677.1128211	-
	Obtuse	-1677.1040611	-
SV Triplet	Undistorted	-1677.1412177	2.0230

Table S2. Computed values for the nine molecules considered in this work with various methods.

	NV ⁻ Triplet Undis- torted	NV ⁻ Singlet Acute	NV ⁻ Singlet Obtuse	OV Triplet Undis- torted	OV Singlet Acute	OV Singlet Obtuse	SV Triplet Undis- torted	SV Singlet Acute	SV Singlet Obtuse
E/a.u. from CAM-B3LYP- D3BJ/Def2- QZVPP	-1333. 796076 76	1333. 775738 12	-1333. 757422 84	-1354. 163404 98	-1354. 138629 42	-1354. 122586 86	-1677. 141217 65	-1677. 112821 10	-1677. 104061 06
ΔE_{S-T} (kcal mol ⁻¹) from CAM-B3LYP- D3BJ/Def2- QZVPP	0	12.76	24.26	0	15.55	25.62	0	17.82	23.32
E/a.u. from PBE/PBE- D3BJ/Def2- QZVPP	-1332. 828899 16	-1332. 809456 65	-1332. 810802 63	-1353. 174848 54	-1353. 154078 34	-1353. 154725 96	-1676. 047478 55	-1676. 020303 22	-1676. 034031 54
ΔE_{S-T} (kcal mol ⁻¹) from PBE/PBE- D3BJ/Def2- QZVPP	0	12.20	11.35	0	13.03	12.62	0	17.05	8.44
E/a.u. from BP86- D3BJ/Def2- QZVPP	-1334. 618695 01	-1334. 597822 63	-1334. 600493 70	-1354. 977401 73	-1354. 954986 03	-1354. 957164 67	-1677. 990298 07	-1677. 961376 58	-1677. 976586 10
ΔE_{S-T} (kcal mol ⁻¹) from BP86- D3BJ/Def2- QZVPP	0	13.10	11.42	0	14.07	12.70	0	18.15	8.60
E/a.u. from M06-2X/Def2- QZVPP	-1333. 942205 38	-1333. 932203 39	-1333. 911800 53	-1354. 302719 75	-1354. 288285 16	-1354. 270089 82	-1677. 255916 17	-1677. 237430 00	-1677. 225840 03
ΔE_{S-T} (kcal mol ⁻¹) from M06- 2X/Def2-QZVPP	0	6.28	19.08	0	9.06	20.48	0	11.60	18.87
E/a.u. from LC- wPBE- D3BJ/Def2- QZVPP	-1333. 746685 20	-1333. 740758 36	-1333. 702108 53	-1354. 103530 50	-1354. 091751 34	-1354. 057191 40	-1676. 990472 04	-1676. 975607 48	-1676. 946636 86
ΔE_{S-T} (kcal mol ⁻¹)	0	3.72	27.97	0	7.39	29.08	0	9.33	27.51

from LC-wPBE-D3BJ/Def2-QZVPP									
E/a.u. from wB97xD/Def2-QZVPP	-1334.07645411	-1334.06109208	-1334.03829846	-1354.43825883	-1354.41801185	-1354.39806360	-1677.40381301	-1677.38019304	-1677.36790715
ΔE_{S-T} (kcal mol ⁻¹) from wB97xD/Def2-QZVPP	0	9.64	23.94	0	12.70	25.22	0	14.82	22.53
E/a.u. from DLPNO-B2PLYP-D3BJ/Def2-TZVPP	-1333.271410158105	-1333.254905438357	-1333.253184552526	-1353.630841090564	-1353.610705002420	-1353.610224598034	-1676.499272029033	-1676.475362602096	-1676.487598071272
ΔE_{S-T} (kcal mol ⁻¹) from DLPNO-B2PLYP-D3BJ/Def2-TZVPP	0	10.36	11.44	0	12.64	12.94	0	15.00	7.33
E/a.u. from DLPNO-DSDPBEP86-D3BJ/Def2-TZVPP	-1331.910934894611	-1331.904361066435	-1331.897079699419	-1352.255455252912	-1352.244449630160	-1352.238825214667	-1675.008289709208	-1674.994233003239	-1675.002108017921
ΔE_{S-T} (kcal mol ⁻¹) from DLPNO-DSDPBEP86-D3BJ/Def2-TZVPP	0	4.13	8.69	0	6.91	10.44	0	8.83	3.88
E/a.u. from DLPNO-MP2/Def2-TZVPP	-1331.092609554506	-1331.101418877071	-1331.098389247544	-1351.432365975085	-1351.436313911024	-1351.434503495475	-1674.008350358706	-1674.028492306509	-1674.043950508383
ΔE_{S-T} (kcal mol ⁻¹) from DLPNO-MP2/Def2-TZVPP	0	-5.53	-3.63	0	-2.48	-1.34	0	-12.64	-22.34
E/a.u. from DMRG(22,37)M=512	-1325.40107272	-1325.40027225	-1325.38661139	-1345.74187827	-1345.74009336	-1345.72721404	-1668.3522211	-1668.35759471	-1668.35022007
ΔE_{S-T} (kcal mol ⁻¹) from	0	0.50	9.07	0	1.12	9.20	0	-3.37	1.26

