

## Supporting information

### Insights from the Computational Studies on the Oxidized as Isolated State of [NiFeSe] Hydrogenase from *D. vulgaris* Hildenborough

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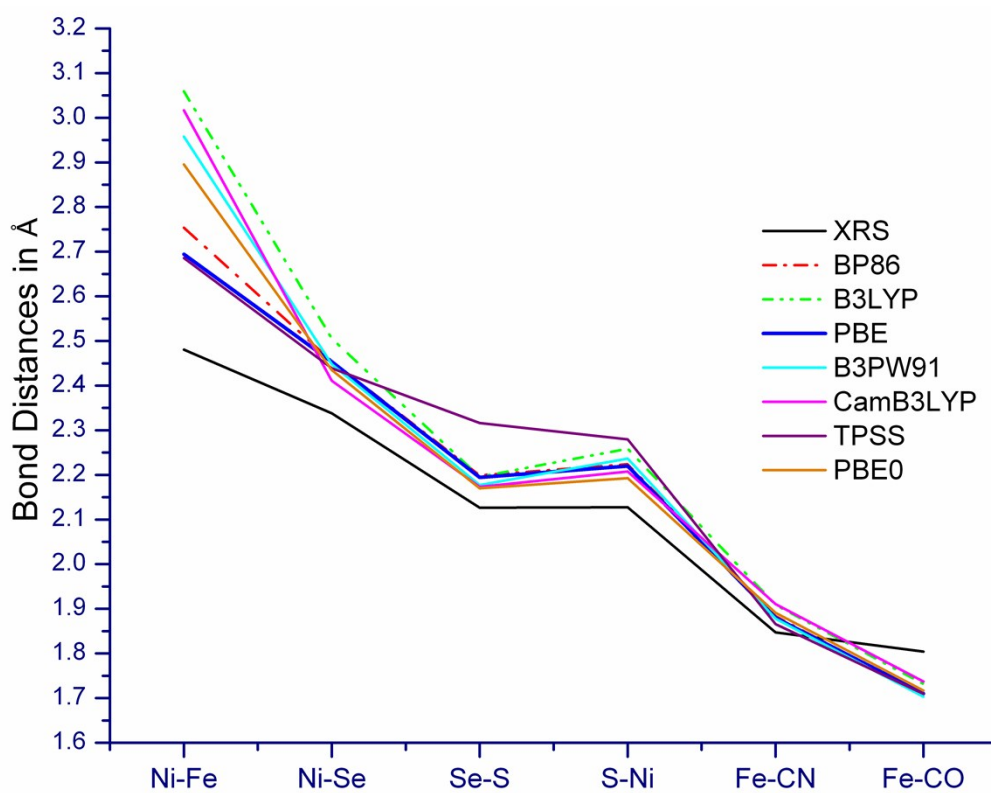
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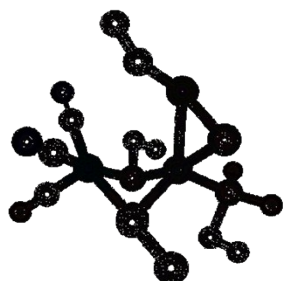
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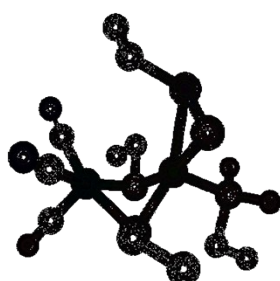
**Figure SF1.** Performance of various Functionals in reproducing the structural features of the oxidized [NiFeSe] Hase in DvH. XRS represents the parameters reported for the crystal structure.



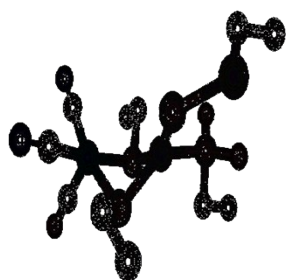
**Figure SF2.** Structures of the geometries proposed for Conf-II and Optimized at BP86/TZVP level. Hydrogens are omitted for clarity. The legends at the bottom of the optimized geometry are the Ni-Fe distances ( $\text{\AA}$ ) and the Ni-S-Se bond angle ( $^\circ$ ).



