## Supporting Information to: Theoretical analysis of the solvent effects on the magnetic exchange coupling in bis-nitroxides

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### 1 Structures

The following coordinates are given in Å.

2	211N-WU		
С	0.079268	0.036911	0.083138
С	0.015650	-0.073673	1.443613
С	2.140799	-0.053382	1.025111
Ν	1.435095	0.052982	-0.219448
Η	-0.657761	0.105748	-0.699934
Η	-0.869075	-0.118685	2.063209
С	3.566952	-0.075183	1.179630
С	4.500079	-0.002004	0.198299
Ο	1.946809	0.144367	-1.378797
Ν	1.279972	-0.129119	2.014531
С	8.120635	-0.011647	0.022753
С	7.876943	-0.116125	1.366186
Η	9.016428	0.029748	-0.574329
Η	8.603044	-0.183993	2.164380
Ν	6.518148	-0.129925	1.647482
$\mathbf{C}$	5.904890	-0.034221	0.491758
Ν	6.866425	0.043194	-0.566379
Ο	6.593898	0.142790	-1.802893
Η	3.886761	-0.161178	2.214060
Η	4.224778	0.084786	-0.845483

	2IN-W1a		
С	-0.044955	0.001282	-0.054271
$\mathbf{C}$	-0.122090	0.005572	1.308697
$\mathbf{C}$	2.010174	-0.009680	0.911171
Ν	1.315176	-0.007759	-0.344291
Η	-0.773348	0.002306	-0.848506
Η	-1.011687	0.012384	1.922717
$\mathbf{C}$	3.436145	-0.016021	1.087385
$\mathbf{C}$	4.363388	0.002751	0.094641
Ο	1.832048	-0.014125	-1.504822
Ν	1.138106	-0.000660	1.893155
$\mathbf{C}$	7.969998	0.003934	-0.237900
$\mathbf{C}$	7.799427	0.015483	1.119813
Η	8.833668	-0.001866	-0.881575
Η	8.564850	0.020820	1.882889
Ν	6.457565	0.019292	1.467886
$\mathbf{C}$	5.775747	0.006353	0.341429
Ν	6.688000	-0.000834	-0.762834
Ο	6.354588	-0.009270	-1.987827
Η	3.741744	-0.042673	2.134066
Η	4.073250	0.015065	-0.948931
Ο	4.996376	-0.066896	3.992887
Η	5.625773	-0.066358	3.245667
Η	4.890945	0.868816	4.206099
	2IN-W1b		
С	-0.074614	-0.152465	-0.065872
С	-0.111015	-0.158846	1.300683
С	2.002300	-0.048774	0.840628
Ν	1.272389	-0.082721	-0.395377
Η	-0.825989	-0.188512	-0.837375
Н	-0.982700	-0.205503	1.938588
С	3.428896	0.024165	0.967507
С	4.341464	0.073540	-0.035045
Ο	1.759954	-0.054097	-1.568421
Ν	1.161640	-0.094803	1.849944
С	7.952927	0.261113	-0.292975
С	7.740683	0.246348	1.059089
Η	8.849830	0.308560	-0.886862
Η	8.494020	0.282183	1.832516
Ν	6.389214	0.175814	1.373732
С	5.750442	0.145356	0.228142
Ν	6.687172	0.196489	-0.854451
0	6.382445	0.183158	-2.088291
Η	3.769432	0.039124	1.998740
Η	4.044477	0.060740	-1.076534
0	10.996334	0.423591	0.300142
Η	11.624957	-0.303700	0.387613
Н	11.540088	$1\ 219471$	0.353783