DMRG(22,37)M =512									
E/a.u. from SF-TDDFT CAM-B3LYP-D3BJ/Def2-QZVPP	- 1333.7 972134 8	- 1333.7 653217 20	- 1333.7 500452 3	- 1354.1 645053 96	Referen ce triplet not conver ged	Referen ce triplet not conver ged	- 1677.1 423941 2	Referen ce triplet not conver ged	- 1677.0 971117 63048
ΔE_{S-T} (kcal mol ⁻¹) from SF-TDDFT CAM-B3LYP-D3BJ/Def2-QZVPP	0	20.01	29.60	---	---	---	0	---	28.42
ZPVE/a.u. from CAM-B3LYP-D3(BJ)/Def2-TZVPP	0.6281 81	0.6313 81	0.6280 36	0.6313 16	0.6337 79	0.6309 87	0.6250 93	0.6286 00	0.6254 97

XYZ file information of 9 computed molecules

NV Acute Distortion Singlet

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-1 1

C	1.908527	-1.119644	1.157992
H	2.428255	-0.985759	2.113591
C	2.879135	-1.060028	0.000000
H	3.593909	-1.887203	0.000000
C	0.977446	0.071560	0.912724
C	1.908526	-1.119645	-1.157992
H	2.428254	-0.985762	-2.113591
C	0.977446	0.071559	-0.912725
C	1.706884	1.401092	-1.158011
H	2.237835	1.364074	-2.114390
C	3.626426	0.291107	-0.000001
H	4.275928	0.345502	0.877941
H	4.275928	0.345501	-0.877945
C	1.706885	1.401093	1.158008
H	2.237836	1.364077	2.114387
C	2.672079	1.504490	-0.000002
H	3.243853	2.437843	-0.000003
C	1.093356	-2.428145	1.225391
H	1.803386	-3.263396	1.247304
C	-1.026524	-1.720802	0.000002
C	1.093355	-2.428147	-1.225389
H	1.803385	-3.263397	-1.247300
C	0.180586	-2.610954	0.000002
H	-0.076556	-3.714247	0.000003
C	0.679486	2.550762	1.220647
H	1.220553	3.501366	1.198531
N	-1.218312	1.453335	-0.000001
C	0.679485	2.550760	-1.220651
H	1.220553	3.501364	-1.198537
C	-0.251789	2.552550	-0.000002
H	-0.783302	3.526968	-0.000002
C	-1.752019	-1.470717	-1.255262
H	-2.466241	-2.297390	-1.573557

C	-0.001538	-0.005746	-2.150120
H	0.725693	0.061311	-2.969473
C	0.228303	-2.457267	-2.466458
H	-0.311024	-3.407132	-2.520815
H	0.836278	-2.371337	-3.373551
C	-0.750953	-1.303758	-2.381433
H	-1.282070	-1.216219	-3.337347
C	-2.660283	-0.208530	-1.208675
C	-0.944550	1.163675	-2.363881
C	-1.931120	1.160836	-1.220627
H	-2.713867	1.927648	-1.410088
C	-0.166625	2.456752	-2.468573
H	0.455555	2.455067	-3.367088
H	-0.841922	3.314563	-2.536553
H	-3.265985	-0.214620	-2.122382
H	-1.496600	0.989936	-3.289862
C	-0.001536	-0.005743	2.150120
C	-1.752018	-1.470715	1.255265
C	-1.931119	1.160838	1.220627
C	-0.166623	2.456755	2.468569
H	-0.841921	3.314566	2.536548
H	0.455557	2.455072	3.367085
C	0.228304	-2.457264	2.466461
H	0.836280	-2.371332	3.373554
H	-0.311022	-3.407129	2.520820
C	-3.562423	-0.286220	0.000001
H	-4.290931	0.531725	0.000001
H	-4.118317	-1.227103	0.000002
C	-2.660282	-0.208528	1.208677
C	-0.750952	-1.303755	2.381435
C	-0.944549	1.163678	2.363880
H	-1.496598	0.989940	3.289862
H	-1.282068	-1.216214	3.337350
H	0.725695	0.061316	2.969473
H	-2.713866	1.927650	1.410087
H	-2.466241	-2.297388	1.573562
H	-3.265984	-0.214617	2.122384