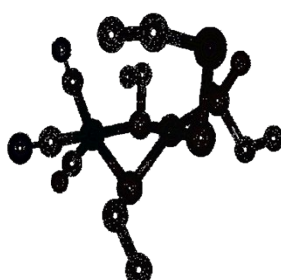
SPY-1  
2.85 $\text{\AA}$ , 71.7 $^\circ$



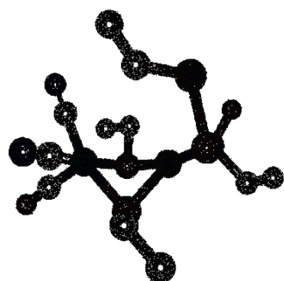
SPY-2  
2.80 $\text{\AA}$ , 68.4 $^\circ$



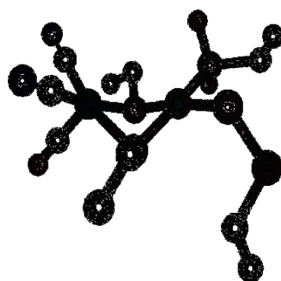
SSW  
3.09 $\text{\AA}$ , 122.1 $^\circ$



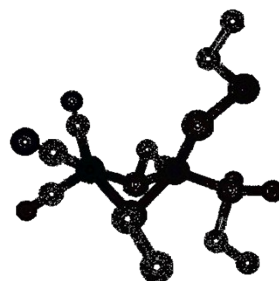
SPL-1  
3.09 $\text{\AA}$ , 106.1 $^\circ$