	211N- W 1C		
С	-0.047460	0.115155	-0.185706
С	-0.045304	-0.138281	1.156798
С	2.057878	-0.012560	0.652027
Ν	1.291283	0.209924	-0.542827
Η	-0.821880	0.251647	-0.922442
Η	-0.898600	-0.277599	1.805633
$\mathbf{C}$	3.490728	-0.011336	0.738831
$\mathbf{C}$	4.366485	-0.031822	-0.296692
Ο	1.740500	0.508112	-1.692784
Ν	1.245763	-0.208432	1.664407
$\mathbf{C}$	7.978138	0.050119	-0.647114
$\mathbf{C}$	7.795591	0.004463	0.710369
Η	8.845998	0.089614	-1.284192
Η	8.557676	-0.006039	1.477245
Ν	6.452246	-0.032146	1.052071
С	5.784454	-0.016207	-0.076088
Ν	6.702349	0.039057	-1.182430
Ο	6.392260	0.098734	-2.414016
Η	3.864648	-0.012806	1.758582
Η	4.031905	-0.108252	-1.323484
Ο	3.750087	-0.970488	-3.464081
Η	3.101189	-0.256551	-3.416994
Η	4.606097	-0.521804	-3.404672
	2IN-W1d		
$\alpha$	0.004005	0.045032	-0.034877
C	-0.004905	0.040302	0.001011
C C	-0.004905 -0.037231	-0.058680	1.326507
C C C	-0.004905 -0.037231 2.078655	-0.058680 -0.023983	$\begin{array}{c} 0.004011\\ 1.326507\\ 0.859623\end{array}$
C C C N	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\end{array}$	$\begin{array}{c} -0.040332 \\ -0.058680 \\ -0.023983 \\ 0.070810 \end{array}$	1.326507 0.859623 -0.368268
C C C N H	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\end{array}$	$\begin{array}{c} 0.043332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203 \end{array}$	1.326507 0.859623 -0.368268 -0.801875
C C C N H H	-0.004905 -0.037231 2.078655 1.344642 -0.759522 -0.906818	-0.058680 -0.023983 0.070810 0.105203 -0.107565	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\end{array}$
C C C N H H C	-0.004905 -0.037231 2.078655 1.344642 -0.759522 -0.906818 3.508107	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\end{array}$
C C C N H H C C	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\end{array}$	$\begin{array}{c} -0.043332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374 \end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\end{array}$
C C C N H H C C O	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451 \end{array}$	$\begin{array}{c} -0.043332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797 \end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\end{array}$
C C C N H H C C O N	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\end{array}$	$\begin{array}{c} -0.043332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855 \end{array}$	$\begin{array}{c} 1.326507\\ 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\\ 1.868607\end{array}$
C C C N H H C C O N C	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\end{array}$	$\begin{array}{c} 1.326507\\ 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\\ 1.868607\\ -0.296592 \end{array}$
C C C N H H C C O N C C	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\\ 1.868607\\ -0.296592\\ 1.055515\end{array}$
C C C N H H C C O N C C H	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\end{array}$	$\begin{array}{c} -0.04332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325 \end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\\ 1.868607\\ -0.296592\\ 1.055515\\ -0.937075 \end{array}$
C C C N H H C C O N C C H H	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325\\ -0.104271\end{array}$	$\begin{array}{c} 1.326507\\ 0.859623\\ -0.368268\\ -0.801875\\ 1.966756\\ 0.982143\\ -0.022339\\ -1.539558\\ 1.868607\\ -0.296592\\ 1.055515\\ -0.937075\\ 1.833938 \end{array}$
C C C N H H C C O N C C H H N	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\end{array}$	$\begin{array}{c} -0.04332\\ -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325\\ -0.104271\\ -0.066037 \end{array}$	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715
C C C N H H C C O N C C H H N C	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325\\ -0.104271\\ -0.066037\\ 0.018442\end{array}$	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736
C C C N H H C C O N C C H H N C N	$\begin{array}{r} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325\\ -0.104271\\ -0.066037\\ 0.018442\\ 0.097197\end{array}$	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100
C C C N H H C C O N C C H H N C N O	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\\ 6.767179\\ 6.446631\end{array}$	-0.058680 -0.023983 0.070810 0.105203 -0.107565 -0.034535 0.039374 0.161797 -0.100855 0.055096 -0.044892 0.098325 -0.104271 -0.066037 0.018442 0.097197 0.189159	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100 -2.077382
C C C N H H C C O N C C H H N C N O H	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\\ 6.446631\\ 3.852681\end{array}$	$\begin{array}{c} -0.058680\\ -0.023983\\ 0.070810\\ 0.105203\\ -0.107565\\ -0.034535\\ 0.039374\\ 0.161797\\ -0.100855\\ 0.055096\\ -0.044892\\ 0.098325\\ -0.104271\\ -0.066037\\ 0.018442\\ 0.097197\\ 0.189159\\ -0.112056\end{array}$	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100 -2.077382 2.009205
C C C N H H C C O N C C H H N C N O H H	$\begin{array}{c} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\\ 6.446631\\ 3.852681\\ 4.114412\end{array}$	-0.058680 -0.023983 0.070810 0.105203 -0.107565 -0.034535 0.039374 0.161797 -0.100855 0.055096 -0.044892 0.098325 -0.104271 -0.066037 0.018442 0.097197 0.189159 -0.112056 0.116393	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100 -2.077382 2.009205 -1.059086
C C C N H H C C O N C C H H N C N O H H O	$\begin{array}{r} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\\ 6.446631\\ 3.852681\\ 4.114412\\ 9.162473\end{array}$	-0.058680 -0.023983 0.070810 0.105203 -0.107565 -0.034535 0.039374 0.161797 -0.100855 0.055096 -0.044892 0.098325 -0.104271 -0.066037 0.018442 0.097197 0.189159 -0.112056 0.316301	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100 -2.077382 2.009205 -1.059086 -3.202651
C C C N H H C C O N C C H H N C N O H H O H	$\begin{array}{r} -0.004905\\ -0.037231\\ 2.078655\\ 1.344642\\ -0.759522\\ -0.906818\\ 3.508107\\ 4.417396\\ 1.828451\\ 1.241072\\ 8.034882\\ 7.821858\\ 8.903950\\ 8.569845\\ 6.471263\\ 5.827197\\ 6.767179\\ 6.767179\\ 6.446631\\ 3.852681\\ 4.114412\\ 9.162473\\ 9.279801 \end{array}$	-0.058680 -0.023983 0.070810 0.105203 -0.107565 -0.034535 0.039374 0.161797 -0.100855 0.055096 -0.044892 0.098325 -0.104271 -0.066037 0.018442 0.097197 0.189159 -0.112056 0.316301 1.243345	1.326507 0.859623 -0.368268 -0.801875 1.966756 0.982143 -0.022339 -1.539558 1.868607 -0.296592 1.055515 -0.937075 1.833938 1.375715 0.237736 -0.847100 -2.077382 2.009205 -1.059086 -3.202651 -3.445267

