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Table S1. Obs. ^{1}H Shifts[a] vs Calc. (B3LYP/6-31G (d)) Shielding tensor (Hiso) and Shifts for Alkanes

Compound	^{1}H	^{1}H obs	Siso	^{1}H calc	obs-calc
methane	–	0.22	31.93	0.17	0.06
ethane	–	0.86	31.22	0.88	-0.02
propane	C2	1.34	30.76	1.34	0.00
	Me	0.90	31.21	0.89	0.01
2,2-dimethylbutane	CH2	1.21	30.78	1.32	-0.11
	Me	0.82	31.23	0.87	-0.05
	t-Bu	0.86	31.21	0.89	-0.03
Cyclopropane	-	0.22	31.97	0.13	0.09
Cyclobutane	-	1.96	30.25	1.85	0.11
Cyclopentane	-	1.51	30.62	1.48	0.03
Cyclohexane	ax	1.19	30.86	1.24	-0.05
	eq	1.68	30.62	1.48	0.20
1,1-dimethylcyclohexane	1ax-Me	0.87	31.18	0.92	-0.05
	1eq-Me	0.87	31.26	0.84	0.03
	2,6ax	1.09	30.85	1.25	-0.16
	2,6eq	1.32	30.75	1.35	-0.03
	3,5ax	1.36	30.58	1.52	-0.16
	3,5eq	1.48	30.74	1.36	0.12
	4ax	1.04	30.95	1.15	-0.11
	4eq	1.65	30.59	1.51	0.14
trans 1,2-dimethylcyhexane	1,2ax (CH)	0.94	30.98	1.12	-0.18
	1,2eq (Me)	0.88	31.26	0.84	0.04
	3,6ax	0.93	31.05	1.05	-0.12
	3,6eq	1.62	30.60	1.50	0.12
	4,5ax	1.21	30.83	1.27	-0.06
	4,5eq	1.65	30.59	1.51	0.14
cis 1,3-dimethylcyclohexane	1,3ax(CH)	1.34	30.67	1.40	-0.06
	1,3eq(Me)	0.86	31.29	0.81	0.05
	2ax	0.54	31.42	0.68	-0.14
	2eq	1.63	30.51	1.59	0.04
	4,6ax	0.76	31.20	0.90	-0.14
	4,6eq	1.63	30.57	1.53	0.10
	5ax	1.25	30.78	1.32	-0.07
	5eq	1.69	30.53	1.57	0.12
trans 1,4-dimethylcyclohexane	1,4ax(CH)	1.26	30.76	1.34	-0.08
	1,4eq(Me)	0.86	31.31	0.79	0.07
	2,3,5,6ax	0.90	31.08	1.02	-0.12
	2,3,5,6eq	1.60	30.52	1.58	0.02
norbornane	1,4(CH)	2.19	30.12	1.98	0.21
	endo H	1.16	30.93	1.17	-0.01
	exo H	1.47	30.64	1.46	0.01
	7a,s	1.18	30.98	1.12	0.06

Table S2. Obs. vs Calc. (B3LYP/6-31G (d) [a]) NMR tensor (Hiso) and ^{1}H Shift[b] for Alkenes

Compound	Nucleus	^{1}H obs	Hiso	^{1}H calc	Obs-calc
Ethylene	–	5.405	26.66	5.44	-0.04
benzene	–	7.341	24.81	7.29	0.05
Propene CH_2=CH.Me	1_{cis}	4.941	27.09	5.01	-0.07
	1_{trans}	5.031	27.25	4.85	0.18
	CH	5.834	26.22	5.88	-0.05
	Me	1.725	30.55	1.55	0.17
trans-2-butene	CH	5.550	26.63	5.47	0.08
	Me	1.578	30.66	1.44	0.14
cis-2-butene	CH	5.368	26.69	5.41	-0.04
	Me	1.541	30.68	1.42	0.12
3,3-dimethyl-1-butene (t-butylethylene)	t-Bu	1.011	31.09	1.01	0.00
	=CH	5.850	26.03	6.07	-0.22
	$=CH_2$ cis	4.912	27.20	4.90	0.01
	$=CH_2$ tr	4.825	27.27	4.83	0.00
cyclohexene	$H_{1,2}$	5.68	26.49	5.61	0.07
	$H_{3,6}$	1.99	30.27	1.83	0.16
	$H_{4,5}$	1.61	30.61	1.49	0.12
cyclopentene	$H_{1,2}$	5.74	26.53	5.57	0.17
	$H_{3,5}$	2.31	30.00	2.10	0.21
	H_4	1.82	30.45	1.65	0.17
butadiene	$H_{1,4tr}$	5.082	26.94	5.16	-0.08
	$H_{1,4cis}$	5.194	27.00	5.10	0.09
	$H_{2,3}$	6.326	25.67	6.43	-0.10
cyclopentadiene	CH_2	2.797	29.32	2.78	0.02
	$H_{2,5}$	6.283	25.80	6.30	-0.02
	$H_{3,4}$	6.427	25.66	6.44	-0.01
Tetramethyl cyclopentadiene	CH_2	2.693	29.59	2.51	0.18
	$Me_{2,5}$	1.879	30.27	1.83	0.05
	$Me_{3,4}$	1.767	30.37	1.78	-0.01
1,3-cyclohexadiene	$H_{1,4}$	5.894	26.73	5.37	0.52
	$H_{2,3}$	5.798	26.43	5.67	0.33
	$H_{5,6}$	2.151	29.65	2.45	0.30
1,4-cyclohexadiene	$H_{1,2,4,5}$	5.70	26.58	5.52	0.18
	$H_{3,6}$	2.67	29.69	2.41	0.26
3-Me-1,2-butadiene Me_2.C=C=CH_2	Me	1.682	30.44	1.66	0.02
	CH_2	4.515	27.78	4.32	0.20

