

Torsional barriers of substituted biphenyls calculated using density functional theory: a benchmarking study

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Table 1 Activation parameters for the torsional isomerization of biphenyls **1** – **8** calculated at the B97–D/def2–TZVPP level,^a and deviations from experimental data.

	R ¹	R ²	R ³	R ⁴	T ^b	ΔE ^c	ΔH ^d	ΔS ^e	ΔG ^f	ΔG ^{ref,f,g}	ΔΔG ^h	Ref.
1a	ⁱ Pr	CH ₃			–120 ⁱ	7.0	7.0	–3.1	7.5	7.4	0.1	2a
1b	ⁱ Pr	C ₂ H ₅			–95 ⁱ	7.9	7.9	–3.4	8.5	8.7	–0.2	2a
1c	ⁱ Pr	ⁱ Pr			–45 ⁱ	10.4	10.3	–4.3	11.3	11.1	0.2	2a
1d	ⁱ Pr	ⁱ Bu			38 ⁱ	13.9	13.8	–5.1	15.4	15.4	0.0	2a
1e	ⁱ Pr	Cl			–118 ⁱ	7.3	7.1	–3.7	7.7	7.7	0.0	2a
1f	ⁱ Pr	Br			–95 ⁱ	8.3	8.1	–3.7	8.7	8.8	0.0	2a
1g	ⁱ Pr	I			–70 ⁱ	9.6	9.3	–3.9	10.1	9.9	0.2	2a
1h	Si	C≡CH			–150	5.5	5.3	–3.7	5.8	6.0	–0.2	3a
1i	Si	N(CH ₃) ₂			–133	7.5	7.3	–2.5	7.6	6.9	0.7	3b
2a	H	CF ₃	CF ₃	H	64 ⁱ	25.1	24.7	–8.1	27.4	26.2	1.2	8c
2b	H	ⁱ Pr	CF ₃	H	78 ⁱ	24.9	24.6	–7.1	27.1	26.8	0.3	8c
2c	H	ⁱ Pr	ⁱ Pr	H	83 ⁱ	25.4	24.9	–4.6	26.5	27.4	–0.9	8c
2d	H	ⁱ Bu	ⁱ Pr	H	160 ⁱ	30.9	30.4	–5.5	32.8	32.7	0.1	8c
2e	H	OCH ₃	COOH	NO ₂	24	20.3	19.5	–7.2	21.7	21.9	–0.2	7
2f^j	H	N(CH ₃) ₂	N(CH ₃) ₃ ⁺	H	90	27.3	26.8	–4.8	28.6	28.9	–0.3	11a
2g^j	OCH ₃	COO [–]	COO [–]	OCH ₃	90	25.1	24.2	–8.9	27.4	29.8	–2.4	11b
2h	OCH ₃	CONH ₂	CONH ₂	OCH ₃	109	30.6	29.2	–10.1	33.1	32.2	0.2	11c
2i	OCH ₃	COOCH ₃	COOCH ₃	OCH ₃	100	27.7	27.4	–6.6	29.8	30.4	–0.6	11c
3a	ⁱ Pr	OCH ₃	H	H	86	18.2	18.0	–4.3	19.5	19.2	0.3	5a
3b	ⁱ Pr	OCH ₃	OCH ₃	OCH ₃	61	16.9	16.8	–4.4	18.2	17.9	0.3	5a
3c	Br	Br	COOH	COOH	–8 ⁱ	19.3	19.0	–6.0	20.6	19.9	0.7	11d
4a	CH ₃	Br	H		78 ⁱ	18.3	18.1	–5.4	20.0	20.0	0.0	5b
4b	CH ₃	CF ₃	H		134 ⁱ	20.7	20.5	–7.3	23.5	23.3	0.2	5b
4c	CH ₃	Cl	H		62 ⁱ	17.0	16.8	–5.7	18.7	18.7	0.0	5b
4d	CH ₃	Cl	NO ₂		54 ⁱ	16.3	16.1	–5.5	17.9	18.3	–0.4	5b
4e	CH ₃	CN	H		–24 ⁱ	12.1	12.0	–5.0	13.3	14.1	–0.8	5b
4f	CH ₃	COCH ₃	H		2 ⁱ	15.0	14.6	–4.4	15.8	15.5	0.3	5b
4g	CH ₃	F	H		–32 ⁱ	11.2	11.1	–5.0	12.3	12.4	–0.1	5b
4h	CH ₃	F	NO ₂		–45 ⁱ	10.7	10.6	–4.5	11.7	11.6	0.0	5b
4i	CH ₃	I	H		112 ⁱ	19.9	19.6	–5.2	21.6	21.5	0.1	5b
4j	CH ₃	I	H		39 ⁱ	15.9	15.5	–4.2	16.8	16.7	0.1	5b
4k	CH ₃	ⁱ Pr	H		165 ⁱ	21.0	20.7	–5.6	23.1	24.1	–0.9	5b
4l	CH ₃	NH ₂	H		69 ⁱ	17.5	17.3	–6.2	19.4	19.3	0.1	5b
4m	CH ₃	N(CH ₃) ₂	H		46 ⁱ	16.0	15.7	–5.8	17.5	17.1	0.4	5b
4n	CH ₃	NO ₂	H		16 ⁱ	14.6	14.4	–3.3	15.3	16.4	–1.1	5b
4o	CH ₃	OCH ₃	H		–3 ⁱ	13.5	13.4	–4.7	14.7	14.7	0.0	5b
4p	CH ₃	Ph	H		29 ⁱ	15.4	15.2	–4.1	16.4	16.9	–0.4	5b
4q	CH ₃	SH	H		68 ⁱ	18.4	18.2	–5.6	20.1	19.4	0.7	5b
4r	CH ₃	Si(CH ₃) ₃	H		123 ⁱ	19.1	18.9	–5.6	21.1	22.0	–0.9	5b
5a	H				29 ⁱ	23.6	23.0	–6.2	24.9	23.4	1.5	11e
5b	I				90 ⁱ	30.1	29.1	–9.2	32.5	30.2	2.3	11e
6^j					81 ⁱ	22.4	21.5	–9.2	24.8	27.2	–2.4	11f
7a	Cl	H	H	Cl	300	41.7	40.1	–9.6	45.7	44.0	1.7	9b
7b	Cl	Cl	Cl	H	300	43.1	41.5	–9.4	46.9	45.2	1.7	9b
7c	Cl	H	Cl	Cl	300	41.0	39.5	–9.8	45.1	44.0	1.1	9b
8					44	18.0	17.3	–1.9	17.9	16.1	1.9	5c

^a Both structure optimization and vibrational analysis were carried out at this level of theory. ^b in °C; enthalpies and Gibbs energies of activation are calculated at this temperature. ^c Electronic contribution to the torsional barriers [kcal/mol]. ^d Enthalpy of activation at temperature *T* [kcal/mol]. ^e Entropy of activation at temperature *T* [cal/mol·K]. ^f Gibbs energy of activation at temperature *T* [kcal/mol]. ^g Experimental data. ^h Deviation from experimental data [kcal/mol]. ⁱ Mean value of a reported temperature interval. ^j Solvation term added to energy, enthalpy and Gibbs energy of activation.

Table 2 Activation parameters for the torsional isomerization of biphenyls **1** – **8** calculated at the TPSS–D3/def2–TZVPP level,^a and deviations from experimental data.

	R ¹	R ²	R ³	R ⁴	T ^b	ΔE ^c	ΔH ^d	ΔS ^e	ΔG ^f	ΔG ^{ref,f,g}	ΔΔG ^h	Ref.