	2IN-W2a		
Ν	0.010125	0.037493	0.023989
$\mathbf{C}$	-0.002988	0.030908	1.409397
$\mathbf{C}$	1.315514	-0.017309	1.775142
Ν	2.162180	-0.041424	0.674320
$\mathbf{C}$	1.384612	-0.008712	-0.382197
$\mathbf{C}$	1.727339	-0.013624	-1.775552
$\mathbf{C}$	3.017366	-0.056722	-2.193640
Ċ	3.495379	-0.066637	-3.545758
Ň	2.675641	-0.032010	-4.724963
C	3.534849	-0.056646	-5.814717
Ċ	4.791622	-0.103352	-5.280756
Ň	4.762594	-0.109329	-3.891562
0	1.405617	0.012503	-4.764291
Õ	-0.986228	0.076505	-0.764318
Õ	-0.740597	0.040661	4.441820
H	3.172590	-0.039251	-6.828547
Н	5.723629	-0.133394	-5.825639
Н	-0.914174	0.059870	1.982276
Н	1.705787	-0.036226	2.782424
Н	3.813992	-0.088372	-1.455910
Η	0.902781	0.018865	-2.476956
Н	-0.997692	0.811507	4.962761
Η	-1.052820	-0.713143	4.957550
0	5.065950	-0.131787	-8.537142
Η	5.314225	0.602104	-9.112809
		0.001000	0.000100
Н	5.246585	-0.921289	-9.062189
Н	5.246585 2IN-W2b	-0.921289	-9.062189
H C	5.246585 2IN-W2b 0.524880	-0.921289 0.226441	-9.062189 -0.916810
H C C	5.246585 2IN-W2b 0.524880 0.197259	-0.921289 0.226441 -0.150078	-9.062189 -0.916810 0.356943
H C C C	5.246585 2IN-W2b 0.524880 0.197259 2.361668	-0.921289 0.226441 -0.150078 -0.111812	-9.062189 -0.916810 0.356943 0.384373
H C C C N	5.246585 $2IN-W2b$ $0.524880$ $0.197259$ $2.361668$ $1.911850$	-0.921289 0.226441 -0.150078 -0.111812 0.261170	-9.062189 -0.916810 0.356943 0.384373 -0.930569
H C C N H	$\begin{array}{c} 5.246585\\ 2\mathrm{IN-W2b}\\ 0.524880\\ 0.197259\\ 2.361668\\ 1.911850\\ -0.021114\end{array}$	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936
H C C C N H H	$\begin{array}{c} 5.246585\\ 2\mathrm{IN}\text{-}\mathrm{W2b}\\ 0.524880\\ 0.197259\\ 2.361668\\ 1.911850\\ -0.021114\\ -0.792640\end{array}$	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138
H C C C N H H C	$\begin{array}{c} 5.246585\\ 2\mathrm{IN-W2b}\\ 0.524880\\ 0.197259\\ 2.361668\\ 1.911850\\ -0.021114\\ -0.792640\\ 3.728162\end{array}$	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717
H C C C N H H C C	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123
H C C C N H H C C O	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123 -1.919709
H C C C N H H C C O N	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123 -1.919709 1.147043
H C C C C N H H C C O N C	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123 -1.919709 1.147043 0.607441
H C C C N H H C C O N C C	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123 -1.919709 1.147043 0.607441 1.826921
H C C C N H H C C O N C C H	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353	-9.062189 -0.916810 0.356943 0.384373 -0.930569 -1.816936 0.768138 0.807717 0.065123 -1.919709 1.147043 0.607441 1.826921 0.218987
H C C C N H H C C O N C C H H H	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550	$\begin{array}{c} -0.921289\\ 0.226441\\ -0.150078\\ -0.111812\\ 0.261170\\ 0.476739\\ -0.290228\\ -0.206868\\ 0.030786\\ 0.565791\\ -0.355886\\ -0.054760\\ -0.419189\\ 0.078353\\ -0.667941\end{array}$	$\begin{array}{c} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\end{array}$
H C C C N H H C C O N C C H H N	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\end{array}$
H C C C N H H C C O N C C H H N C	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\end{array}$
H CCCNHHCCONCCHHNCN	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302	$\begin{array}{c} -0.921289\\ 0.226441\\ -0.150078\\ -0.111812\\ 0.261170\\ 0.476739\\ -0.290228\\ -0.206868\\ 0.030786\\ 0.565791\\ -0.355886\\ -0.054760\\ -0.419189\\ 0.078353\\ -0.667941\\ -0.447187\\ -0.102990\\ 0.155575\end{array}$	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\end{array}$
H CCCNHHCCONCCHHNCNO	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389	$\begin{array}{c} -0.921289\\ 0.226441\\ -0.150078\\ -0.111812\\ 0.261170\\ 0.476739\\ -0.290228\\ -0.206868\\ 0.030786\\ 0.565791\\ -0.355886\\ -0.054760\\ -0.419189\\ 0.078353\\ -0.667941\\ -0.447187\\ -0.102990\\ 0.155575\\ 0.509184\end{array}$	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\end{array}$
H CCCNHHCCONCCHHNCNOH	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417	$\begin{array}{c} -0.921289\\ 0.226441\\ -0.150078\\ -0.111812\\ 0.261170\\ 0.476739\\ -0.290228\\ -0.206868\\ 0.030786\\ 0.565791\\ -0.355886\\ -0.054760\\ -0.419189\\ 0.078353\\ -0.667941\\ -0.447187\\ -0.102990\\ 0.155575\\ 0.509184\\ -0.505996\end{array}$	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\end{array}$
H C C C N H H C C O N C C H H N C N O H H	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\end{array}$
H CCCNHHCCONCCHHNCNOHHO	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434 0.463355	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.30786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802 1.027998	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\\ -3.916317\end{array}$
H CCCNHHCCONCCHHNCNOHHOH	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434 0.463355 1.351089 2.246585 1.224858 1.351089	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802 1.027998 1.011898	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\\ -3.916317\\ -3.526669\end{array}$
H CCCNHHCCONCCHHNCNOHHOHH	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434 0.463355 1.351089 0.436455 5.246552 0.436455 0.4	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.30786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802 1.027998 1.011898 0.242468	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\\ -3.916317\\ -3.526669\\ -4.491233\\ -4.9123\\ -4.91232\\ -4.91233\\ -4.91232\\ -4.91232\\ -4.9123\\ -4.9123\\ -4.91232\\ -4.9123\\ -4.9123\\ -4.91232\\ -4.9123\\ -4.9122\\ -4.9123\\ -4.9122\\ -4.9122\\ -4.9122\\ -4.9122\\ -4.9122\\ -4.9122\\ -4.9$
H CCCNHHCCONCCHHNCNOHHOHHO	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434 0.463355 1.351089 0.436455 0.274280	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.30786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802 1.027998 1.011898 0.242468 -0.674364	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\\ -3.916317\\ -3.526669\\ -4.491233\\ -6.188811\\ -0.05141\end{array}$
H CCCNHHCCONCCHHNCNOHHOHHOH	5.246585 2IN-W2b 0.524880 0.197259 2.361668 1.911850 -0.021114 -0.792640 3.728162 4.838284 2.655325 1.322401 8.420991 7.916218 9.417000 8.469550 6.528621 6.156444 7.308302 7.286389 3.836417 4.776434 0.463355 1.351089 0.436455 0.274280 0.503429 2.02440	-0.921289 0.226441 -0.150078 -0.111812 0.261170 0.476739 -0.290228 -0.206868 0.030786 0.565791 -0.355886 -0.054760 -0.419189 0.078353 -0.667941 -0.447187 -0.102990 0.155575 0.509184 -0.505996 0.330802 1.027998 1.011898 0.242468 -0.674364 0.166895 -0.505958	$\begin{array}{r} -9.062189\\ -0.916810\\ 0.356943\\ 0.384373\\ -0.930569\\ -1.816936\\ 0.768138\\ 0.807717\\ 0.065123\\ -1.919709\\ 1.147043\\ 0.607441\\ 1.826921\\ 0.218987\\ 2.721835\\ 1.826775\\ 0.616670\\ -0.193475\\ -1.413167\\ 1.846226\\ -0.973479\\ -3.916317\\ -3.526669\\ -4.491233\\ -6.188811\\ -6.607288\\ \end{array}$