a) Use 6-31G(d) except for conj. C=C (inc Ar) use 6-31+G (d),
b) Hshif=32.10-Hiso (H sat and HC=),

Table S3. Obs. vs Calc. (B3LYP/6-31G (d)) NMR tensor (Hiso) and ^{1}H Shift[a] for Aromatics

Compound	Atom	^{1}H obs	Hiso	^{1}H calc	Obs-calc	Hiso +	^{1}H calc(+)	Obs-calc
Ethylene	–	5.405	26.66	5.44	-0.04	26.51	5.59	-0.19
benzene	–	7.341	24.99	7.11	0.23	24.81	7.29	0.05
Toluene	H_o	7.180	25.12	6.98	0.20	25.05	7.05	0.13
	H_m	7.260	25.06	7.04	0.24	24.90	7.20	0.06
	H_p	7.165	25.22	6.88	0.28	25.03	7.07	0.10
	Me	2.343	29.96	2.14	0.20	29.74	2.36	-0.02
Fluorobenzene	H_o	7.05	25.50	6.60	0.45	25.21	6.89	0.16
	H_m	7.32	24.91	7.19	0.13	24.78	7.32	0.00
	H_p	7.11	25.22	6.88	0.23	25.11	6.99	0.12
chlorobenzene	H_o	7.34	25.16	6.94	0.40	24.92	7.18	0.16
	H_m	7.30	25.01	7.09	0.21	24.85	7.25	0.05
	H_p	7.24	25.17	6.93	0.31	25.01	7.09	0.15
bromobenzene	H_o	7.50	25.05	7.05	0.45	24.72	7.38	0.12
	H_m	7.24	25.02	7.08	0.16	24.87	7.23	0.01
	H_p	7.30	25.15	6.95	0.35	24.97	7.13	0.17
phenol	H_o	6.824	25.83	6.27	0.55	25.54	6.56	0.26
	H_m	7.239	25.07	7.03	0.21	24.92	7.18	0.06
	H_p	6.927	25.51	6.59	0.34	25.42	6.68	0.25
anisole	H_o	6.897	25.66	6.44	0.46	25.42	6.68	0.22
	H_m	7.277	25.02	7.08	0.20	24.84	7.26	0.02
	H_p	6.934	25.45	6.65	0.28	25.30	6.80	0.13
	OMe	3.789	28.60	3.50	0.29	28.43	3.67	0.12
aniline	H_o	6.635	25.98	6.12	0.52	25.62	6.48	0.16
	H_m	7.127	25.20	6.90	0.23	25.02	7.08	0.05
	H_p	6.733	25.72	6.38	0.35	25.59	6.61	0.12
N,N-dimethylaniline	H_o	6.730	25.86	6.24	0.49	25.67	6.43	0.29
	H_m	7.231	25.10	7.00	0.23	24.85	7.25	-0.03
	H_p	6.713	25.69	6.41	0.30	25.48	6.62	0.09
	NMe_2	2.926	29.40	2.70	0.23	29.27	2.83	0.07
acetophenone	H_o	7.950	24.21	7.89	0.06	24.00	8.10	-0.15
	H_m	7.445	24.85	7.25	0.19	24.75	7.35	0.10
	H_p	7.551	24.84	7.26	0.29	24.61	7.49	0.06
	CO.Me	2.591	29.87	2.23	0.36	29.71	2.39	0.20
Methyl benzoate	H_o	8.033	24.11	7.99	0.04	23.90	8.20	-0.17
	H_m	7.415	24.90	7.20	0.22	24.70	7.40	0.02
	H_p	7.534	24.86	7.24	0.29	24.60	7.50	0.03
	OMe	3.898	28.45	3.65	0.25	28.33	3.80	0.10

a) Hshif=32.10-Hiso (H sat and HC=) b) Hiso + = 6-31$^+$G(d).