SPL-2  
3.03 $\text{\AA}$ , 99 $^\circ$

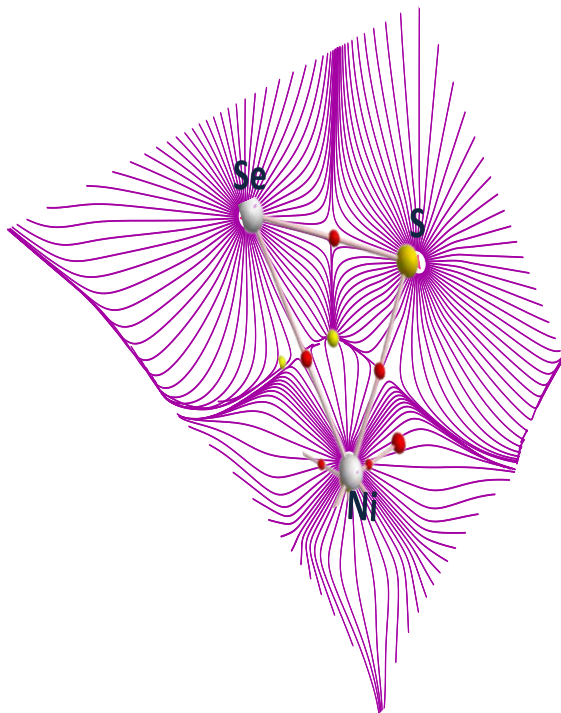


SPL-3  
3.15 $\text{\AA}$ , 106.2 $^\circ$

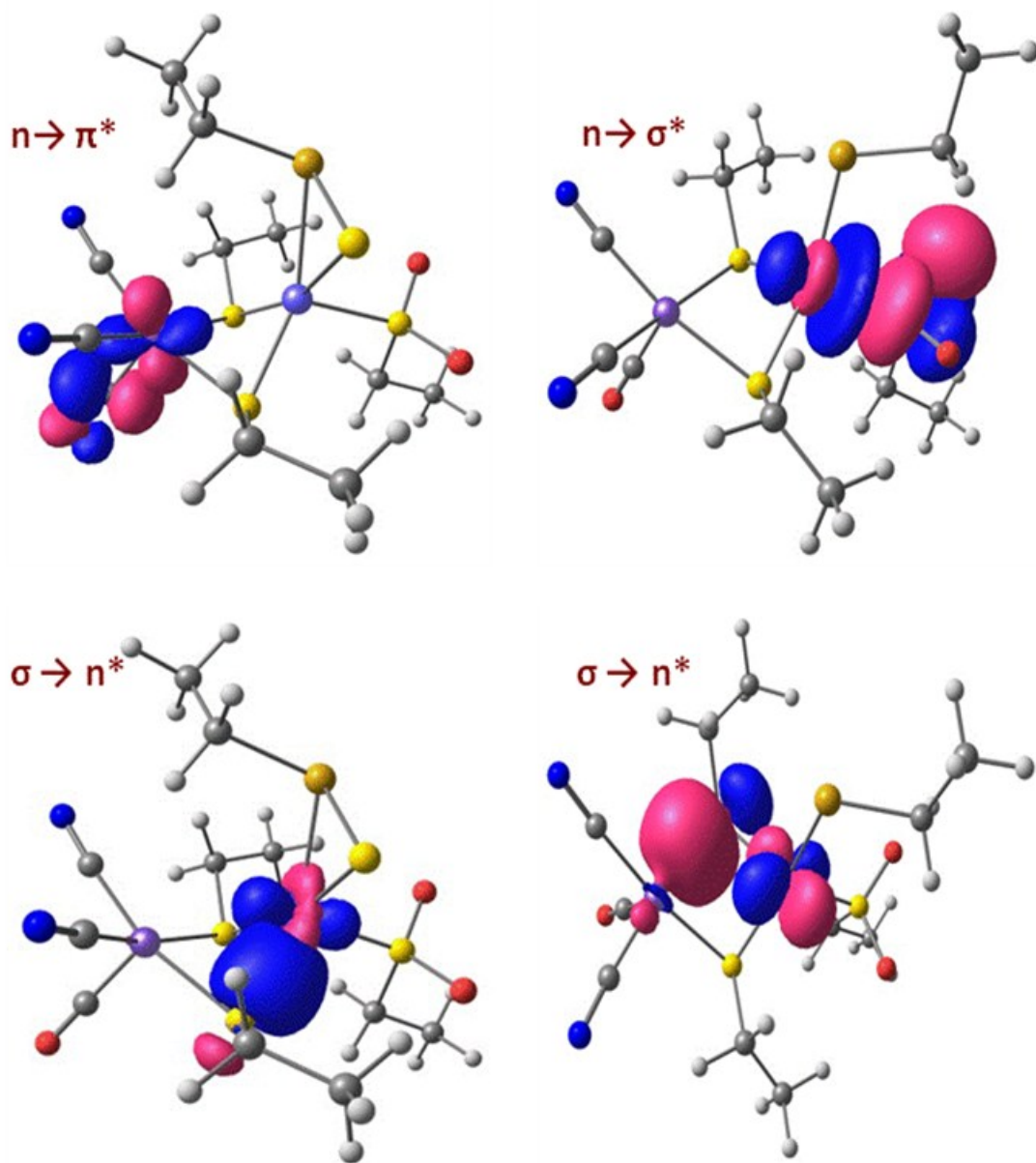


Conf-II  
2.77 $\text{\AA}$ , 106.7 $^\circ$

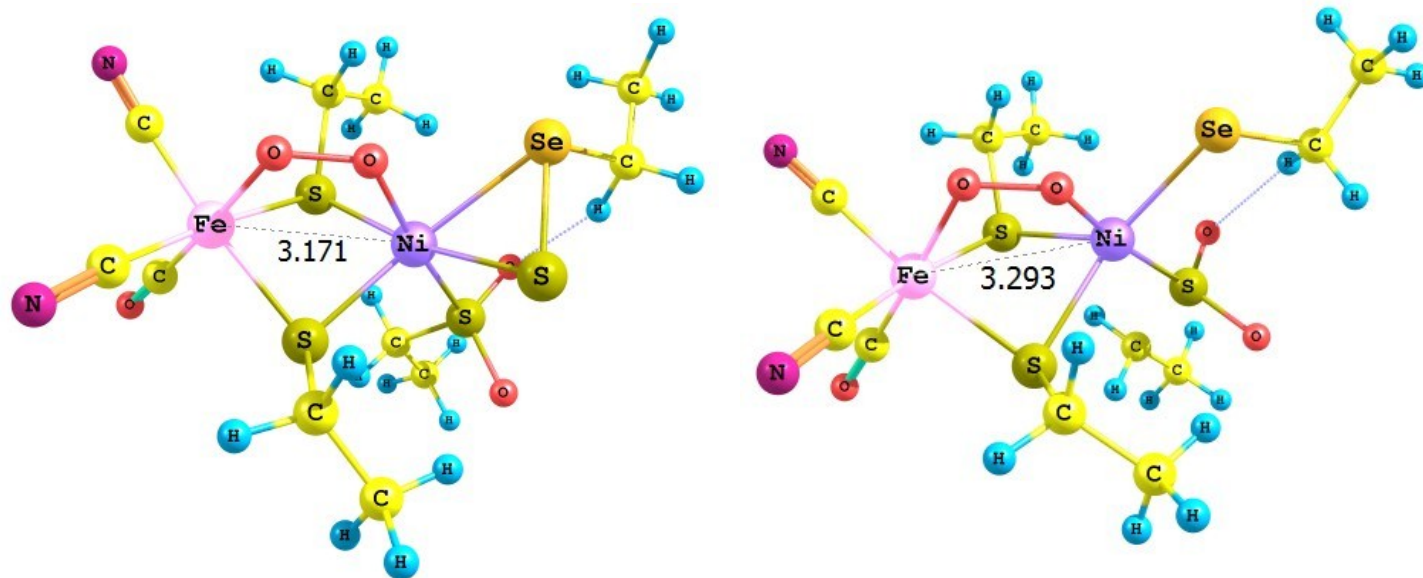
**Figure SF3.** Gradient path of the electron density between the Ni-S-Se in Conf I.



**Figure SF4.** NBO interactions that contribute majorly to the ground state stabilization of the Conf-I, Conf-II & Conf-III of Ni-IS state of [NiFeSe] Hase.



**Figure SF5.** Optimized Geometries of the Peroxo inhibited states of Conf-I and Conf-III showing the Ni- Fe distances in Å units.



Peroxo inhibited state of Conf-I/ -153.8560 a.u

Peroxo inhibited state of Conf-III/ -153.8582 a.u

**Table ST1.** Results of the Natural Spin Orbital calculations revealing the type of the molecular orbital and their occupancy numbers in the SSW model.