NV Obtuse Distortion Singlet

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-1 1

C	-0.930936	2.008420	1.292859
H	-1.509068	2.477706	2.129769
C	-1.689037	2.377017	0.000000
H	-1.812656	3.465416	0.000000
C	-0.811450	0.536605	1.487577
C	-0.930936	2.008420	-1.292859
H	-1.509068	2.477706	-2.129769
C	-0.811450	0.536605	-1.487577
C	-2.082885	-0.223928	-1.249292
H	-2.765285	-0.008972	-2.110788
C	-3.046970	1.713157	0.000000
H	-3.618606	2.014041	0.883781
H	-3.618606	2.014041	-0.883781
C	-2.082885	-0.223928	1.249292
H	-2.765285	-0.008972	2.110788
C	-2.836748	0.215580	0.000000
H	-3.810740	-0.287194	-0.000000
C	0.446723	2.659441	1.280719
H	0.341441	3.749457	1.289527
C	1.310124	0.740608	0.000000
C	0.446723	2.659441	-1.280719
H	0.341441	3.749457	-1.289527
C	1.159838	2.226033	0.000000
H	2.167072	2.676694	0.000000
C	-1.922706	-1.747775	1.247922
H	-2.922938	-2.190689	1.218210
N	0.192256	-1.841763	-0.000000
C	-1.922706	-1.747775	-1.247922
H	-2.922938	-2.190689	-1.218210
C	-1.189737	-2.248864	-0.000000
H	-1.267906	-3.360552	-0.000000
C	2.037166	0.234373	-1.231188
H	3.040414	0.695157	-1.193536
C	0.015514	0.011207	-2.587791

H	-0.418885	0.214805	-3.602450
C	1.229023	2.209789	-2.512204
H	2.216261	2.680111	-2.528276
H	0.703699	2.533149	-3.414939
C	1.378412	0.690432	-2.519882
H	1.996288	0.385695	-3.371590
C	2.256988	-1.278068	-1.214614
C	0.154076	-1.527084	-2.487999
C	0.921685	-2.010730	-1.241981
H	1.138191	-3.089074	-1.412427
C	-1.208157	-2.183332	-2.507748
H	-1.772830	-1.874207	-3.390579
H	-1.108866	-3.272486	-2.541936
H	2.792003	-1.555177	-2.126880
H	0.741138	-1.865376	-3.347778
C	0.015514	0.011207	2.587791
C	2.037166	0.234373	1.231188
C	0.921685	-2.010730	1.241981
C	-1.208157	-2.183332	2.507748
H	-1.108866	-3.272486	2.541936
H	-1.772830	-1.874207	3.390579
C	1.229023	2.209789	2.512204
H	0.703699	2.533149	3.414939
H	2.216261	2.680111	2.528276
C	3.059750	-1.686643	-0.000000
H	3.230807	-2.766927	-0.000000
H	4.036967	-1.196920	-0.000000
C	2.256988	-1.278068	1.214614
C	1.378412	0.690432	2.519882
C	0.154076	-1.527084	2.487999
H	0.741138	-1.865376	3.347778
H	1.996288	0.385695	3.371590
H	-0.418885	0.214805	3.602450
H	1.138191	-3.089074	1.412427
H	3.040414	0.695157	1.193536
H	2.792003	-1.555177	2.126880