2	21N-W2c		
С	0.120580	-0.070325	0.086718
С	0.177888	0.009757	1.448759
С	2.259259	-0.059349	0.850073
Ν	1.443216	-0.109856	-0.332778
Η	-0.702942	-0.091138	-0.606978
Н	-0.658131	0.059726	2.130706
$\mathbf{C}$	3.693789	-0.083064	0.879613
Č	4.524641	-0.370633	-0.153831
õ	1 849497	-0.117627	-1536991
N	1 489746	0.023543	1 910299
C	8 113927	-0 478140	-0.662917
$\mathbf{C}$	7995249	-0.203527	0.675514
н	8 951368	-0.612059	-1 327206
н	8 703613	-0.012000	1 300384
N	6 670772	-0.059245 0.120642	1.030384 1.073493
C	5.040884	-0.120042	1.073423
U N	0.949004 6 915149	-0.540070	1.196710
	0.010140	-0.374807	-1.120719
	0.440208	-0.791218	-2.324393
п	4.111942	0.143329	1.800219
П	4.144027	-0.672396	-1.120663
U U	3.747260	-2.011/3/	-3.016912
H	3.101469	-1.293646	-3.040325
H	4.604783	-1.565497	-3.072378
0	-2.960768	-0.095663	0.353408
Н	-3.617295	0.602132	0.236039
Н	-3.473225	-0.913477	0.335343
C <sup>1</sup>	2IN-W2d	0.011954	0 076499
U	-0.041000	-0.011604	-0.070400
$\mathbf{C}$	0.026000	0 074091	
C C	-0.036980	0.074831	1.200022
C C	-0.036980 2.068262 1.208108	0.074831 0.027689	0.764675
C C N	-0.036980 2.068262 1.298108	$\begin{array}{c} 0.074831 \\ 0.027689 \\ -0.035983 \\ 0.044024 \end{array}$	0.764675 -0.446995
C C N H	-0.036980 2.068262 1.298108 -0.816615	0.074831 0.027689 -0.035983 -0.044924	$\begin{array}{c} 1.283822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950002\end{array}$
C C N H H	-0.036980 2.068262 1.298108 -0.816615 -0.888016	$\begin{array}{c} 0.074831 \\ 0.027689 \\ -0.035983 \\ -0.044924 \\ 0.117734 \\ 0.017122 \end{array}$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.052000\end{array}$
C C N H C	-0.036980 2.068262 1.298108 -0.816615 -0.888016 3.502813	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.852092\\ \end{array}$
C C N H C C	-0.036980 2.068262 1.298108 -0.816615 -0.888016 3.502813 4.350950	$\begin{array}{c} 0.074831\\ 0.027689\\ -0.035983\\ -0.044924\\ 0.117734\\ 0.017122\\ -0.299549\\ -0.04554\\ -0.04554\\ -0.017122\\ -0.00054\\ -0.00054\\ -0.00054\\ -0.00054\\ -0.0005\\ -0.00$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ 1.950803\\ 0.852092\\ \end{array}$
C C N H C C O	-0.036980 2.068262 1.298108 -0.816615 -0.888016 3.502813 4.350950 1.741974	$\begin{array}{c} 0.074831\\ 0.027689\\ -0.035983\\ -0.044924\\ 0.117734\\ 0.017122\\ -0.299549\\ -0.034258\\ 0.102024\end{array}$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.502540\end{array}$
C C N H H C C O N	$\begin{array}{c} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ \end{array}$	$\begin{array}{c} 0.074831\\ 0.027689\\ -0.035983\\ -0.044924\\ 0.117734\\ 0.017122\\ -0.299549\\ -0.034258\\ 0.106934\\ -0.05556\end{array}$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ \end{array}$
C C N H H C C O N C	$\begin{array}{c} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\end{array}$	$\begin{array}{c} 0.074831\\ 0.027689\\ -0.035983\\ -0.044924\\ 0.117734\\ 0.017122\\ -0.299549\\ -0.034258\\ 0.106934\\ -0.485596\end{array}$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\end{array}$
C C N H H C C O N C C	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452 \end{array}$	$\begin{array}{c} 0.074831\\ 0.027689\\ -0.035983\\ -0.044924\\ 0.117734\\ 0.017122\\ -0.299549\\ -0.034258\\ 0.106934\\ -0.485596\\ -0.112070\\ -0.01100\\ -0.01100\\ -0.0100\\ -0.0100\\ -0.00$	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ \end{array}$
C C N H H C C O N C C H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\end{array}$
C C N H H C C O N C C H H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272	$\begin{array}{c} 1.283822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912 \end{array}$
C C N H H C C O N C C H H N	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976	$\begin{array}{c} 1.283822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988 \end{array}$
C C N H H C C O N C C H H N C	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\end{array}$
C C N H H C C O N C C H H N C N	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699	$\begin{array}{c} 1.283822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\end{array}$
C C N H H C C O N C C H H N C N O	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.895125	$\begin{array}{c} 1.283822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\\ -2.313393\end{array}$
C C N H H C C O N C C H H N C N O H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.895125 0.267962	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\\ -2.313393\\ 1.843517\end{array}$
C C N H H C C O N C C H H N C N O H H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.274818 -0.595699 -0.895125 0.267962 -0.636580	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\\ -2.313393\\ 1.843517\\ -1.120582\end{array}$
C C N H H C C O N C C H H N C N O H H O	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\\ 3.514386\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.895125 0.267962 -0.636580 -2.164716	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\\ -2.313393\\ 1.843517\\ -1.120582\\ -2.852145\end{array}$
C C N H H C C O N C C H H N C N O H H O H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\\ 3.514386\\ 2.906016\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.895125 0.267962 -0.636580 -2.164716 -1.437856	$\begin{array}{c} 1.263822\\ 0.764675\\ -0.446995\\ -0.824498\\ 1.950803\\ 0.852092\\ -0.162088\\ -1.637039\\ 1.792759\\ -0.717662\\ 0.598264\\ -1.388140\\ 1.283912\\ 1.013988\\ -0.021965\\ -1.143393\\ -2.313393\\ 1.843517\\ -1.120582\\ -2.852145\\ -3.038076\end{array}$
C C N H H C C O N C C H H N C N O H H O H H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\\ 3.514386\\ 2.906016\\ 4.393020\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.274818 -0.595699 -0.895125 0.267962 -0.636580 -2.164716 -1.437856 -1.775122	1.263822 0.764675 -0.446995 -0.824498 1.950803 0.852092 -0.162088 -1.637039 1.792759 -0.717662 0.598264 -1.388140 1.283912 1.013988 -0.021965 -1.143393 -2.313393 1.843517 -1.120582 -2.852145 -3.038076 -2.968094
C C N H H C C O N C C H H N C N O H H O H H O	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\\ 3.514386\\ 2.906016\\ 4.393020\\ 5.259901\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.274818 -0.595699 -0.895125 0.267962 -0.636580 -2.164716 -1.437856 -1.775122 0.754498	1.263822 0.764675 -0.446995 -0.824498 1.950803 0.852092 -0.162088 -1.637039 1.792759 -0.717662 0.598264 -1.388140 1.283912 1.013988 -0.021965 -1.143393 -2.313393 1.843517 -1.120582 -2.852145 -3.038076 -2.968094 3.538938
C C N H H C C O N C C H H N C N O H H O H H O H	$\begin{array}{r} -0.036980\\ 2.068262\\ 1.298108\\ -0.816615\\ -0.888016\\ 3.502813\\ 4.350950\\ 1.741974\\ 1.256483\\ 7.928058\\ 7.847452\\ 8.748031\\ 8.662699\\ 6.533855\\ 5.776175\\ 6.618517\\ 6.222279\\ 3.882477\\ 3.977332\\ 3.514386\\ 2.906016\\ 4.393020\\ 5.259901\\ 5.221896\end{array}$	0.074831 0.027689 -0.035983 -0.044924 0.117734 0.017122 -0.299549 -0.034258 0.106934 -0.485596 -0.112070 -0.681444 0.071272 0.019976 -0.274818 -0.595699 -0.274818 -0.595699 -0.895125 0.267962 -0.636580 -2.164716 -1.437856 -1.775122 0.754498 1.716683	1.263822 0.764675 -0.446995 -0.824498 1.950803 0.852092 -0.162088 -1.637039 1.792759 -0.717662 0.598264 -1.388140 1.283912 1.013988 -0.021965 -1.143393 -2.313393 1.843517 -1.120582 -2.852145 -3.038076 -2.968094 3.538938 3.468975