SSW					
MO no	Atom type	Orbital type	MO Coefficient		Total Occupancy
333	Fe16(1)	d3z2-r2	0.723	0.362	0.362
334	Fe16(1)	dxz	0.614	0.307	0.307
335	Fe16(1)	dyz	0.717	0.358	0.358
336	Fe16(1)	dx2-y2	0.718	0.359	0.359
337	Fe16(1)	dxy	0.670	0.335	0.335
338	Fe16(2)	d3z2-r2	0.282	0.141	0.141
339	Fe16(2)	dxz	0.248	0.124	0.124
340	Fe16(2)	dyz	0.278	0.139	0.139
341	Fe16(2)	dx2-y2	0.282	0.141	0.141
342	Fe16(2)	dxy	0.263	0.132	0.132
343	Fe16(3)	d3z2-r2	0.217	0.109	0.109
344	Fe16(3)	dxz	0.178	0.089	0.089
345	Fe16(3)	dyz	0.214	0.107	0.107
346	Fe16(3)	dx2-y2	0.207	0.104	0.104
347	Fe16(3)	dxy	0.210	0.105	0.105
480	Ni23(1)	d3z2-r2	0.914	0.457	0.457
481	Ni23(1)	dxz	0.938	0.469	0.469
482	Ni23(1)	dyz	0.956	0.478	0.478
483	Ni23(1)	dx2-y2	0.995	0.498	0.498
484	Ni23(1)	dxy	0.706	0.353	0.353
485	Ni23(2)	d3z2-r2	0.337	0.169	0.169
486	Ni23(2)	dxz	0.346	0.173	0.173
487	Ni23(2)	dyz	0.351	0.176	0.176
488	Ni23(2)	dx2-y2	0.362	0.181	0.181
489	Ni23(2)	dxy	0.266	0.133	0.133
490	Ni23(3)	d3z2-r2	0.228	0.114	0.114
491	Ni23(3)	dxz	0.233	0.117	0.117
492	Ni23(3)	dyz	0.240	0.120	0.120
493	Ni23(3)	dx2-y2	0.252	0.126	0.126
494	Ni23(3)	dxy	0.187	0.093	0.093
Total no of electrons in Ni d= 6					



**Table ST2.** Geometric features of the model structures proposed for Conf-II. (Bond lengths (Å) and bond angles (°)).

Selected Bond Parameters of Models of Conf-II											
	Ni-Fe	Fe-S <sub>brdg(p)</sub>	Fe-S <sub>brdg(d)</sub>	Ni-S	Ni-Se	S-Se	Fe-C(N)p	Fe-C(N)d	Fe-C(O)	FeSpNi	Total Energy (Hartrees)
SPY1	2.847	2.270	2.296	2.232	2.603	2.213	1.899	1.899	1.704	77.38	-7534.3569
SPY2	2.798	2.286	2.285	2.221	2.487	2.199	1.886	1.889	1.707	76.21	-7534.3537
SSW	3.091	2.278	2.316	2.183	3.866	2.235	1.900	1.899	1.691	86.11	-7534.3603
SPL1	3.098	2.283	2.299	2.229	3.573	2.241	1.894	1.899	1.688	85.92	-7534.3623
SPL2	3.029	2.283	2.296	2.235	3.400	2.234	1.894	1.897	1.689	83.61	-7534.3621
SPL3	3.153	2.290	2.284	2.231	3.587	2.254	1.895	1.897	1.687	87.22	-7534.3612

**Table ST3.** NPA Net atomic Charges at Ni, Fe, Se and bridging Sulphurs ( $S_{\text{brdg}}$ ) in all the models studied.

<b>NPA Charges</b>									
	Ni	Fe	Se	S12	S3	S15	S8	C21	O22
SPY1	-0.314	-1.205	0.315	-0.268	1.623	0.221	0.204	0.843	-0.524
SPY2	-0.315	-1.206	0.315	-0.268	1.623	0.221	0.204	0.843	-0.524
SSW	-0.227	-1.076	0.149	-0.336	1.621	0.154	0.215	0.859	-0.519
SPL1	-0.171	-1.098	0.193	-0.404	1.631	0.188	0.189	0.859	-0.516
SPL2	-0.173	-1.117	0.185	-0.393	1.629	0.195	0.195	0.858	-0.518
SPL3	-0.130	-1.084	0.087	-0.378	1.632	0.193	0.170	0.860	-0.516
Conf-1	-0.360	-1.094	0.465	-0.181	1.647	0.257	0.298	0.863	-0.465
Conf-II	-0.066	-0.504	-0.081	-0.202	0.527	-0.041	-0.073	0.334	-0.277
Conf-III	-0.219	-1.122	-0.103	-	1.644	0.229	0.143	0.851	-0.519
ICC1	-0.110	-1.163	-0.137	-	-0.219	0.241	0.175	0.841	-0.529

**Table ST4.** Topological properties at the BCPs in Ni-S, Ni-Se, and S-Se bonds.  $\rho(r)$  in units of  $e\text{\AA}^{-3}$ ,  $L(r)$  in units of  $e\text{\AA}^{-3}$ ,  $G(r)$ ,  $V(r)$ ,  $H(r)$  in units of a.u.  $\text{\AA}^{-3}$ .