NV Triplet

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-1 3

C	-0.729946	2.097159	1.266109
H	-1.222444	2.619731	2.119483
C	-1.454974	2.567315	-0.000000
H	-1.464765	3.662960	-0.000000
C	-0.833068	0.624126	1.443569
C	-0.729946	2.097159	-1.266109
H	-1.222444	2.619731	-2.119483
C	-0.833068	0.624126	-1.443569
C	-2.176908	0.006321	-1.251258
H	-2.830563	0.276661	-2.113557
C	-2.886121	2.051373	-0.000000
H	-3.418755	2.421698	0.880841
H	-3.418755	2.421698	-0.880841
C	-2.176908	0.006321	1.251258
H	-2.830563	0.276661	2.113557
C	-2.877650	0.530273	-0.000000
H	-3.909895	0.161118	-0.000000
C	0.729368	2.566314	1.261189
H	0.735138	3.661940	1.270321
C	1.667009	0.622802	-0.000000
C	0.729368	2.566314	-1.261189
H	0.735138	3.661940	-1.270321
C	1.462858	2.096096	-0.000000
H	2.448607	2.617804	-0.000000
C	-2.123651	-1.528034	1.242648
H	-3.151833	-1.900898	1.205228
N	-0.000986	-1.811806	0.000000
C	-2.123651	-1.528034	-1.242648
H	-3.151833	-1.900898	-1.205228
C	-1.421153	-2.083844	0.000000
H	-1.596923	-3.184347	0.000000
C	2.172124	0.004107	-1.259563
H	3.245938	0.273557	-1.394579
C	0.004850	0.005261	-2.510989

H	-0.414775	0.275484	-3.508397
C	1.444673	2.049071	-2.500306
H	2.474121	2.418571	-2.521254
H	0.948597	2.419382	-3.402259
C	1.439255	0.527962	-2.492352
H	1.955136	0.158054	-3.386124
C	2.136866	-1.530201	-1.217150
C	-0.015497	-1.529140	-2.459882
C	0.709023	-2.084800	-1.229867
H	0.796013	-3.185450	-1.381517
C	-1.441068	-2.034751	-2.494250
H	-1.956184	-1.670365	-3.386781
H	-1.459291	-3.128335	-2.524859
H	2.618236	-1.903762	-2.126165
H	0.530682	-1.902830	-3.331454
C	0.004850	0.005261	2.510989
C	2.172124	0.004107	1.259563
C	0.709023	-2.084800	1.229867
C	-1.441068	-2.034751	2.494250
H	-1.459291	-3.128335	2.524859
H	-1.956184	-1.670365	3.386781
C	1.444673	2.049071	2.500306
H	0.948597	2.419382	3.402259
H	2.474121	2.418571	2.521254
C	2.879038	-2.037064	0.000000
H	2.913670	-3.130676	0.000000
H	3.909871	-1.673548	0.000000
C	2.136866	-1.530201	1.217150
C	1.439255	0.527962	2.492352
C	-0.015497	-1.529140	2.459882
H	0.530682	-1.902830	3.331454
H	1.955136	0.158054	3.386124
H	-0.414775	0.275484	3.508397
H	0.796013	-3.185450	1.381517
H	3.245938	0.273557	1.394579
H	2.618236	-1.903762	2.126165

OV Acute Distortion Singlet

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0 1

C	-1.855153	1.218308	1.158970
H	-2.382306	1.113420	2.112895
C	-2.826437	1.207178	0.000000
H	-3.496259	2.068343	0.000000
C	-0.991585	-0.021171	0.919934
C	-1.855152	1.218310	-1.158970
H	-2.382305	1.113423	-2.112895
C	-0.991584	-0.021169	-0.919935
C	-1.792007	-1.308127	-1.162266
H	-2.320754	-1.252073	-2.116173
C	-3.644419	-0.101813	-0.000001
H	-4.295634	-0.123407	0.876064
H	-4.295634	-0.123405	-0.876067
C	-1.792008	-1.308129	1.162263
H	-2.320755	-1.252076	2.116170
C	-2.757237	-1.364902	-0.000002
H	-3.377167	-2.265211	-0.000003
C	-0.970898	2.481058	1.225388
H	-1.636946	3.348848	1.247447
C	1.104059	1.635284	0.000001
C	-0.970897	2.481060	-1.225385
H	-1.636945	3.348850	-1.247444
C	-0.051914	2.610768	0.000002
H	0.281842	3.679432	0.000002
C	-0.820830	-2.505040	1.230379
H	-1.396094	-3.433987	1.205051
O	1.114831	-1.471867	-0.000001
C	-0.820829	-2.505038	-1.230382
H	-1.396094	-3.433985	-1.205056
C	0.063344	-2.582047	-0.000002
H	0.658992	-3.496238	-0.000002
C	1.827119	1.389341	-1.261005
H	2.574702	2.177043	-1.574331
C	-0.004488	0.013844	-2.152553