1a	ⁱ Pr	CH ₃			–120 ⁱ	6.5	6.5	–5.9	7.5	7.4	0.1	2a
1b	ⁱ Pr	C ₂ H ₅			–95 ⁱ	7.3	7.3	–5.6	8.3	8.7	–0.4	2a
1c	ⁱ Pr	ⁱ Pr			–45 ⁱ	9.7	9.6	–8.0	11.4	11.1	0.3	2a
1d	ⁱ Pr	ⁱ Bu			38 ⁱ	13.2	13.0	–10.1	16.2	15.4	0.8	2a
1e	ⁱ Pr	Cl			–118 ⁱ	6.4	6.2	–6.2	7.2	7.7	–0.5	2a
1f	ⁱ Pr	Br			–95 ⁱ	7.4	7.1	–5.6	8.1	8.8	–0.6	2a
1g	ⁱ Pr	I			–70 ⁱ	8.6	8.2	–6.5	9.5	9.9	–0.4	2a
1h	Si	C≡CH			–150	5.2	5.0	–5.0	5.6	6.0	–0.4	3a
1i	Si	N(CH ₃) ₂			–133	7.1	6.6	–10.3	8.0	6.9	1.1	3b
2a	H	CF ₃	CF ₃	H	64 ⁱ	22.3	21.9	–9.0	24.9	26.2	–1.3	8c
2b	H	CF ₃	CF ₃	H	78 ⁱ	23.3	23.0	–10.6	26.7	26.8	–0.1	8c
2c	H	ⁱ Pr	ⁱ Pr	H	83 ⁱ	24.5	24.2	–11.1	28.1	27.4	0.8	8c
2d	H	ⁱ Bu	ⁱ Pr	H	160 ⁱ	29.2	28.8	–9.1	32.7	32.7	0.0	8c
2e	H	OCH ₃	COOH	NO ₂	24	19.3	18.5	–8.0	20.9	21.9	–1.0	7
2f^j	H	N(CH ₃) ₂	N(CH ₃) ₃ ⁺	H	90	26.6	26.0	–4.3	27.5	28.9	–1.4	11a
2g^j	OCH ₃	COO [–]	COO [–]	OCH ₃	90	25.5	24.6	–9.0	27.8	29.8	–2.0	11b
2h	OCH ₃	CONH ₂	CONH ₂	OCH ₃	109	29.3	28.6	–2.3	29.5	32.2	–3.4	11c
2i	OCH ₃	COOCH ₃	COOCH ₃	OCH ₃	100	27.6	27.2	–6.9	29.8	30.4	–0.6	11c
3a	ⁱ Pr	OCH ₃	H	H	86	17.1	16.8	–7.1	19.4	19.2	0.2	5a
3b	ⁱ Pr	OCH ₃	OCH ₃	OCH ₃	61	15.8	15.7	–7.2	18.1	17.9	0.2	5a
3c	Br	Br	COOH	COOH	–8 ⁱ	17.7	17.3	–6.1	18.9	19.9	–1.0	11d
4a	CH ₃	Br	H		78 ⁱ	17.0	16.7	–8.6	19.8	20.0	–0.3	5b
4b	CH ₃	CF ₃	H		134 ⁱ	18.9	18.6	–10.2	22.8	23.3	–0.5	5b
4c	CH ₃	Cl	H		62 ⁱ	15.8	15.5	–8.5	18.4	18.7	–0.3	5b
4d	CH ₃	Cl	NO ₂		54 ⁱ	15.2	14.9	–8.8	17.8	18.3	–0.5	5b
4e	CH ₃	CN	H		–24 ⁱ	11.0	10.9	–7.2	12.7	14.1	–1.3	5b
4f	CH ₃	COCH ₃	H		2 ⁱ	14.5	14.1	–8.2	16.3	15.5	0.8	5b
4g	CH ₃	F	H		–32 ⁱ	10.2	10.1	–7.0	11.8	12.4	–0.6	5b
4h	CH ₃	F	NO ₂		–45 ⁱ	9.8	9.7	–6.4	11.1	11.6	–0.5	5b
4i	CH ₃	I	H		112 ⁱ	18.5	18.1	–8.4	21.3	21.5	–0.2	5b
4j	CH ₃	I	H		39 ⁱ	14.3	13.8	–6.3	15.8	16.7	–0.9	5b
4k	CH ₃	ⁱ Pr	H		165 ⁱ	20.0	19.8	–11.8	25.0	24.1	0.9	5b
4l	CH ₃	NH ₂	H		69 ⁱ	16.6	16.4	–8.7	19.4	19.3	0.1	5b
4m	CH ₃	N(CH ₃) ₂	H		46 ⁱ	15.3	15.0	–8.9	17.8	17.1	0.8	5b
4n	CH ₃	NO ₂	H		16 ⁱ	14.4	14.2	–5.4	15.7	16.4	–0.7	5b
4o	CH ₃	OCH ₃	H		–3 ⁱ	12.4	12.3	–7.2	14.3	14.7	–0.4	5b
4p	CH ₃	Ph	H		29 ⁱ	14.5	14.3	–6.0	16.1	16.9	–0.7	5b
4q	CH ₃	SH	H		68 ⁱ	17.0	16.7	–8.3	19.6	19.4	0.1	5b
4r	CH ₃	Si(CH ₃) ₃	H		123 ⁱ	17.8	17.5	–11.2	21.9	22.0	–0.1	5b
5a	H				29 ⁱ	21.6	20.9	–6.0	22.7	23.4	–0.7	11e
5b	I				90 ⁱ	27.8	26.8	–8.5	29.9	30.2	–0.3	11e
6^j					81 ⁱ	21.6	20.7	–9.3	24.0	27.2	–3.2	11f
7a	Cl	H	H	Cl	300	39.8	38.3	–9.9	44.0	44.0	0.0	9b
7b	Cl	Cl	Cl	H	300	41.1	39.5	–10.0	45.2	45.2	0.1	9b
7c	Cl	H	Cl	Cl	300	39.2	37.6	–10.0	43.4	44.0	–0.6	9b
8					44	17.0	16.4	–2.5	17.2	16.1	1.2	5c

^a Both structure optimization and vibrational analysis were carried out at this level of theory. ^b in °C; enthalpies and Gibbs energies of activation are calculated at this temperature. ^c Electronic contribution to the torsional barriers [kcal/mol]. ^d Enthalpy of activation at temperature *T* [kcal/mol]. ^e Entropy of activation at temperature *T* [cal/mol·K]. ^f Gibbs energy of activation at temperature *T* [kcal/mol]. ^g Experimental data. ^h Deviation from experimental data [kcal/mol]. ⁱ Mean value of a reported temperature interval. ^j Solvation term added to energy, enthalpy and Gibbs energy of activation.

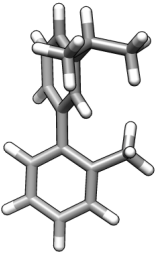
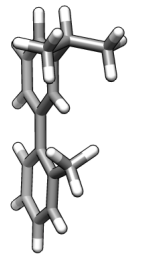
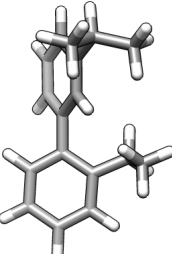
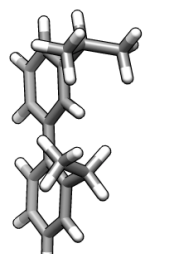
Table 3a Deviations from experimentally determined Gibbs energies of activation, calculated with dispersion-corrected and uncorrected GGAs, meta-GGAs and hybrids.