2	21N-W2e		
С	3.814949	-0.026284	-0.468911
С	3.987642	-1.250571	0.109215
С	1.837811	-1.060349	-0.073319
Ν	2.442662	0.122102	-0.612655
Η	4.486958	0.747524	-0.801200
Н	4.916710	-1.730505	0.382345
С	0.428209	-1.314560	0.008016
С	-0.550004	-0.390977	-0.162140
Ο	1.853310	1.093900	-1.176091
Ν	2.771092	-1.884484	0.338096
С	-4.161017	-0.251086	-0.048729
С	-3.894361	-1.581337	0.174804
Η	-5.067988	0.326351	-0.115732
Н	-4.610884	-2.374004	0.341328
Ν	-2.537448	-1.849436	0.170447
С	-1.940071	-0.702074	-0.051208
N	-2.925880	0.342048	-0.196098
0	-2.685310	1.571623	-0.423726
Н	0.173351	-2.337570	0.268009
Н	-0.299336	0.639802	-0.357621
0	-0.132543	3.092337	0.061326
H	0.420634	2.851591	-0.694958
Н	-0.997752	2.693088	-0.128495
0	1.425515	1.487916	1.819636
Н	1.027702	1.438891	2.696582
Н	0.870901	2.130433	1.335697
4	2IN-W2f		
С	0.040761	-0.000142	-0.062334
С	0.021000	-0.034612	1.310371
$\mathbf{C}$	2.129889	-0.016335	0.846093
Ν	1.382068	0.011472	-0.390639
Η	-0.739741	0.012957	-0.821332
H H	-0.739741 -0.850444	0.012957 -0.055097	-0.821332 1.949981
H H C	-0.739741 -0.850444 3.557144	0.012957 -0.055097 -0.014549	$\begin{array}{c} -0.821332 \\ 1.949981 \\ 0.962494 \end{array}$
Н Н С С	$\begin{array}{c} -0.739741 \\ -0.850444 \\ 3.557144 \\ 4.468352 \end{array}$	0.012957 -0.055097 -0.014549 0.013160	-0.821332 1.949981 0.962494 -0.043038
H H C C O	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\end{array}$	$\begin{array}{c} 0.012957 \\ -0.055097 \\ -0.014549 \\ 0.013160 \\ 0.038874 \end{array}$	-0.821332 1.949981 0.962494 -0.043038 -1.557961
H H C O N	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\end{array}$	$\begin{array}{c} 0.012957\\ -0.055097\\ -0.014549\\ 0.013160\\ 0.038874\\ -0.043391 \end{array}$	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698
H C C O N C	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\end{array}$	$\begin{array}{c} 0.012957 \\ -0.055097 \\ -0.014549 \\ 0.013160 \\ 0.038874 \\ -0.043391 \\ 0.026399 \end{array}$	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335
H H C C O N C C	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993 \end{array}$	$\begin{array}{c} 0.012957 \\ -0.055097 \\ -0.014549 \\ 0.013160 \\ 0.038874 \\ -0.043391 \\ 0.026399 \\ -0.002057 \end{array}$	$\begin{array}{c} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\end{array}$
H C C O N C C H	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\end{array}$	$\begin{array}{c} 0.012957\\ -0.055097\\ -0.014549\\ 0.013160\\ 0.038874\\ -0.043391\\ 0.026399\\ -0.002057\\ 0.041271 \end{array}$	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123
H H C C O N C C H H	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607
H H C C O N C C H H N	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$	$\begin{array}{c} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\\ -0.928123\\ 1.828607\\ 1.360658\end{array}$
H H C C O N C C H H N C	$\begin{array}{c} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700	$\begin{array}{c} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\\ -0.928123\\ 1.828607\\ 1.360658\\ 0.217158\end{array}$
H H C C O N C C H H N C N	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957	$\begin{array}{r} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\\ -0.928123\\ 1.828607\\ 1.360658\\ 0.217158\\ -0.866190\end{array}$
H H C C O N C C H H N C N O N C O N C C H H O N C O N O N	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396	$\begin{array}{r} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\\ -0.928123\\ 1.828607\\ 1.360658\\ 0.217158\\ -0.866190\\ -2.099704 \end{array}$
H H C C O N C C H H N C N O H	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$	$\begin{array}{c} -0.821332\\ 1.949981\\ 0.962494\\ -0.043038\\ -1.557961\\ 1.857698\\ -0.306335\\ 1.045595\\ -0.928123\\ 1.828607\\ 1.360658\\ 0.217158\\ -0.866190\\ -2.099704\\ 1.992116\end{array}$
H H C C O N C C H H N C N O H H	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186
H H C C O N C C H H N C N O H H O	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\\ 0.197348\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508 0.069399	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186 -3.880907
H H C C O N C C H H N C N O H H O H	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\\ 0.197348\\ 0.816518\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508 0.069399 0.110951	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186 -3.880907 -3.127573
H H C C O N C C H H N C N O H H O H H	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\\ 0.197348\\ 0.816518\\ 0.383474\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508 0.069399 0.110951 - $0.779135$	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186 -3.880907 -3.127573 -4.302109
H H C C O N C C H H N C N O H H O H H O	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\\ 0.197348\\ 0.816518\\ 0.383474\\ -2.111023\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508 0.069399 0.110951 - $0.779135$ 0.029073	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186 -3.880907 -3.127573 -4.302109 -2.360781
HHCCONCCHHNCNOHHOHHOH	$\begin{array}{r} -0.739741\\ -0.850444\\ 3.557144\\ 4.468352\\ 1.897669\\ 1.295712\\ 8.083793\\ 7.874993\\ 8.963535\\ 8.620216\\ 6.522132\\ 5.879859\\ 6.813468\\ 6.511027\\ 3.902274\\ 4.168965\\ 0.197348\\ 0.816518\\ 0.383474\\ -2.111023\\ -2.482032\end{array}$	0.012957 - $0.055097$ - $0.014549$ 0.013160 0.038874 - $0.043391$ 0.026399 - $0.002057$ 0.041271 - $0.016409$ - $0.011676$ 0.010700 0.034957 0.058396 - $0.039127$ 0.038508 0.069399 0.110951 - $0.779135$ 0.029073 0.916406	-0.821332 1.949981 0.962494 -0.043038 -1.557961 1.857698 -0.306335 1.045595 -0.928123 1.828607 1.360658 0.217158 -0.866190 -2.099704 1.992116 -1.083186 -3.880907 -3.127573 -4.302109 -2.360781 -2.442708