H	-0.726510	-0.022648	-2.975162
C	-0.106842	2.469551	-2.467955
H	0.477754	3.390118	-2.523903
H	-0.716778	2.414630	-3.374076
C	0.814990	1.269637	-2.385950
H	1.334740	1.154247	-3.344124
C	2.675355	0.092877	-1.210255
C	0.878561	-1.201828	-2.364739
C	1.888494	-1.221758	-1.260366
H	2.578197	-2.068379	-1.327773
C	0.049118	-2.462133	-2.465088
H	-0.563194	-2.431278	-3.365310
H	0.678424	-3.353289	-2.528405
H	3.284769	0.047021	-2.120557
H	1.444011	-1.057510	-3.285606
C	-0.004490	0.013841	2.152553
C	1.827118	1.389339	1.261007
C	1.888494	-1.221760	1.260365
C	0.049117	-2.462136	2.465085
H	0.678422	-3.353293	2.528400
H	-0.563196	-2.431283	3.365307
C	-0.106844	2.469548	2.467958
H	-0.716780	2.414625	3.374078
H	0.477752	3.390114	2.523908
C	3.578792	0.114626	0.000001
H	4.270904	-0.733007	0.000001
H	4.175196	1.026960	0.000002
C	2.675355	0.092875	1.210256
C	0.814989	1.269634	2.385952
C	0.878559	-1.201832	2.364737
H	1.444009	-1.057514	3.285606
H	1.334738	1.154242	3.344126
H	-0.726512	-0.022653	2.975161
H	2.578196	-2.068381	1.327771
H	2.574701	2.177040	1.574335
H	3.284768	0.047018	2.120559

OV Obtuse Distortion Singlet

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0 1

C	-0.957735	1.999555	1.293052
H	-1.539815	2.451656	2.127103
C	-1.720400	2.355418	0.000000
H	-1.859463	3.440275	0.000000
C	-0.811726	0.523502	1.486733
C	-0.957735	1.999555	-1.293052
H	-1.539815	2.451656	-2.127103
C	-0.811726	0.523502	-1.486733
C	-2.085009	-0.244854	-1.252807
H	-2.769965	-0.047100	-2.109161
C	-3.070731	1.676010	0.000000
H	-3.647564	1.968451	0.881262
H	-3.647564	1.968451	-0.881262
C	-2.085009	-0.244854	1.252807
H	-2.769965	-0.047100	2.109161
C	-2.842492	0.181228	0.000000
H	-3.810391	-0.332043	-0.000000
C	0.410268	2.667938	1.281145
H	0.293514	3.754758	1.287383
C	1.292710	0.756484	0.000000
C	0.410268	2.667938	-1.281145
H	0.293514	3.754758	-1.287383
C	1.124905	2.241126	0.000000
H	2.127136	2.696620	0.000000
C	-1.901671	-1.764472	1.254487
H	-2.888392	-2.232846	1.213970
O	0.210002	-1.784982	-0.000000
C	-1.901671	-1.764472	-1.254487
H	-2.888392	-2.232846	-1.213970
C	-1.204677	-2.255766	-0.000000
H	-1.131099	-3.348368	-0.000000
C	2.035839	0.272684	-1.234991
H	3.030563	0.742956	-1.196608
C	0.015008	0.021826	-2.602493

H	-0.413967	0.214248	-3.614770
C	1.200084	2.233092	-2.513134
H	2.179683	2.715886	-2.528594
H	0.673988	2.551186	-3.415580
C	1.371864	0.716179	-2.526296
H	1.997413	0.424076	-3.375477
C	2.278707	-1.234463	-1.214851
C	0.167164	-1.512719	-2.500319
C	0.968313	-1.976568	-1.289394
H	1.127166	-3.057604	-1.339193
C	-1.179544	-2.200132	-2.509178
H	-1.750060	-1.898633	-3.386916
H	-1.066016	-3.286839	-2.548469
H	2.810916	-1.516453	-2.125646
H	0.764340	-1.860569	-3.348237
C	0.015008	0.021826	2.602493
C	2.035839	0.272684	1.234991
C	0.968313	-1.976568	1.289394
C	-1.179544	-2.200132	2.509178
H	-1.066016	-3.286839	2.548469
H	-1.750060	-1.898633	3.386916
C	1.200084	2.233092	2.513134
H	0.673988	2.551186	3.415580
H	2.179683	2.715886	2.528594
C	3.077721	-1.648584	-0.000000
H	3.262201	-2.725752	-0.000000
H	4.047041	-1.151530	-0.000000
C	2.278707	-1.234463	1.214851
C	1.371864	0.716179	2.526296
C	0.167164	-1.512719	2.500319
H	0.764340	-1.860569	3.348237
H	1.997413	0.424076	3.375477
H	-0.413967	0.214248	3.614770
H	1.127166	-3.057604	1.339193
H	3.030563	0.742956	1.196608
H	2.810916	-1.516453	2.125646