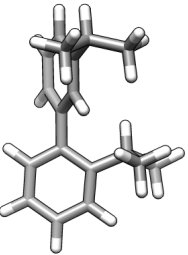
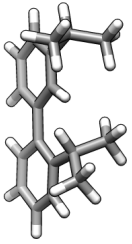
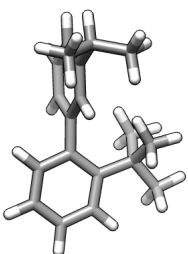
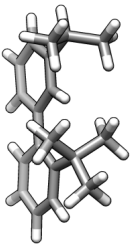
	BP86			TPSS			B3LYP		
		-D	-D3		-D	-D3		-D	-D3
1a	0.1	-0.8	0.6	-0.3	-1.0	0.1	0.9	-0.1	1.3
1c	1.2	-1.3	0.6	1.1	-1.4	0.3	2.1	-0.2	2.0
2a	-1.6	-1.6	-1.0	-2.1	-1.6	-1.3	0.4	0.7	0.8
2d	-1.0	-2.3	1.3	-3.2	-2.4	0.0	1.9	0.5	3.2
2i	1.2	-3.8	-2.3	1.7	-3.4	-0.6	4.9	-1.1	0.7
3b	-0.1	-1.7	0.3	-0.3	-0.9	0.2	1.7	0.1	1.9
4a	-0.7	-1.9	0.3	-1.0	-2.2	-0.3	1.2	0.0	2.0
4b	-0.7	-2.1	0.1	-1.4	-2.6	-0.5	0.8	-0.3	1.4
4e	-1.5	-2.4	-0.8	-1.8	-2.6	-1.3	0.4	-0.8	0.9
4k	0.9	-2.9	1.6	0.3	-3.1	0.9	3.1	-0.9	3.4
4r	0.1	-3.7	0.7	0.4	-4.3	-0.1	2.6	-1.1	3.4
7a	-1.6	-0.4	-0.2	-0.9	0.9	0.0	2.0	3.1	3.1
8	-0.2	1.0	1.7	-0.1	1.0	1.2	1.0	2.1	2.5
MD	-0.31	-2.08	0.10	-0.64	-2.05	-0.21	1.83	0.00	2.00
RMSD	0.30	0.30	0.30	0.40	0.39	0.18	0.38	0.33	0.30

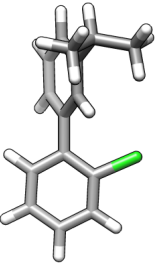
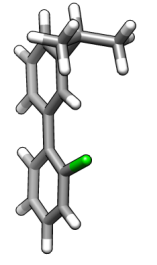
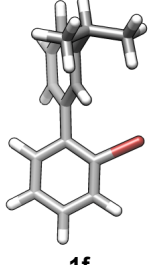
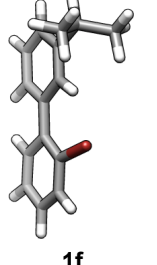
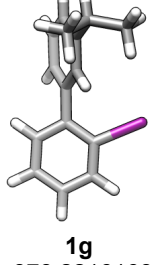
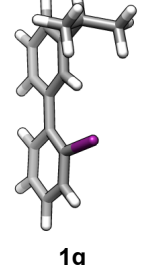
Table 3b Deviations from experimentally determined Gibbs energies of activation, calculated with dispersion-corrected and uncorrected GGAs, hybrids and double hybrids.

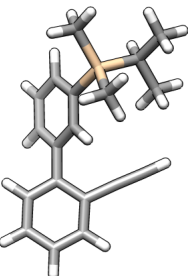
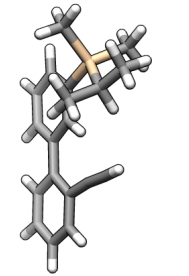
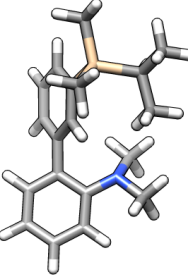
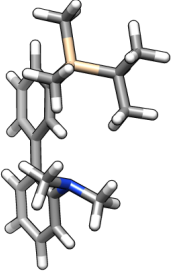
	PBE0		B97		ω B97XD	BMK	M06-2X	B2PLYP		
		-D3		-D	-D3				-D	-D3
1a	0.6	0.8	0.1	1.4	1.8	2.1	1.3	0.7	-0.1	0.9
1c	1.5	1.2	0.2	1.9	2.0	2.8	1.3	1.5	-0.3	1.4
2a	0.0	0.5	1.2	-0.2	1.9	-2.9	0.9	0.0	0.1	0.1
2d	1.3	2.7	0.1	2.2	3.4	0.5	0.8	1.5	0.0	1.9
2i	5.0	0.8	-0.6	-0.4	5.5	2.6	1.8	0.1	-3.6	-2.7
3b	0.8	1.3	0.3	1.4	2.6	0.3	1.8	1.3	-0.1	1.2
4a	0.7	1.2	0.0	1.4	2.8	1.0	2.0	0.7	-0.2	1.2
4b	0.7	1.1	0.2	0.9	2.1	-0.1	2.7	0.3	-0.5	0.7
4e	-0.5	-0.2	-0.8	0.5	1.6	1.0	1.0	0.1	-0.8	0.4
4k	1.9	2.2	-0.9	2.9	3.7	0.3	2.8	2.4	-1.1	2.6
4r	1.1	1.3	-0.9	2.8	2.8	1.3	2.5	1.5	-1.2	2.2
7a	1.9	2.6	1.7	1.0	4.5	0.7	3.3	0.3	1.1	0.9
8	0.9	1.9	1.9	2.4	2.2	1.8	2.6	1.4	2.1	2.4
MD	1.24	1.30	0.04	1.32	2.89	0.79	1.85	0.86	-0.55	0.91
RMSD	0.40	0.25	0.23	0.30	0.35	0.43	0.24	0.21	0.32	0.39

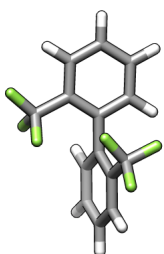
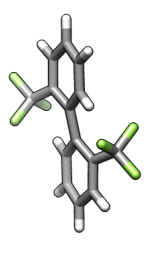
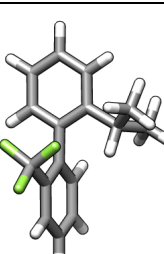
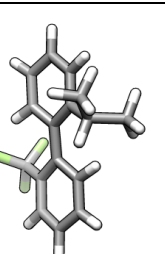
Table 4 Structures and Cartesian coordinates of ground and transition states of biphenyls **1** – **8**, optimized at the B3LYP–D level.^a Energies obtained after optimization with the B3LYP–D hybrid (top value), B97–D GGA (middle value) and TPSS–D3 meta-GGA (bottom value).^b

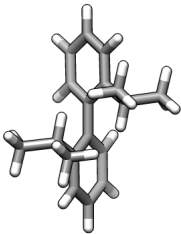
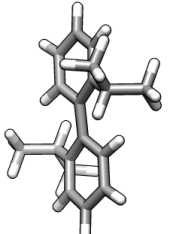
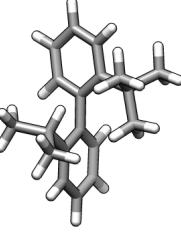
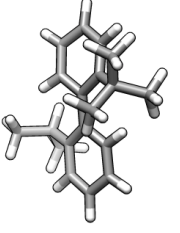
Ground State				Transition State					
 <p>1a -620.4223161 -620.3234761 -620.9195148</p>	H	0.74674	1.20097	-3.68552	 <p>1a -620.4114782 -620.3122976 -620.9092183</p>	H	-0.00305	2.13579	-3.53938
	C	0.67438	1.13866	-2.60631		C	-0.00233	1.74834	-2.52781
	C	0.47763	0.97964	0.18033		C	-0.00066	0.73208	0.13078
	C	0.33384	-0.07568	-2.01390		C	-0.00140	0.37823	-2.30880
	C	0.92028	2.26300	-1.82302		C	-0.00238	2.61089	-1.43659
	C	0.82485	2.18581	-0.44017		C	-0.00157	2.11708	-0.14330
	C	0.24054	-0.13553	-0.62404		C	-0.00055	-0.10156	-0.99727
	H	1.18097	3.20259	-2.29340		H	-0.00311	3.68233	-1.59184
	H	1.00442	3.06193	0.16903		H	-0.00164	2.84308	0.65227
	H	-0.00927	-1.07639	-0.15356		H	0.00017	-1.16592	-0.89196
	C	0.39864	0.89662	1.65925		C	0.00009	0.23180	1.54848
	C	0.37126	0.80672	4.46282		C	0.00121	-0.46990	4.31230
	C	1.45031	1.43180	2.41344		C	-0.00032	1.18733	2.58477
	C	-0.69501	0.31503	2.32946		C	0.00114	-1.13269	1.95355
	C	-0.68436	0.28520	3.72559		C	0.00165	-1.43640	3.32090
	C	1.44697	1.38781	3.80057		C	0.00021	0.86302	3.93046
	H	2.28867	1.87391	1.89077		H	-0.00112	2.23750	2.34730
	H	-1.53378	-0.14756	4.24073		H	0.00241	-2.48037	3.60879
	H	2.27738	1.80127	4.35803		H	-0.00016	1.65319	4.66993
	H	0.34937	0.76622	5.54419		H	0.00161	-0.75474	5.35622
C	0.07239	-1.30846	-2.85281	C	-0.00095	-0.59858	-3.46692		
H	0.18363	-1.02085	-3.90204	H	-0.00306	-0.01097	-4.38926		
C	1.09145	-2.41553	-2.55210	C	1.26017	-1.47274	-3.46363		
H	1.01030	-2.73367	-1.50996	H	1.29600	-2.08502	-2.55922		
H	2.11207	-2.06685	-2.72023	H	2.16356	-0.86077	-3.49319		
H	0.90945	-3.28544	-3.18768	H	1.26281	-2.14341	-4.32618		
C	-1.35696	-1.82841	-2.65024	C	-1.25864	-1.47762	-3.46102		
H	-1.50812	-2.12999	-1.61086	H	-1.29001	-2.09049	-2.55685		
H	-1.54130	-2.69817	-3.28524	H	-1.26065	-2.14793	-4.32386		
H	-2.09333	-1.05875	-2.88919	H	-2.16449	-0.86919	-3.48824		
C	-1.89315	-0.24408	1.60229	C	0.00180	-2.33690	1.03891		
H	-1.73191	-1.28275	1.30049	H	0.88577	-2.36614	0.39794		
H	-2.11090	0.32061	0.69558	H	-0.88252	-2.36754	0.39851		
H	-2.77003	-0.22389	2.25128	H	0.00272	-3.24926	1.63562		
 <p>1b -659.7263740 -659.6236733 -660.2556184</p>	H	1.39722	0.98023	-3.64721	 <p>1b -659.7141359 -659.6110411 -660.2439795</p>	H	-2.21993	3.62125	0.21160
	C	1.22531	0.91293	-2.57963		C	-1.85625	2.60253	0.15385
	C	0.76915	0.74516	0.17667		C	-0.90079	-0.07695	0.00787
	C	0.63645	-0.23482	-2.05328		C	-0.50146	2.35627	-0.01755
	C	1.59086	1.96534	-1.74459		C	-2.73295	1.52755	0.25339
	C	1.36589	1.88412	-0.37674		C	-2.26891	0.22466	0.18290
	C	0.42138	-0.30122	-0.67762		C	-0.05396	1.03616	-0.08606
	H	2.04534	2.85418	-2.16350		H	-3.79269	1.70234	0.38922
	H	1.63620	2.70793	0.27078		H	-3.00616	-0.55542	0.27028
	H	-0.01922	-1.19356	-0.25705		H	1.00028	0.91146	-0.21163
	C	0.54609	0.65540	1.64094		C	-0.43224	-1.50616	-0.06379
	C	0.27415	0.53149	4.43182		C	0.18539	-4.29098	-0.16281
	C	1.61800	0.96151	2.49132		C	-1.41008	-2.51768	0.03300
	C	-0.69047	0.29363	2.20747		C	0.91130	-1.94962	-0.22702
	C	-0.79765	0.24052	3.60018		C	1.17168	-3.32577	-0.26899
	C	1.49392	0.89835	3.87101		C	-1.12747	-3.87176	-0.01154
	H	2.56630	1.23675	2.04802		H	-2.44718	-2.25282	0.14735
	H	-1.75468	-0.02452	4.03473		H	2.20036	-3.64196	-0.39274
	H	2.34142	1.13049	4.50280		H	-1.93452	-4.58814	0.07002
	H	0.15755	0.48046	5.50670		H	0.43862	-5.34231	-0.20224
C	0.23610	-1.39153	-2.94382	C	0.49657	3.49104	-0.12295		
H	0.46894	-1.10915	-3.97438	H	-0.06283	4.42737	-0.04366		
C	1.03288	-2.65831	-2.60471	C	1.51615	3.44585	1.02324		
H	0.82428	-2.97466	-1.57986	H	2.09947	2.52307	0.97812		
H	2.10671	-2.48285	-2.69203	H	1.01824	3.48254	1.99401		
H	0.75593	-3.47538	-3.27523	H	2.20835	4.28829	0.95291		
C	-1.27069	-1.66856	-2.85313	C	1.21731	3.48107	-1.47749		
H	-1.54395	-1.95770	-1.83543	H	1.79838	2.56272	-1.59240		
H	-1.55057	-2.48448	-3.52367	H	1.90470	4.32720	-1.55115		
H	-1.85017	-0.78268	-3.12001	H	0.50535	3.53549	-2.30308		
C	-1.92752	-0.01444	1.39491	C	2.15231	-1.08402	-0.32087		
H	-1.81138	0.34212	0.37280	H	2.02206	-0.27459	-1.03815		
H	-2.76848	0.53286	1.83009	H	2.95837	-1.69794	-0.72706		
C	-2.27700	-1.50916	1.38674	C	2.60701	-1.04991	1.04649		
H	-1.46940	-2.10266	0.95419	H	1.81548	0.01261	1.54192		
H	-3.18491	-1.69245	0.80775	H	3.47890	0.10028	0.94131		
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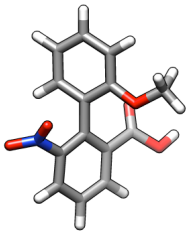
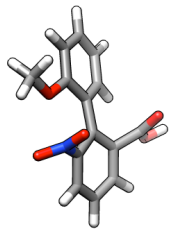
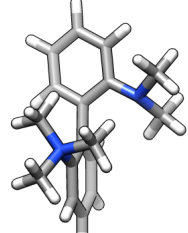
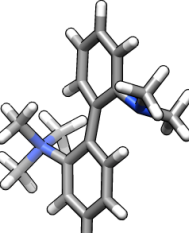
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<tr><td>C</td><td>-0.59242</td><td>0.27857</td><td>2.20554</td></tr> <tr><td>C</td><td>-0.75862</td><td>0.11848</td><td>3.58424</td></tr> <tr><td>C</td><td>1.57578</td><td>0.50759</td><td>3.98577</td></tr> <tr><td>H</td><td>2.75352</td><td>0.86071</td><td>2.23144</td></tr> <tr><td>H</td><td>-1.74965</td><td>-0.08401</td><td>3.96964</td></tr> <tr><td>H</td><td>2.41536</td><td>0.59780</td><td>4.66273</td></tr> <tr><td>H</td><td>0.13774</td><td>0.09231</td><td>5.53283</td></tr> <tr><td>C</td><td>0.44683</td><td>-1.27011</td><td>-2.96921</td></tr> <tr><td>H</td><td>0.76282</td><td>-0.97042</td><td>-3.97237</td></tr> <tr><td>C</td><td>1.09850</td><td>-2.62139</td><td>-2.64750</td></tr> <tr><td>H</td><td>0.80333</td><td>-2.95718</td><td>-1.65054</td></tr> <tr><td>H</td><td>2.18738</td><td>-2.54859</td><td>-2.67083</td></tr> <tr><td>H</td><td>0.78271</td><td>-3.37940</td><td>-3.36828</td></tr> <tr><td>C</td><td>-1.08232</td><td>-1.40133</td><td>-2.96911</td></tr> <tr><td>H</td><td>-1.43808</td><td>-1.70238</td><td>-1.98074</td></tr> <tr><td>H</td><td>-1.40159</td><td>-2.15854</td><td>-3.68913</td></tr> <tr><td>H</td><td>-1.55834</td><td>-0.45287</td><td>-3.22546</td></tr> <tr><td>C</td><td>-1.81844</td><td>0.19596</td><td>1.31206</td></tr> <tr><td>H</td><td>-1.53066</td><td>0.48978</td><td>0.30459</td></tr> <tr><td>C</td><td>-2.92079</td><td>1.16267</td><td>1.76670</td></tr> <tr><td>H</td><td>-3.29581</td><td>0.89729</td><td>2.75738</td></tr> <tr><td>H</td><td>-3.76067</td><td>1.12526</td><td>1.06894</td></tr> <tr><td>H</td><td>-2.54874</td><td>2.18797</td><td>1.80833</td></tr> <tr><td>C</td><td>-2.36273</td><td>-1.23744</td><td>1.24931</td></tr> <tr><td>H</td><td>-1.60391</td><td>-1.93647</td><td>0.89238</td></tr> <tr><td>H</td><td>-3.22534</td><td>-1.28998</td><td>0.58051</td></tr> <tr><td>H</td><td>-2.67915</td><td>-1.56780</td><td>2.24172</td></tr> </tbody> </table>	