## 2 Basis set and integration grid sizes

Electronic density integration. Several integration grids are available in ORCA:

- grid0: product grid
- grid1: Lebedev 50 (not recommended)
- grid2: Lebedev 110 points (default for SCF iterations)
- grid3: Lebedev 194 points (more accurate)
- grid4: Lebedev 302 points (default for FinalGrid)
- grid5: Lebedev 434 points (large)
- grid6: Lebedev 590 points (larger)
- grid7: Lebedev 770 points (very large)

Table 1: Effect of the grid s	ize on the mag	netic couplin	ng consta	ant $J$ (in	$\mathrm{cm}^{-1}$	) for various	implicit	solvents.
	2IN model	$Solvent^*$	grid1	grid4	grid7			

ZIN model	Solvent	gnui	griu4	griui
	vacuum	-658	-663	-663
	hexane	-706	-710	-710
W0	acetone	-801	-806	-806
	acetonitrile	-808	-812	-812
	dmso	-810	-814	-814
	water	-812	-817	-817
	vacuum	-685	-687	-687
	hexane	-730	-732	-732
W1a	acetone	-823	-824	-824
	acetonitrile	-829	-830	-831
	dmso	-831	-832	-832
	water	-834	-835	-835
	vacuum	-701	-707	-707
	hexane	-747	-754	-754
W2a	acetone	-835	-841	-841
	acetonitrile	-839	-846	-846
	dmso	-842	-848	-848
	water	-845	-850	-851

 $*\varepsilon(hexane) = 2, \varepsilon(acetone) = 20, \varepsilon(acetonitrile) = 37, \varepsilon(dmso) = 47, \varepsilon(water) = 80.$ 

Enlarging the size of the DFT electronic density integration grid alters very slightly the magnetic exchange value. Using the standard grid4 gives J values in perfect agreement with larger ones.