OV Triplet

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0 3

C	0.732656	1.262807	-2.098576
H	1.226888	2.114648	-2.609370
C	-0.725567	1.262874	-2.568574
H	-0.730431	1.271300	-3.661991
C	0.833735	1.436910	-0.620755
C	-1.459951	0.003095	-2.098576
H	-2.444782	0.005192	-2.609370
C	-1.661268	0.003581	-0.620755
C	-2.176017	1.268872	-0.014439
H	-3.244827	1.406860	-0.280599
C	-1.439091	2.504835	-2.055514
H	-0.942791	3.404859	-2.425492
H	-2.466623	2.529393	-2.425413
C	-0.000000	2.518957	-0.014424
H	0.419104	3.511804	-0.280617
C	-1.436640	2.500819	-0.534389
H	-1.950564	3.395414	-0.167577
C	1.456465	-0.003077	-2.568574
H	1.466194	-0.003078	-3.661991
C	0.827533	-1.440491	-0.620755
C	-0.730897	-1.259797	-2.568574
H	-0.735762	-1.268222	-3.661991
C	0.727295	-1.265902	-2.098576
H	1.217895	-2.119840	-2.609370
C	0.024540	2.467737	1.517623
H	-0.523619	3.330769	1.904238
O	0.000000	0.000000	1.755313
C	-2.144077	1.221903	1.517541
H	-2.613414	2.130232	1.904065
C	-0.731959	1.274179	2.067683
H	-0.750452	1.306416	3.161516
C	-0.010866	-2.518922	-0.014439
H	0.404037	-3.513532	-0.280599
C	-2.181481	-1.259479	-0.014424

H	-3.250864	-1.392948	-0.280617
C	-1.449705	-2.498707	-2.055514
H	-0.957207	-3.400855	-2.425413
H	-2.477299	-2.518910	-2.425492
C	-1.447453	-2.494576	-0.534389
H	-1.965233	-3.386944	-0.167577
C	0.013839	-2.467777	1.517541
C	-2.149393	-1.212616	1.517623
C	-0.737492	-1.270984	2.067683
H	-0.756163	-1.303119	3.161516
C	-2.879784	0.006248	2.036655
H	-3.907242	0.008456	1.674257
H	-2.917548	0.006345	3.129165
H	-0.538128	-3.328399	1.904065
H	-2.622721	-2.118852	1.904238
C	2.186884	1.250050	-0.014439
C	2.181481	-1.259479	-0.014424
C	1.469451	-0.003194	2.067683
C	1.445303	2.490842	2.036655
H	1.464269	2.523498	3.129165
H	1.960944	3.379542	1.674257
C	2.888797	-0.006128	-2.055514
H	3.423831	0.871462	-2.425413
H	3.420089	-0.885949	-2.425492
C	1.434481	-2.497090	2.036655
H	1.453279	-2.529843	3.129165
H	1.946298	-3.387998	1.674257
C	2.124853	-1.255121	1.517623
C	2.884093	-0.006243	-0.534389
C	2.130238	1.245874	1.517541
H	3.151542	1.198167	1.904065
H	3.915796	-0.008469	-0.167577
H	2.840790	2.106672	-0.280599
H	1.506615	-0.003297	3.161516
H	2.831760	-2.118857	-0.280617
H	3.146341	-1.211917	1.904238

SV Acute Distortion Singlet

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0 1

C	1.919939	1.234185	-1.166097
H	2.455983	1.136882	-2.115885
C	2.885489	1.213812	-0.000197
H	3.562746	2.069455	-0.000343
C	1.046055	0.003138	-0.943130
C	1.920031	1.234537	1.165769
H	2.456119	1.137480	2.115561
C	1.046138	0.003465	0.943102
C	1.834413	-1.294205	1.171760
H	2.378936	-1.229631	2.117439
C	3.692724	-0.100500	-0.000066
H	4.343626	-0.127737	-0.876124
H	4.343665	-0.127530	0.875968
C	1.834359	-1.294538	-1.171553
H	2.378822	-1.230184	-2.117283
C	2.793420	-1.354139	0.000092
H	3.407070	-2.258573	0.000202
C	1.040293	2.500422	-1.223431
H	1.709506	3.365576	-1.224850
C	-1.046072	1.632886	-0.000181
C	1.040348	2.500771	1.222779
H	1.709544	3.365938	1.223944
C	0.116495	2.612620	-0.000327
H	-0.239915	3.671620	-0.000475
C	0.898923	-2.523581	-1.273016
H	1.523364	-3.413715	-1.380153
S	-1.101269	-1.359129	0.000186
C	0.898985	-2.523224	1.273595
H	1.523432	-3.413328	1.380940
C	0.069342	-2.738321	0.000340
H	-0.414045	-3.715598	0.000489
C	-1.784934	1.475910	1.272943
H	-2.465126	2.330552	1.552575
C	0.042611	0.066731	2.182560