H	1.85312	1.01117	-3.50455	C	1.61978	0.91598	-2.45085	C	1.00530	0.67827	0.26799	C	0.90415	-0.19451	-2.00734	C	2.03251	1.89582	-1.55208	C	1.72908	1.77969	-0.20163	C	0.61219	-0.29748	-0.64851	H	2.58607	2.75563	-1.90756	H	2.03798	2.54722	0.49596	H	0.06792	-1.15989	-0.28875	C	0.70137	0.53740	1.71400	C	0.30310	0.22441	4.47130	C	1.76332	0.66134	2.62055	C	-0.59242	0.27857	2.20554	C	-0.75862	0.11848	3.58424	C	1.57578	0.50759	3.98577	H	2.75352	0.86071	2.23144	H	-1.74965	-0.08401	3.96964	H	2.41536	0.59780	4.66273	H	0.13774	0.09231	5.53283	C	0.44683	-1.27011	-2.96921	H	0.76282	-0.97042	-3.97237	C	1.09850	-2.62139	-2.64750	H	0.80333	-2.95718	-1.65054	H	2.18738	-2.54859	-2.67083	H	0.78271	-3.37940	-3.36828	C	-1.08232	-1.40133	-2.96911	H	-1.43808	-1.70238	-1.98074	H	-1.40159	-2.15854	-3.68913	H	-1.55834	-0.45287	-3.22546	C	-1.81844	0.19596	1.31206	H	-1.53066	0.48978	0.30459	C	-2.92079	1.16267	1.76670	H	-3.29581	0.89729	2.75738	H	-3.76067	1.12526	1.06894	H	-2.54874	2.18797	1.80833	C	-2.36273	-1.23744	1.24931	H	-1.60391	-1.93647	0.89238	H	-3.22534	-1.28998	0.58051	H	-2.67915	-1.56780	2.24172	 <p>1c -699.0153518 -698.9081020 -699.5767849</p>	<table border="1"> <tbody> <tr><td>H</td><td>-0.05430</td><td>2.09151</td><td>-3.93390</td></tr> <tr><td>C</td><td>-0.03110</td><td>1.81238</td><td>-2.88747</td></tr> <tr><td>C</td><td>0.02614</td><td>1.07726</td><td>-0.12849</td></tr> <tr><td>C</td><td>0.04585</td><td>0.47625</td><td>-2.52393</td></tr> <tr><td>C</td><td>-0.08577</td><td>2.77961</td><td>-1.88997</td></tr> <tr><td>C</td><td>-0.05961</td><td>2.42290</td><td>-0.55238</td></tr> <tr><td>C</td><td>0.07051</td><td>0.13822</td><td>-1.16979</td></tr> <tr><td>H</td><td>-0.15332</td><td>3.82773</td><td>-2.15266</td></tr> <tr><td>H</td><td>-0.11552</td><td>3.23052</td><td>0.15698</td></tr> <tr><td>H</td><td>0.11711</td><td>-0.90905</td><td>-0.96426</td></tr> <tr><td>C</td><td>0.05248</td><td>0.74117</td><td>1.34468</td></tr> <tr><td>C</td><td>0.03733</td><td>0.42919</td><td>4.18049</td></tr> <tr><td>C</td><td>0.03243</td><td>1.82718</td><td>2.24394</td></tr> <tr><td>C</td><td>0.09640</td><td>-0.55953</td><td>1.93556</td></tr> <tr><td>C</td><td>0.07990</td><td>-0.66429</td><td>3.33169</td></tr> <tr><td>C</td><td>0.02257</td><td>1.69547</td><td>3.62126</td></tr> <tr><td>H</td><td>0.02818</td><td>2.83552</td><td>1.86884</td></tr> <tr><td>H</td><td>0.10663</td><td>-1.64528</td><td>3.77972</td></tr> <tr><td>H</td><td>0.00535</td><td>2.58137</td><td>4.24265</td></tr> <tr><td>H</td><td>0.02585</td><td>0.28763</td><td>5.25341</td></tr> <tr><td>C</td><td>0.08903</td><td>-0.62144</td><td>-3.56721</td></tr> <tr><td>H</td><td>0.06954</td><td>-0.14054</td><td>-4.54921</td></tr> <tr><td>C</td><td>1.37981</td><td>-1.44487</td><td>-3.46697</td></tr> <tr><td>H</td><td>1.43319</td><td>-1.95356</td><td>-2.50123</td></tr> <tr><td>H</td><td>2.26170</td><td>-0.80874</td><td>-3.56246</td></tr> <tr><td>H</td><td>1.40971</td><td>-2.20528</td><td>-4.25097</td></tr> <tr><td>C</td><td>-1.13721</td><td>-1.53826</td><td>-3.46046</td></tr> <tr><td>H</td><td>-1.15496</td><td>-2.03875</td><td>-2.48930</td></tr> <tr><td>H</td><td>-1.11010</td><td>-2.30583</td><td>-4.23761</td></tr> <tr><td>H</td><td>-2.06329</td><td>-0.96948</td><td>-3.56286</td></tr> <tr><td>C</td><td>0.12074</td><td>-1.87395</td><td>1.16151</td></tr> <tr><td>H</td><td>0.81592</td><td>-1.75910</td><td>0.33302</td></tr> <tr><td>C</td><td>-1.28325</td><td>-2.20041</td><td>0.62268</td></tr> <tr><td>H</td><td>-1.94239</td><td>-2.43020</td><td>1.46313</td></tr> <tr><td>H</td><td>-1.25193</td><td>-3.07254</td><td>-0.03575</td></tr> <tr><td>H</td><td>-1.71630</td><td>-1.36564</td><td>0.07323</td></tr> <tr><td>C</td><td>0.64612</td><td>-3.08780</td><td>1.93995</td></tr> <tr><td>H</td><td>1.60577</td><td>-2.87741</td><td>2.41502</td></tr> <tr><td>H</td><td>0.77874</td><td>-3.91865</td><td>1.24411</td></tr> <tr><td>H</td><td>-0.05602</td><td>-3.41701</td><td>2.70865</td></tr> </tbody> </table>	H	-0.05430	2.09151	-3.93390	C	-0.03110	1.81238	-2.88747	C	0.02614	1.07726	-0.12849	C	0.04585	0.47625	-2.52393	C	-0.08577	2.77961	-1.88997	C	-0.05961	2.42290	-0.55238	C	0.07051	0.13822	-1.16979	H	-0.15332	3.82773	-2.15266	H	-0.11552	3.23052	0.15698	H	0.11711	-0.90905	-0.96426	C	0.05248	0.74117	1.34468	C	0.03733	0.42919	4.18049	C	0.03243	1.82718	2.24394	C	0.09640	-0.55953	1.93556	C	0.07990	-0.66429	3.33169	C	0.02257	1.69547	3.62126	H	0.02818	2.83552	1.86884	H	0.10663	-1.64528	3.77972	H	0.00535	2.58137	4.24265	H	0.02585	0.28763	5.25341	C	0.08903	-0.62144	-3.56721	H	0.06954	-0.14054	-4.54921	C	1.37981	-1.44487	-3.46697	H	1.43319	-1.95356	-2.50123	H	2.26170	-0.80874	-3.56246	H	1.40971	-2.20528	-4.25097	C	-1.13721	-1.53826	-3.46046	H	-1.15496	-2.03875	-2.48930	H	-1.11010	-2.30583	-4.23761	H	-2.06329	-0.96948	-3.56286	C	0.12074	-1.87395	1.16151	H	0.81592	-1.75910	0.33302	C	-1.28325	-2.20041	0.62268	H	-1.94239	-2.43020	1.46313	H	-1.25193	-3.07254	-0.03575	H	-1.71630	-1.36564	0.07323	C	0.64612	-3.08780	1.93995	H	1.60577	-2.87741	2.41502	H	0.77874	-3.91865	1.24411	H	-0.05602	-3.41701	2.70865																								
H	1.85312	1.01117	-3.50455																																																																																																																																																																																																																																																																																																																																																								
C	1.61978	0.91598	-2.45085																																																																																																																																																																																																																																																																																																																																																								
C	1.00530	0.67827	0.26799																																																																																																																																																																																																																																																																																																																																																								
C	0.90415	-0.19451	-2.00734																																																																																																																																																																																																																																																																																																																																																								
C	2.03251	1.89582	-1.55208																																																																																																																																																																																																																																																																																																																																																								
C	1.72908	1.77969	-0.20163																																																																																																																																																																																																																																																																																																																																																								
C	0.61219	-0.29748	-0.64851																																																																																																																																																																																																																																																																																																																																																								
H	2.58607	2.75563	-1.90756																																																																																																																																																																																																																																																																																																																																																								