**Basis set.** The effect of the basis set size (from double- $\zeta$  to triple- $\zeta$  including diffuse and polarization functions) on the J solvent shift has been studied.

2IN model	$\operatorname{Solvent}^*$	6-31G	6-31G(d,p)	6-311G(d,p)	6-311G(2d,2p)	6-311+G(2d,2p)
	vacuum	-567	-663	-608	-623	-643
	hexane	-614	-710	-656	-672	-708
W0	acetone	-706	-806	-754	-772	-852
	acetonitrile	-712	-812	-761	-779	-862
	dmso	-714	-814	-763	-780	-866
	water	-717	-817	-766	-784	-870
	vacuum	-589	-687	-629	-645	-660
	hexane	-634	-732	-674	-691	-721
W1a	acetone	-725	-824	-770	-788	-858
	acetonitrile	-731	-830	-777	-795	-868
	dmso	-733	-832	-779	-797	-871
	water	-736	-835	-782	-800	-876
	vacuum	-610	-707	-651	-665	-690
	hexane	-656	-754	-698	-712	-754
W2a	acetone	-742	-841	-788	-803	-886
	acetonitrile	-748	-846	-793	-809	-894
	dmso	-749	-848	-795	-811	-897
	water	-752	-850	-798	-813	-901

Table 2: Influence of the basis set size on the magnetic coupling constant J (in  $\text{cm}^{-1}$ ) for various implicit solvents

 $\varepsilon(hexane) = 2, \varepsilon(acetone) = 20, \varepsilon(acetonitrile) = 37, \varepsilon(dmso) = 47, \varepsilon(water) = 80.$ 

The J shifts due to the solvent (implicit or explicit) are almost identical whatever the chosen basis set, with the exception of the largest basis set that includes diffuse functions on non-hydrogen atomic centers. Despite the COSMO outlying charge correction, special care must be taken when electrons are free to flow outside the molecular cavity.

#### 3 PBE0 versus B3LYP

The effect of the choice of a DFT functional is checked by comparison of J values obtained with B3LYP and PBE0 functionals. As expected, the absolute values largely depend on the functional. However the solvent contribution is almost independent of the choice of the functional.

$Solvent^*$	$J_{B3LYP}$	$J_{PBE0}$	$\%_{B3LYP}$	$\%_{PBE0}$
Vacuum	-663	-1168	0	0
Hexane	-710	-1236	7	6
Acetone	-806	-1370	21	17
Acetonitrile	-812	-1379	22	18
Dmso	-814	-1382	23	18
Water	-817	-1386	23	19

Table 3: Magnetic coupling constant  $J_{B3LYP}$  and  $J_{PBE0}$  (in cm<sup>-1</sup>); proportions  $\%_{B3LYP}$  and  $\%_{PBE0}$  in implicit solvents.

 $\varepsilon(hexane) = 2, \varepsilon(acetone) = 20, \varepsilon(acetonitrile) = 37, \varepsilon(dmso) = 47, \varepsilon(water) = 80.$ 

## 4 Geometry optimizations

The dependence of the J values with the geometry of 2IN in different solvents is analyzed. As expected from a completely conjugated system, 2IN geometry remains almost the same, justifying our choice to keep the gas phase one.

Table 4: Magnetic coupling constant J (in cm<sup>-1</sup>); overlap  $S_{ab}$  between the magnetic orbitals; square of the singly occupied molecular orbital (SOMO) energy splitting in the triplet state (in  $eV^2$ ) for various implicit solvents with geometry optimizations.

			without optimization			with optimization	
2IN model	$\operatorname{Solvent}^*$	J	$S_{ab}$	$(\varepsilon_1 - \varepsilon_2)^2$	J	$S_{ab}$	$(\varepsilon_1 - \varepsilon_2)^2$
	vacuum	-663	0.2465	1.2010	-664	0.2469	1.2010
	hexane	-710	0.2589	1.2348	-707	0.2582	1.2263
W0	acetone	-806	0.2840	1.2971	-805	0.2839	1.2764
	acetonitrile	-812	0.2857	1.3010	-811	0.2857	1.2794
	dmso	-814	0.2862	1.3021	-813	0.2862	1.2807
	water	-817	0.2871	1.3037	-817	0.2870	1.2823
	vacuum	-687	0.2553	1.2371	-690	0.2561	1.2398
	hexane	-732	0.2668	1.2674	-730	0.2663	1.2604
W1a	acetone	-825	0.2905	1.3240	-819	0.2892	1.3055
	acetonitrile	-831	0.2921	1.3276	-825	0.2908	1.3085
	dmso	-833	0.2926	1.3285	-827	0.2914	1.3096
	water	-836	0.2933	1.3301	-830	0.2921	1.3108
	vacuum	-707	0.2579	1.2448	-710	0.2588	1.2467
	hexane	-754	0.2699	1.2726	-752	0.2696	1.2623
W2a	acetone	-841	0.2927	1.3207	-821	0.2914	1.3057
	acetonitrile	-847	0.2941	1.3234	-842	0.2933	1.3064
	dmso	-848	0.2946	1.3243	-838	0.2937	1.3083
	water	-851	0.2952	1.3255	-845	0.2941	1.3075