H	0.776468	0.046266	2.995102
C	0.180745	2.520170	2.467770
H	-0.382653	3.453855	2.515617
H	0.790634	2.460002	3.373452
C	-0.765895	1.339189	2.396497
H	-1.286095	1.242617	3.356057
C	-2.724855	0.241744	1.279134
C	-0.854825	-1.130689	2.476436
C	-2.014501	-1.130247	1.480096
H	-2.741610	-1.919384	1.672958
C	-0.029225	-2.422419	2.486621
H	0.575373	-2.426988	3.393052
H	-0.677748	-3.300799	2.537093
H	-3.401836	0.333026	2.134177
H	-1.281171	-0.986241	3.469845
C	0.042506	0.066121	-2.182577
C	-1.784981	1.475569	-1.273240
C	-2.014582	-1.130642	-1.479732
C	-0.029359	-2.423092	-2.486015
H	-0.677889	-3.301482	-2.536221
H	0.575189	-2.427903	-3.392479
C	0.180659	2.519498	-2.468406
H	0.790522	2.459086	-3.374089
H	-0.382730	3.453177	-2.516483
C	-3.569703	0.232474	0.000046
H	-4.260989	-0.616242	0.000172
H	-4.180966	1.135608	-0.000059
C	-2.724912	0.241408	-1.279083
C	-0.765988	1.338543	-2.396799
C	-0.854955	-1.131355	-2.476127
H	-1.281340	-0.987150	-3.469554
H	-1.286225	1.241736	-3.356315
H	0.776339	0.045440	-2.995135
H	-2.741705	-1.919826	-1.672347
H	-2.465177	2.330141	-1.553076
H	-3.401931	0.332480	-2.134118

SV Obtuse Distortion Singlet

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0 1

C	1.644215	1.490371	1.283884
H	1.903588	2.173818	2.121165
C	1.770573	2.328468	-0.000000
H	2.774650	2.761165	-0.000000
C	0.263718	0.944729	1.502660
C	1.644215	1.490371	-1.283884
H	1.903588	2.173818	-2.121165
C	0.263718	0.944729	-1.502660
C	-0.825147	1.981346	-1.275550
H	-0.773139	2.706399	-2.115543
C	0.746987	3.440675	-0.000000
H	0.870610	4.074993	0.880946
H	0.870610	4.074993	-0.880946
C	-0.825147	1.981346	1.275550
H	-0.773139	2.706399	2.115543
C	-0.627078	2.808823	0.000000
H	-1.387482	3.596838	0.000000
C	2.705560	0.394436	1.280265
H	3.695039	0.857882	1.294629
C	1.258384	-1.122236	-0.000000
C	2.705560	0.394436	-1.280265
H	3.695039	0.857882	-1.294629
C	2.570247	-0.439341	-0.000000
H	3.383713	-1.185682	-0.000000
C	-2.259447	1.436014	1.318717
H	-2.949051	2.276829	1.422719
S	-1.404536	-0.549189	0.000000
C	-2.259447	1.436014	-1.318717
H	-2.949051	2.276829	-1.422719
C	-2.618794	0.712470	0.000000
H	-3.652295	0.358631	0.000000
C	0.942835	-1.903451	-1.262983
H	1.680064	-2.724367	-1.297333