H	2.03798	2.54722	0.49596																																																																																																																																																																																																																																																																																																																																																								
H	0.06792	-1.15989	-0.28875																																																																																																																																																																																																																																																																																																																																																								
C	0.70137	0.53740	1.71400																																																																																																																																																																																																																																																																																																																																																								
C	0.30310	0.22441	4.47130																																																																																																																																																																																																																																																																																																																																																								
C	1.76332	0.66134	2.62055																																																																																																																																																																																																																																																																																																																																																								
C	-0.59242	0.27857	2.20554																																																																																																																																																																																																																																																																																																																																																								
C	-0.75862	0.11848	3.58424																																																																																																																																																																																																																																																																																																																																																								
C	1.57578	0.50759	3.98577																																																																																																																																																																																																																																																																																																																																																								
H	2.75352	0.86071	2.23144																																																																																																																																																																																																																																																																																																																																																								
H	-1.74965	-0.08401	3.96964																																																																																																																																																																																																																																																																																																																																																								
H	2.41536	0.59780	4.66273																																																																																																																																																																																																																																																																																																																																																								
H	0.13774	0.09231	5.53283																																																																																																																																																																																																																																																																																																																																																								
C	0.44683	-1.27011	-2.96921																																																																																																																																																																																																																																																																																																																																																								
H	0.76282	-0.97042	-3.97237																																																																																																																																																																																																																																																																																																																																																								
C	1.09850	-2.62139	-2.64750																																																																																																																																																																																																																																																																																																																																																								
H	0.80333	-2.95718	-1.65054																																																																																																																																																																																																																																																																																																																																																								
H	2.18738	-2.54859	-2.67083																																																																																																																																																																																																																																																																																																																																																								
H	0.78271	-3.37940	-3.36828																																																																																																																																																																																																																																																																																																																																																								
C	-1.08232	-1.40133	-2.96911																																																																																																																																																																																																																																																																																																																																																								
H	-1.43808	-1.70238	-1.98074																																																																																																																																																																																																																																																																																																																																																								
H	-1.40159	-2.15854	-3.68913																																																																																																																																																																																																																																																																																																																																																								
H	-1.55834	-0.45287	-3.22546																																																																																																																																																																																																																																																																																																																																																								
C	-1.81844	0.19596	1.31206																																																																																																																																																																																																																																																																																																																																																								
H	-1.53066	0.48978	0.30459																																																																																																																																																																																																																																																																																																																																																								