 ${}^*\varepsilon(hexane)=2, \varepsilon(acetone)=20, \varepsilon(acetonitrile)=37, \varepsilon(dmso)=47, \varepsilon(water)=80.$ 

## 5 Mulliken spin population analysis

sen spin	population	analysis on	water molec	ules 101 2111-
Atom	W1a	W1b	W1c	W1d
H1	-0.000274	-0.000005	-0.000342	0.000011
Ο	-0.000143	0.000017	0.003251	-0.000504
H2	0.000016	-0.000004	-0.001676	-0.002601

Table 5: Mulliken spin population analysis on water molecules for 2IN-cis-W1 (in  $|\mathbf{e}|$ )

Table 6: Mulliken spin population analysis on water molecules for 2IN-cis-W1 frozen (in |e|)

Atom	W1a*	W1b*	W1c*	W1d*
H1	-0.000284	-0.000006	-0.000780	0.000003
Ο	-0.000063	0.000019	0.002015	-0.000431
H2	0.000006	-0.000005	-0.000463	-0.002281

Table 7: Mülliken spin population analysis for W1 (in |e|).

	W1a		W1b		W1c		W1d	
Atom	Vacuum	Water	Vacuum	Water	Vacuum	Water	Vacuum	Water
0	0.5275	0.4931	0.5467	0.5270	0.5432	0.5261	0.5577	0.5379
N1	0.1731	0.1843	0.1862	0.1980	0.1945	0.2029	0.1862	0.1982
$\mathbf{C}$	0.1471	0.1621	0.0859	0.0907	0.0756	0.0836	0.0680	0.0741
$\mathbf{C}$	-0.1982	-0.2088	0.0387	0.0483	0.0650	0.0679	0.0692	0.0757
$\mathbf{C}$	0.1808	0.1974	0.0427	0.0399	0.0234	0.0250	0.0169	0.0168
$\mathbf{C}$	-0.1668	-0.1794	0.0906	0.1039	0.1069	0.1168	0.1137	0.1251
N2	-0.1504	-0.1663	0.1740	0.1889	0.1914	0.2002	0.1988	0.2036
0	-0.5243	-0.4872	0.5597	0.5304	0.5283	0.5067	0.5141	0.4945

Table 8: Mülliken spin population analysis for W2 (in |e|).

	W2a		W2b		W2c		W2d		W2e		W2f
Atom	Vacuum	Water	Vacuum	Water	Vacuum	Water	Vacuum	Water	Vacuum	Water	Vacuum
0	0.5522	0.5263	0.5218	0.5047	0.5397	0.5261	0.5489	0.5316	0.5359	0.5220	0.4801
N1	0.1760	0.1893	0.2092	0.2136	0.1986	0.2029	0.1967	0.2043	0.2059	0.2105	0.2209
$\mathbf{C}$	0.0982	0.1081	0.0857	0.0968	0.0702	0.0836	0.0565	0.0700	0.0598	0.0728	0.1128
$\mathbf{C}$	0.0339	0.0355	0.0414	0.0432	0.0739	0.0679	0.0983	0.0924	0.1023	0.0985	0.0182
$\mathbf{C}$	0.0472	0.0528	0.0426	0.0478	0.0161	0.0250	0.0012	0.0072	-0.0035	0.0024	0.0736
$\mathbf{C}$	0.0813	0.0884	0.0927	0.1004	0.1136	0.1168	0.1276	0.1330	0.1304	0.1375	0.0781
N2	0.1888	0.1993	0.1729	0.1876	0.1912	0.2002	0.1822	0.1925	0.1969	0.2013	0.1743
Ο	0.5459	0.5263	0.5598	0.5344	0.5210	0.5067	0.5173	0.4990	0.4918	0.4795	0.5659

atoms	vacuum	$\cosmo^*$	%	_
$0\mathrm{C}$	-0.091537	-0.096695	6	-
$1\mathrm{C}$	0.196222	0.201226	2	
$2\mathrm{C}$	0.078970	0.086579	10	
3N	0.185286	0.198009	$\overline{7}$	
6C	0.046851	0.052721	12	
$7\mathrm{C}$	0.033402	0.034985	5	
80	0.553630	0.530887	-4	$\varepsilon(water) = 80.$
9N	0.049223	0.050507	2	
10C	-0.094432	-0.10404	10	
11C	0.197670	0.208135	5	
14N	0.036597	0.032751	-10	
15C	0.096033	0.106561	11	
16N	0.171742	0.187785	9	
170	0.560355	0.530701	-5	

Table 9: Mulliken population analysis for 2IN-W0 system ; proportions %.

# 6 Molcas input for computing exchange integrals over molecular orbitals or magnetic orbitals

Note that the correctness of the magnetic orbitals has been checked by visual inspection (using the Grid\_it utility).

```
&Gateway
Coord = W0.xyz
Basis = 6-31G**
Group = nosym
&Seward
&Scf
charge = 0
uhf
zspin = 2
ksdft = b3lyp
> LINK bisnitro.UnaOrb INPORB
&Grid_it
ASCII
Select = 1:1-50
Name = Natural
&Motra
LumOrb
Frozen = 48
Deleted = 190
Print = 10
&Localisation
NOrbitals = 2
NFrozen = 48
> LINK bisnitro.LocOrb INPORB
&Grid_it
ASCII
Select = 1:1-50
Name = Local
&Motra
LumOrb
Frozen = 48
Deleted = 190
Print = 10
```

By default, the Motra module cannot handle UhfOrb files. In order to compute the exchange integral between the two SOMOs, we copy their coefficients from the UhfOrb file to a fake UnaOrb file that can be read by Motra.