<b>Ni-S BCP</b>							
	$\rho(r)$	$L(r)$	$G(r)$	$H(r)$	E	$V(r)$	$ -V(r) /G(r)$
SPL1	0.084	-0.041	0.069	-0.027	0.053	-0.096	1.391
SPL2	0.084	-0.041	0.067	-0.027	0.059	-0.095	1.417
SPL3	0.084	-0.043	0.069	-0.027	0.036	-0.097	1.405
SPY1	0.083	-0.039	0.066	-0.027	0.096	-0.093	1.409
SPY2	0.085	-0.040	0.068	-0.028	0.051	-0.097	1.426
SSW	0.09	-0.046	0.077	-0.031	0.026	-0.108	1.402
Conf-II	0.098	-0.049	0.085	-0.036	0.047	-0.122	1.435
Conf-I	0.083	-0.041	0.067	-0.027	0.023	-0.095	1.418
<b>S-Se BCPs</b>							
SPL1	0.107	0.002	0.041	-0.043	0.043	-0.085	2.073
SPL2	0.108	0.003	0.041	-0.044	0.037	-0.086	2.097
SPL3	0.107	0.001	0.040	-0.041	0.022	-0.081	2.025
SPY1	0.112	0.003	0.045	-0.048	0.068	-0.094	2.089
SPY2	0.115	0.004	0.047	-0.051	0.094	-0.099	2.106
SSW	0.108	0.002	0.042	-0.044	0.059	-0.087	2.071
Conf-I	0.116	0.004	0.048	-0.053	0.095	-0.101	2.104
Conf-II	0.112	0.003	0.044	-0.047	0.047	-0.091	2.068
<b>Ni-Se BCP</b>							
SPY1	0.051	-0.026	0.041	-0.015	1.063	-0.056	1.380
SPY2	0.058	-0.029	0.047	-0.018	0.515	-0.064	1.361
Conf-III	0.075	-0.030	0.052	-0.022	0.061	-0.074	1.423
Conf-I	0.060	-0.034	0.048	-0.014	0.354	-0.062	1.291

**Table ST5.** Volume(Vol), Charge and average number of electrons(NVol) present in the atomic basins of Ni and Se in Conf-I & Conf-III along with the average electron density at Ni (Avr  $\rho(r)$ ) and Delocalization Index  $\delta$  ( $\Omega_{Ni}$ ,  $\Omega_{Se}$ ) values in Ni/Se atomic basins (DI).

	Vol @ Ni	Charge @ Ni	NVol @ Ni	$\delta$ ( $\Omega_{Ni}$ , $\Omega_{Se}$ )	Avr $\rho(r)$
Conf-I	85.79	0.496	27.50	1.6062	0.314
Conf-III	102.90	0.558	27.44	2.7677	0.262
	Vol @ Se	Charge @ Se	NVol @ Se		Avr $\rho(r)$
Conf-I	204.95	0.0765	33.88		0.166
Conf-III	256.07	-33.83	34.27		0.133

**Table ST6.** bond parameters of the optimized geometries of conf-I, conf-II and conf-III obtained by solvating the structures in water by polarizable Continuum Model at BP86/TZVP.