C	-2.92079	1.16267	1.76670																																																																																																																																																																																																																																																																																																																																																								
H	-3.29581	0.89729	2.75738																																																																																																																																																																																																																																																																																																																																																								
H	-3.76067	1.12526	1.06894																																																																																																																																																																																																																																																																																																																																																								
H	-2.54874	2.18797	1.80833																																																																																																																																																																																																																																																																																																																																																								
C	-2.36273	-1.23744	1.24931																																																																																																																																																																																																																																																																																																																																																								
H	-1.60391	-1.93647	0.89238																																																																																																																																																																																																																																																																																																																																																								
H	-3.22534	-1.28998	0.58051																																																																																																																																																																																																																																																																																																																																																								
H	-2.67915	-1.56780	2.24172																																																																																																																																																																																																																																																																																																																																																								
H	-0.05430	2.09151	-3.93390																																																																																																																																																																																																																																																																																																																																																								
C	-0.03110	1.81238	-2.88747																																																																																																																																																																																																																																																																																																																																																								
C	0.02614	1.07726	-0.12849																																																																																																																																																																																																																																																																																																																																																								
C	0.04585	0.47625	-2.52393																																																																																																																																																																																																																																																																																																																																																								
C	-0.08577	2.77961	-1.88997																																																																																																																																																																																																																																																																																																																																																								
C	-0.05961	2.42290	-0.55238																																																																																																																																																																																																																																																																																																																																																								
C	0.07051	0.13822	-1.16979																																																																																																																																																																																																																																																																																																																																																								
H	-0.15332	3.82773	-2.15266																																																																																																																																																																																																																																																																																																																																																								
H	-0.11552	3.23052	0.15698																																																																																																																																																																																																																																																																																																																																																								
H	0.11711	-0.90905	-0.96426																																																																																																																																																																																																																																																																																																																																																								
C	0.05248	0.74117	1.34468																																																																																																																																																																																																																																																																																																																																																								
C	0.03733	0.42919	4.18049																																																																																																																																																																																																																																																																																																																																																								
C	0.03243	1.82718	2.24394																																																																																																																																																																																																																																																																																																																																																								
C	0.09640	-0.55953	1.93556																																																																																																																																																																																																																																																																																																																																																								
C	0.07990	-0.66429	3.33169																																																																																																																																																																																																																																																																																																																																																								
