

SUPPLEMENTARY MATERIAL TO
Calculations of optical rotation: Influence of molecular structure

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TABLE SI. Comparison of $[\alpha]_D$ ($\text{dm}^{-1} \text{g}^{-1} \text{cm}^3$) obtained using HF and DFT with different basis sets

Compd.	Configuration	Method	$[\alpha]_{\text{cal}}$	Expt.
1	S	HF/6-311++G(3df,2pd)	1.49	-19
		HF/aug-cc-pVDZ	-0.80	
		DFT/B3LYP/6-31G(d)	2.77	
		DFT/B3PW91/6-311++G(3df,2pd)	-1.62	
2	S	HF/6-311+G(d)	-42.45	-46.5
		HF/aug-cc-pVDZ	-43.12	
		DFT/B3LYP/6-311++G(3df,2pd)	-114.33	
		DFT/B3PW91/6-311++G(3df,2pd)	-112.33	
3	S	HF/6-311++G(3df,2pd)	17.61	22.75
		HF/aug-cc-pVDZ	14.56	
		DFT/B3LYP/6-311++G(3df,2pd)	20.48	
		DFT/B3PW91/6-311++G(3df,2pd)	23.67	
4	R	HF/6-31G(d)	43.40	44
		HF/aug-cc-pVDZ	42.13	
		DFT/B3LYP/6-31G(d)	49.90	
		DFT/B3PW91/6-31G(d)	54.71	
5	S	HF/6-31G(d)	-74.57	-72.7
		HF/cc-pVDZ	-79.09	
		DFT/B3LYP/6-31G(d)	-109.88	
		DFT/B3PW91/6-31G(d)	-111.71	

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TABLE SI. Continued

Compd.	Conf.	Method	$[\alpha]_{\text{cal}}$	Expt.
6	<i>S</i>	HF/6-311++G(3df,2pd)	-60.82	-115
		HF/cc-pVTZ	-79.11	
		DFT/B3LYP/6-311+G(d)	-106.84	
		DFT/B3PW91/6-311++G(3df,2pd)	-107.50	
7	<i>S</i>	HF/6-31G(d)	10.30	-118
		HF/cc-pVDZ	19.91	
		DFT/B3LYP/6-31G(d)	-38.95	
		DFT/B3PW91/6-31G(d)	-31.04	
8	<i>R</i>	HF/6-311++G(3df,2pd)	-87.98	35.9
		HF/cc-pVDZ	-85.56	
		DFT/B3LYP/6-311++G(3df,2pd)	-106.34	
		DFT/B3PW91/6-311++G(3df,2pd)	-109.52	
9	<i>S</i>	HF/6-311++G(3df,2pd)	6.02	-20
		HF/aug-cc-pVDZ	3.70	
		DFT/B3LYP/6-311+G(d)	-18.03	
		DFT/B3PW91/6-311+G(d)	-1.16	
10	<i>S</i>	HF/6-31G(d)	-45.94	-21
		HF/cc-pVDZ	-49.62	
		DFT/B3LYP/6-311++G(3df,2pd)	-86.06	
		DFT/B3PW91/6-31G(d)	-73.19	
11	<i>S</i>	HF/6-31G(d)	23.06	-90.1
		HF/cc-pVDZ	40.22	
		DFT/B3LYP/6-31G(d)	28.37	
		DFT/B3PW91/6-31G(d)	28.32	
12	<i>S</i>	HF/6-31G(d)	-24.00	-6.5
		HF/cc-pVDZ	-23.87	
		DFT/B3LYP/6-31G(d)	-49.64	
		DFT/B3PW91/6-31G(d)	-45.23	

TABLE SI. Continued

Compd.	Conf.	Method	$[\alpha]_{\text{cal}}$	Expt.
13	<i>S</i>	HF/6-311++G(3df,2pd)	-47.52	-40.1
		HF/cc-pVTZ	-38.07	
		DFT/B3LYP/6-31G(d)	-100.51	
		DFT/B3PW91/6-31G(d)	-95.25	
14	<i>S</i>	HF/6-31G(d)	14.28	11.69
		HF/cc-pVTZ	11.06	
		DFT/B3LYP/6-31G(d)	11.52	
		DFT/B3PW91/6-31G(d)	13.56	
15	<i>S</i>	HF/6-31G(d)	-14.21	-6.5
		HF/cc-pVTZ	-3.93	
		DFT/B3LYP	-14.53	
		DFT/B3PW91/6-31G(d)	-15.34	
16	<i>R</i>	HF/6-31G(d)	-8.71	-13.5
		HF/cc-pVDZ	6.14	
		DFT/B3LYP/6-31G(d)	-8.55	
		DFT/B3PW91/6-31G(d)	-5.35	
17	<i>S</i>	HF/6-311+G(d)	-10.21	20.5
		HF/cc-pVTZ	-10.21	
		DFT/B3LYP/6-311+G(d)	-14.00	
		DFT/B3PW91/6-311+G(d)	-16.06	
18	<i>S</i>	HF/6-311++G(3df,2pd)	-13.45	3
		HF/cc-pVDZ	-2.51	
		DFT/B3LYP/6-311++G(3df,2pd)	0.27	
		DFT/B3PW91/6-311++G(3df,2pd)	0.34	
19	<i>S</i>	HF/6-311+G(d)	46.94	2.3
		HF/cc-pVTZ	58.03	
		DFT/B3LYP/6-311+G(d)	54.82	
		DFT/B3PW91/6-311+G(d)	55.75	

TABLE SI. Continued

Compd.	Conf.	Method	$[\alpha]_{\text{cal}}$	Expt.
20	<i>S</i>	HF/6-31G(d)	61.85	12.15
		HF/cc-pVDZ	51.74	
		DFT/B3LYP/6-31G(d)	87.43	
		DFT/B3PW91/6-31G(d)	86.28	
21	<i>S</i>	HF/6-31G(d)	-19.43	-3.8
		HF/cc-pVDZ	-26.99	
		DFT/B3LYP/6-31G(d)	-10.39	
		DFT/B3PW91/6-31G(d)	-14.51	
22	<i>R</i>	HF/6-31G(d)	17.14	31.2
		HF/cc-pVTZ	-421.52	
		DFT/B3LYP/6-31G(d)	32.06	
		DFT/B3PW91/6-31G(d)	30.45	
23	<i>S</i>	HF/6-311++G(3df,2pd)	6.66	11.2
		HF/cc-pVDZ	27.88	
		DFT/B3LYP/6-311+G(d)	12.88	
		DFT/B3PW91/6-311+G(d)	14.05	
24	<i>R</i>	HF/6-311+G(d)	-11.4	-10.8
		HF/cc-pVTZ	-7.7	
		DFT/B3LYP/6-311+G(d)	-2.29	
		DFT/B3PW91/6-311+G(d)	-2.55	
25	<i>S</i>	HF/6-31G(d)	-32.00	-26.7
		HF/cc-pVDZ	-23.13	
		DFT/B3LYP/6-31G(d)	-71.08	
		DFT/B3PW91/6-31G(d)	-69.26	
26	<i>R</i>	HF/6-311++G(3df,2pd)	-1.30	-3.4
		HF/aug-cc-pVDZ	-1.72	
		DFT/B3LYP/6-31G(d)	-0.34	
		DFT/B3PW91/6-31G(d)	-0.51	