C	0.065122	0.003810	-2.630859
H	0.176600	0.487283	-3.626364
C	2.534884	-0.474382	-2.521881
H	3.287997	-1.264806	-2.542863
H	2.684756	0.132387	-3.416725
C	1.139636	-1.090446	-2.540014
H	1.047847	-1.761231	-3.399273
C	-0.429591	-2.596967	-1.267000
C	-1.362688	-0.595708	-2.605555
C	-1.563825	-1.582046	-1.440707
H	-2.534767	-2.077957	-1.509305
C	-2.420263	0.515776	-2.539022
H	-2.329642	1.130790	-3.434607
H	-3.422457	0.079433	-2.557007
H	-0.463702	-3.258948	-2.134671
H	-1.515212	-1.166696	-3.523951
C	0.065122	0.003810	2.630859
C	0.942835	-1.903451	1.262983
C	-1.563825	-1.582046	1.440707
C	-2.420263	0.515776	2.539022
H	-3.422457	0.079433	2.557007
H	-2.329642	1.130790	3.434607
C	2.534884	-0.474382	2.521881
H	2.684756	0.132387	3.416725
H	3.287997	-1.264806	2.542863
C	-0.617276	-3.431684	0.000000
H	-1.601879	-3.905627	0.000000
H	0.120437	-4.234746	-0.000000
C	-0.429591	-2.596967	1.267000
C	1.139636	-1.090446	2.540014
C	-1.362688	-0.595708	2.605555
H	-1.515212	-1.166696	3.523951
H	1.047847	-1.761231	3.399273
H	0.176600	0.487283	3.626364
H	-2.534767	-2.077957	1.509305
H	1.680064	-2.724367	1.297333
H	-0.463702	-3.258948	2.134671

SV Triplet

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0 3

C	1.267917	0.732032	-2.142050
H	2.115108	1.221158	-2.666052
C	0.000000	1.454681	-2.611884
H	0.000000	1.455104	-3.705151
C	1.460323	0.843118	-0.666849
C	-1.267917	0.732032	-2.142050
H	-2.115108	1.221158	-2.666052
C	-1.460323	0.843118	-0.666849
C	-1.268958	2.210484	-0.071489
H	-2.114936	2.857299	-0.380587
C	0.000000	2.890810	-2.112317
H	0.878517	3.420688	-2.486610
H	-0.878517	3.420688	-2.486610
C	1.268958	2.210484	-0.071489
H	2.114936	2.857299	-0.380587
C	0.000000	2.896190	-0.591707
H	0.000000	3.930616	-0.233012
C	1.259791	-0.727341	-2.611884
H	1.260157	-0.727552	-3.705151
C	-0.000000	-1.686236	-0.666849
C	-1.259791	-0.727341	-2.611884
H	-1.260157	-0.727552	-3.705151
C	-0.000000	-1.464065	-2.142050
H	-0.000000	-2.442317	-2.666052
C	1.302645	2.228886	1.468673
H	1.385255	3.268126	1.793888
S	0.000000	0.000000	1.574658
C	-1.302645	2.228886	1.468673
H	-1.385255	3.268126	1.793888
C	0.000000	1.688620	2.087047
H	0.000000	1.809774	3.172443
C	-1.279856	-2.204192	-0.071489
H	-1.417026	-3.260238	-0.380587

C	-2.548814	-0.006292	-0.071489
H	-3.531962	0.402939	-0.380587
C	-2.503515	-1.445405	-2.112317
H	-2.523145	-2.471162	-2.486610
H	-3.401662	-0.949526	-2.486610
C	-2.508174	-1.448095	-0.591707
H	-3.404014	-1.965308	-0.233012
C	-1.278949	-2.242566	1.468673
C	-2.581594	0.013681	1.468673
C	-1.462388	-0.844310	2.087047
H	-1.567310	-0.904887	3.172443
C	-2.522933	1.456616	1.985576
H	-3.420798	1.974999	1.648450
H	-2.543975	1.468765	3.078664
H	-2.137653	-2.833729	1.793888
H	-3.522908	-0.434397	1.793888
C	2.548814	-0.006292	-0.071489
C	1.279856	-2.204192	-0.071489
C	1.462388	-0.844310	2.087047
C	2.522933	1.456616	1.985576
H	2.543975	1.468765	3.078664
H	3.420798	1.974999	1.648450
C	2.503515	-1.445405	-2.112317
H	3.401662	-0.949526	-2.486610
H	2.523145	-2.471162	-2.486610
C	-0.000000	-2.913232	1.985576
H	-0.000000	-2.937530	3.078664
H	-0.000000	-3.949997	1.648450
C	1.278949	-2.242566	1.468673
C	2.508174	-1.448095	-0.591707
C	2.581594	0.013681	1.468673
H	3.522908	-0.434397	1.793888
H	3.404014	-1.965308	-0.233012
H	3.531962	0.402939	-0.380587
H	1.567310	-0.904887	3.172443
H	1.417026	-3.260238	-0.380587
H	2.137653	-2.833729	1.793888