C	0.02257	1.69547	3.62126																																																																																																																																																																																																																																																																																																																																																								
H	0.02818	2.83552	1.86884																																																																																																																																																																																																																																																																																																																																																								
H	0.10663	-1.64528	3.77972																																																																																																																																																																																																																																																																																																																																																								
H	0.00535	2.58137	4.24265																																																																																																																																																																																																																																																																																																																																																								
H	0.02585	0.28763	5.25341																																																																																																																																																																																																																																																																																																																																																								
C	0.08903	-0.62144	-3.56721																																																																																																																																																																																																																																																																																																																																																								
H	0.06954	-0.14054	-4.54921																																																																																																																																																																																																																																																																																																																																																								
C	1.37981	-1.44487	-3.46697																																																																																																																																																																																																																																																																																																																																																								
H	1.43319	-1.95356	-2.50123																																																																																																																																																																																																																																																																																																																																																								
H	2.26170	-0.80874	-3.56246																																																																																																																																																																																																																																																																																																																																																								
H	1.40971	-2.20528	-4.25097																																																																																																																																																																																																																																																																																																																																																								
C	-1.13721	-1.53826	-3.46046																																																																																																																																																																																																																																																																																																																																																								
H	-1.15496	-2.03875	-2.48930																																																																																																																																																																																																																																																																																																																																																								
H	-1.11010	-2.30583	-4.23761																																																																																																																																																																																																																																																																																																																																																								
H	-2.06329	-0.96948	-3.56286																																																																																																																																																																																																																																																																																																																																																								
C	0.12074	-1.87395	1.16151																																																																																																																																																																																																																																																																																																																																																								
H	0.81592	-1.75910	0.33302																																																																																																																																																																																																																																																																																																																																																								
C	-1.28325	-2.20041	0.62268																																																																																																																																																																																																																																																																																																																																																								
H	-1.94239	-2.43020	1.46313																																																																																																																																																																																																																																																																																																																																																								
H	-1.25193	-3.07254	-0.03575																																																																																																																																																																																																																																																																																																																																																								
H	-1.71630	-1.36564	0.07323																																																																																																																																																																																																																																																																																																																																																								
C	0.64612	-3.08780	1.93995																																																																																																																																																																																																																																																																																																																																																								
H	1.60577	-2.87741	2.41502																																																																																																																																																																																																																																																																																																																																																								