Selected Bond lengths (Å) and Bond angles											
	Ni-Fe	Fe-S <sub>brdg(p)</sub>	Fe-S <sub>brdg(d)</sub>	Ni-S	Ni-Se	S-Se	Fe-C(N)p	Fe-C(N)d	Fe-C(O)	FeSpNi	Total Energy (Hartrees)
Conf-I	2.773	2.269	2.292	2.233	2.437	2.188	1.888	1.888	1.709	75.7	-7534.32082
Conf-II	2.831	2.269	2.288	2.233	2.567	2.209	1.897	1.897	1.703	76.9	-7534.47173
Conf-III	3.021	2.322	2.257	-	2.345	-	1.900	1.898	1.694	82.4	-7096.89197

## Table ST4 Output :

Record of properties at a point in space

Coordinates of point: 0.166063 4.413734 0.230132

Analyzed density function: RHO, electron density

Density value: 0.11249925

Gradient: 0.00000000 -0.00000000 0.00000000

Hessian matrix: -0.03336347 0.00350564 0.13259656  
0.00350564 -0.10131648 0.00507167  
0.13259656 0.00507167 0.12239378

Eigenvalues of Hessian: -0.10929525 -0.10140756 0.19841664

First Eigenvector: -0.86662465 0.06643094 0.49451860

Second Eigenvector: -0.04750786 -0.99758060 0.05075386

Third Eigenvector: 0.49669379 0.02049103 0.86768393

Properties:

Rho 1.1249924646e-001

KEG 4.4194140144e-002

KEK 4.7265682480e-002 EOA -4.7354383623e-002

Lap 3.0715423368e-003

I 3.1614837170e-003

VNET -6.2247624568e+000 VNET(Cor) -6.2305978315e+000

EHF -3.0887483871e+000

VREP(Cor) 6.1330379236e+000

V(Atom) -9.7559907979e-002

VIR 9.1459822624e-002

Overlap matrix, number of orbitals: 139

0.00011702					-0.00037633	0.00002812	-0.00068883	-0.00136568	-0.00024698
-0.00000874	0.00000065				0.00035760	-0.00002672	0.00065456	0.00129773	0.00023469
0.00021420	-0.00001601	0.00039207			-0.00058585	0.00004378	-0.00107236	-0.00212606	-0.00038449
0.00042467	-0.00003174	0.00077732	0.00154111		0.00047848	-0.00003576	0.00087581	0.00173638	0.00031402
0.00007680	-0.00000574	0.00014057	0.00027870	0.00005040	0.00019446	-0.00001453	0.00035595	0.00070570	0.00012762
0.00007110	-0.00000531	0.00013014	0.00025801	0.00004666	0.00035465	-0.00002650	0.00064916	0.00128702	0.00023275
-0.00002966	0.00000222	-0.00005429	-0.00010763	-0.00001946	-0.00008006	0.00000598	-0.00014654	-0.00029052	-0.00005254
-0.00040633	0.00003036	-0.00074375	-0.00147455	-0.00026666	0.00034525	-0.00002580	0.00063195	0.00125291	0.00022658
0.00008302	-0.00000620	0.00015196	0.00030128	0.00005449	0.00015416	-0.00001152	0.00028218	0.00055945	0.00010117
0.00017926	-0.00001340	0.00032812	0.00065053	0.00011764	0.00020416	-0.00001526	0.00037370	0.00074089	0.00013399
0.00016350	-0.00001222	0.00029927	0.00059333	0.00010730	0.00024003	-0.00001794	0.00043936	0.00087107	0.00015753
0.00009041	-0.00000676	0.00016549	0.00032810	0.00005933	0.00012969	-0.00000969	0.00023738	0.00047064	0.00008511
0.00009488	-0.00000709	0.00017366	0.00034430	0.00006227	-0.00013728	0.00001026	-0.00025128	-0.00049819	-0.00009009
0.00017226	-0.00001287	0.00031531	0.00062514	0.00011305	0.00001941	-0.00000145	0.00003553	0.00007044	0.00001274
0.00003330	-0.00000249	0.00006095	0.00012084	0.00002185	0.00004081	-0.00000305	0.00007469	0.00014809	0.00002678
-0.00016503	0.00001233	-0.00030208	-0.00059890	-0.00010831	0.00011410	-0.00000853	0.00020885	0.00041406	0.00007488
0.00035854	-0.00002679	0.00065629	0.00130115	0.00023531	0.00005703	-0.00000426	0.00010439	0.00020697	0.00003743
0.00035973	-0.00002688	0.00065846	0.00130547	0.00023609	-0.00009597	0.00000717	-0.00017566	-0.00034827	-0.00006298
-0.00048112	0.00003595	-0.00088066	-0.00174599	-0.00031575	0.00043137	-0.00003224	0.00078959	0.00156543	0.00028310
0.00016137	-0.00001206	0.00029538	0.00058562	0.00010591	0.00025422	-0.00001900	0.00046534	0.00092257	0.00016684
-0.00020960	0.00001566	-0.00038365	-0.00076063	-0.00013756	-0.00028893	0.00002159	-0.00052887	-0.00104853	-0.00018962
0.00004280	-0.00000320	0.00007834	0.00015532	0.00002809	0.00008688	-0.00000649	0.00015902	0.00031527	0.00005701
-0.00021404	0.00001599	-0.00039177	-0.00077673	-0.00014047	-0.00015932	0.00001191	-0.00029163	-0.00057818	-0.00010456
-0.00016910	0.00001264	-0.00030952	-0.00061365	-0.00011097	0.00004539	-0.00000339	0.00008308	0.00016472	0.00002979
0.00019265	-0.00001440	0.00035263	0.00069912	0.00012643	0.00006088	-0.00000455	0.00011143	0.00022093	0.00003995
0.00022950	-0.00001715	0.00042009	0.00083287	0.00015062	0.00011968	-0.00000894	0.00021906	0.00043431	0.00007854
-0.00017823	0.00001332	-0.00032623	-0.00064678	-0.00011697	-0.00023233	0.00001736	-0.00042526	-0.00084312	-0.00015247
0.00025195	-0.00001883	0.00046117	0.00091432	0.00016535	-0.00011281	0.00000843	-0.00020649	-0.00040939	-0.00007404
0.00029664	-0.00002217	0.00054298	0.00107652	0.00019468	0.00012448	-0.00000930	0.00022785	0.00045174	0.00008169
0.00008140	-0.00000608	0.00014900	0.00029540	0.00005342	-0.00003163	0.00000236	-0.00005790	-0.00011479	-0.00002076
-0.00024389	0.00001823	-0.00044641	-0.00088506	-0.00016006	-0.00018346	0.00001371	-0.00033580	-0.00066577	-0.00012040
-0.00001663	0.00000124	-0.00003045	-0.00006036	-0.00001092	0.00011346	-0.00000848	0.00020768	0.00041175	0.00007446
-0.00005180	0.00000387	-0.00009482	-0.00018800	-0.00003400	0.00004397	-0.00000329	0.00008048	0.00015955	0.00002885
0.00007676	-0.00000574	0.00014050	0.00027856	0.00005038	-0.00001944	0.00000145	-0.00003557	-0.00007053	-0.00001275
0.00006517	-0.00000487	0.00011928	0.00023649	0.00004277	-0.00003766	0.00002814	-0.00068934	-0.00136668	-0.00024716
0.00010032	-0.00000750	0.00018362	0.00036405	0.00006584	-0.00020642	0.00001543	-0.00037783	-0.00074909	-0.00013547
0.00033426	-0.00002498	0.00061183	0.00121301	0.00021937	-0.00005127	0.00000383	-0.00009384	-0.00018605	-0.00003365
-0.00036778	0.00002748	-0.00067320	-0.00133468	-0.00024137	0.00009138	-0.00000683	0.00016726	0.00033161	0.00005997
-0.00018453	0.00001379	-0.00033776	-0.00066965	-0.00012110	0.00006893	-0.00000515	0.00012616	0.00025013	0.00004523
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0.00050506	-0.00003774	0.00092447	0.00183286	0.00033146	0.00010230	-0.00000764	0.00018725	0.00037125	0.00006714





















0.00011370	0.00005521	-0.00006092	0.00001548	0.00008978	-0.00027710	-0.00010737	0.00004746	0.00091973	0.00050412
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