H	0.77874	-3.91865	1.24411																																																																																																																																																																																																																																																																																																																																																								
H	-0.05602	-3.41701	2.70865																																																																																																																																																																																																																																																																																																																																																								
 <p>1d -738.3282311 -738.2173902 -738.9201264</p>	<table border="1"> <tbody> <tr><td>H</td><td>1.82471</td><td>0.65778</td><td>-3.60744</td></tr> <tr><td>C</td><td>1.57840</td><td>0.60207</td><td>-2.55387</td></tr> <tr><td>C</td><td>0.92156</td><td>0.46493</td><td>0.15837</td></tr> <tr><td>C</td><td>1.11379</td><td>-0.59929</td><td>-2.02467</td></tr> <tr><td>C</td><td>1.73500</td><td>1.72060</td><td>-1.73933</td></tr> <tr><td>C</td><td>1.41347</td><td>1.65255</td><td>-0.39014</td></tr> <tr><td>C</td><td>0.80105</td><td>-0.65044</td><td>-0.66517</td></tr> <tr><td>H</td><td>2.10722</td><td>2.64670</td><td>-2.15866</td></tr> <tr><td>H</td><td>1.52727</td><td>2.52167</td><td>0.24428</td></tr> <tr><td>H</td><td>0.45065</td><td>-1.57978</td><td>-0.23606</td></tr> <tr><td>C</td><td>0.64855</td><td>0.36923</td><td>1.62421</td></tr> <tr><td>C</td><td>0.48075</td><td>0.12526</td><td>4.40453</td></tr> <tr><td>C</td><td>1.78634</td><td>0.15035</td><td>2.40924</td></tr> <tr><td>C</td><td>-0.61929</td><td>0.48203</td><td>2.24133</td></tr> <tr><td>C</td><td>-0.65506</td><td>0.35099</td><td>3.63648</td></tr> <tr><td>C</td><td>1.71862</td><td>0.02584</td><td>3.78924</td></tr> <tr><td>H</td><td>2.74385</td><td>0.07360</td><td>1.90982</td></tr> <tr><td>H</td><td>-1.59645</td><td>0.43174</td><td>4.15554</td></tr> <tr><td>H</td><td>2.61721</td><td>-0.14555</td><td>4.36749</td></tr> <tr><td>H</td><td>0.38945</td><td>0.03310</td><td>5.47924</td></tr> <tr><td>C</td><td>0.94239</td><td>-1.82530</td><td>-2.89536</td></tr> <tr><td>H</td><td>1.24605</td><td>-1.55246</td><td>-3.90992</td></tr> <tr><td>C</td><td>1.83725</td><td>-2.97881</td><td>-2.42374</td></tr> <tr><td>H</td><td>1.56184</td><td>-3.28476</td><td>-1.41173</td></tr> <tr><td>H</td><td>2.88787</td><td>-2.68273</td><td>-2.41352</td></tr> <tr><td>H</td><td>1.72379</td><td>-3.84357</td><td>-3.08181</td></tr> <tr><td>C</td><td>-0.52560</td><td>-2.27072</td><td>-2.94006</td></tr> <tr><td>H</td><td>-0.86815</td><td>-2.55226</td><td>-1.94143</td></tr> <tr><td>H</td><td>-0.64303</td><td>-3.13694</td><td>-3.59548</td></tr> <tr><td>H</td><td>-1.16947</td><td>-1.46759</td><td>-3.30356</td></tr> <tr><td>C</td><td>-1.93100</td><td>0.73734</td><td>1.47067</td></tr> <tr><td>C</td><td>-3.12170</td><td>0.96921</td><td>2.41744</td></tr> <tr><td>H</td><td>-3.33801</td><td>0.08708</td><td>3.02300</td></tr> <tr><td>H</td><td>-4.00580</td><td>1.18484</td><td>1.81537</td></tr> <tr><td>H</td><td>-2.94770</td><td>1.81635</td><td>3.08383</td></tr> <tr><td>C</td><td>-2.29354</td><td>-0.47732</td><td>0.59439</td></tr> <tr><td>H</td><td>-1.57531</td><td>-0.62466</td><td>-0.20676</td></tr> <tr><td>H</td><td>-3.27569</td><td>-0.31604</td><td>0.14207</td></tr> <tr><td>H</td><td>-2.33928</td><td>-1.38642</td><td>1.19837</td></tr> <tr><td>C</td><td>-1.82669</td><td>1.99095</td><td>0.58119</td></tr> <tr><td>H</td><td>-1.52775</td><td>2.85888</td><td>1.17334</td></tr> <tr><td>H</td><td>-2.80500</td><td>2.19813</td><td>0.14013</td></tr> <tr><td>H</td><td>-1.11433</td><td>1.86243</td><td>-0.22823</td></tr> </tbody> </table>	H	1.82471	0.65778	-3.60744	C	1.57840	0.60207	-2.55387	C	0.92156	0.46493	0.15837	C	1.11379	-0.59929	-2.02467	C	1.73500	1.72060	-1.73933	C	1.41347	1.65255	-0.39014	C	0.80105	-0.65044	-0.66517	H	2.10722	2.64670	-2.15866	H	1.52727	2.52167	0.24428	H	0.45065	-1.57978	-0.23606	C	0.64855	0.36923	1.62421	C	0.48075	0.12526	4.40453	C	1.78634	0.15035	2.40924	C	-0.61929	0.48203	2.24133	C	-0.65506	0.35099	3.63648	C	1.71862	0.02584	3.78924	H	2.74385	0.07360	1.90982	H	-1.59645	0.43174	4.15554	H	2.61721	-0.14555	4.36749	H	0.38945	0.03310	5.47924	C	0.94239	-1.82530	-2.89536	H	1.24605	-1.55246	-3.90992	C	1.83725	-2.97881	-2.42374	H	1.56184	-3.28476	-1.41173	H	2.88787	-2.68273	-2.41352	H	1.72379	-3.84357	-3.08181	C	-0.52560	-2.27072	-2.94006	H	-0.86815	-2.55226	-1.94143	H	-0.64303	-3.13694	-3.59548	H	-1.16947	-1.46759	-3.30356	C	-1.93100	0.73734	1.47067	C	-3.12170	0.96921	2.41744	H	-3.33801	0.08708	3.02300	H	-4.00580	1.18484	1.81537	H	-2.94770	1.81635	3.08383	C	-2.29354	-0.47732	0.59439	H	-1.57531	-0.62466	-0.20676	H	-3.27569	-0.31604	0.14207	H	-2.33928	-1.38642	1.19837	C	-1.82669	1.99095	0.58119	H	-1.52775	2.85888	1.17334	H	-2.80500	2.19813	0.14013	H	-1.11433	1.86243	-0.22823	 <p>1d -738.3067746 -738.1952291 -738.8991152</p>	<table border="1"> <tbody> <tr><td>H</td><td>2.14217</td><td>0.03088</td><td>-4.01763</td></tr> <tr><td>C</td><td>1.87377</td><td>0.02521</td><td>-2.96825</td></tr> <tr><td>C</td><td>1.16358</td><td>0.01063</td><td>-0.19283</td></tr> <tr><td>C</td><td>0.54103</td><td>0.01519</td><td>-2.58784</td></tr> <tr><td>C</td><td>2.85089</td><td>0.02796</td><td>-1.98013</td></tr> <tr><td>C</td><td>2.50693</td><td>0.02099</td><td>-0.36396</td></tr> <tr><td>C</td><td>0.21812</td><td>0.00809</td><td>-1.22945</td></tr> <tr><td>H</td><td>3.89902</td><td>0.03581</td><td>-2.25095</td></tr> <tr><td>H</td><td>3.33088</td><td>0.02411</td><td>0.05196</td></tr> <tr><td>H</td><td>-0.82713</td><td>0.00049</td><td>-1.02063</td></tr> <tr><td>C</td><td>0.85488</td><td>0.00394</td><td>1.29718</td></tr> <tr><td>C</td><td>0.70274</td><td>-0.00392</td><td>4.15429</td></tr> <tr><td>C</td><td>1.98212</td><td>0.00845</td><td>2.14581</td></tr> <tr><td>C</td><td>-0.42148</td><td>-0.00589</td><td>1.96202</td></tr> <tr><td>C</td><td>-0.43413</td><td>-0.00915</td><td>3.36344</td></tr> <tr><td>C</td><td>1.93370</td><td>0.00480</td><td>3.52804</td></tr> <tr><td>H</td><td>2.96994</td><td>0.01530</td><td>1.72341</td></tr> <tr><td>H</td><td>-1.38052</td><td>-0.01626</td><td>3.87609</td></tr> <tr><td>H</td><td>2.85548</td><td>0.00889</td><td>4.09495</td></tr> <tr><td>H</td><td>0.61538</td><td>-0.00687</td><td>5.23298</td></tr> <tr><td>C</td><td>-0.57018</td><td>0.01261</td><td>-3.61735</td></tr> <tr><td>H</td><td>-0.10096</td><td>0.01778</td><td>-4.60512</td></tr> <tr><td>C</td><td>-1.43320</td><td>-1.25145</td><td>-3.50663</td></tr> <tr><td>H</td><td>-1.92239</td><td>-1.29480</td><td>-2.53107</td></tr> <tr><td>H</td><td>-0.82716</td><td>-2.15238</td><td>-3.61955</td></tr> <tr><td>H</td><td>-2.20891</td><td>-1.25305</td><td>-4.27615</td></tr> <tr><td>C</td><td>-1.44502</td><td>1.26787</td><td>-3.49902</td></tr> <tr><td>H</td><td>-1.93422</td><td>1.30076</td><td>-2.52304</td></tr> <tr><td>H</td><td>-2.22092</td><td>1.26687</td><td>-4.26834</td></tr> <tr><td>H</td><td>-0.84740</td><td>2.17506</td><td>-3.60666</td></tr> <tr><td>C</td><td>-1.80128</td><td>-0.01370</td><td>1.27579</td></tr> <tr><td>C</td><td>-2.99676</td><td>-0.02488</td><td>2.25569</td></tr> <tr><td>H</td><td>-3.00392</td><td>-0.91533</td><td>2.88583</td></tr> <tr><td>H</td><td>-3.91322</td><td>-0.03013</td><td>1.66104</td></tr> <tr><td>H</td><td>-3.01699</td><td>0.86226</td><td>2.89019</td></tr> <tr><td>C</td><td>-1.97270</td><td>-1.33248</td><td>0.46920</td></tr> <tr><td>H</td><td>-1.05977</td><td>-1.68827</td><td>0.00217</td></tr> <tr><td>H</td><td>-2.73733</td><td>-1.21315</td><td>-0.30273</td></tr> <tr><td>H</td><td>-2.30402</td><td>-2.11896</td><td>1.14988</td></tr> <tr><td>C</td><td>-1.99155</td><td>1.30674</td><td>0.47603</td></tr> <tr><td>H</td><td>-2.33652</td><td>2.08428</td><td>1.16016</td></tr> <tr><td>H</td><td>-2.75252</td><td>1.17984</td><td>-0.29833</td></tr> <tr><td>H</td><td>-1.08322</td><td>1.67917</td><td>0.01300</td></tr> </tbody> </table>	H	2.14217	0.03088	-4.01763	C	1.87377	0.02521	-2.96825	C	1.16358	0.01063	-0.19283	C	0.54103	0.01519	-2.58784	C	2.85089	0.02796	-1.98013	C	2.50693	0.02099	-0.36396	C	0.21812	0.00809	-1.22945	H	3.89902	0.03581	-2.25095	H	3.33088	0.02411	0.05196	H	-0.82713	0.00049	-1.02063	C	0.85488	0.00394	1.29718	C	0.70274	-0.00392	4.15429	C	1.98212	0.00845	2.14581	C	-0.42148	-0.00589	1.96202	C	-0.43413	-0.00915	3.36344	C	1.93370	0.00480	3.52804	H	2.96994	0.01530	1.72341	H	-1.38052	-0.01626	3.87609	H	2.85548	0.00889	4.09495	H	0.61538	-0.00687	5.23298	C	-0.57018	0.01261	-3.61735	H	-0.10096	0.01778	-4.60512	C	-1.43320	-1.25145	-3.50663	H	-1.92239	-1.29480	-2.53107	H	-0.82716	-2.15238	-3.61955	H	-2.20891	-1.25305	-4.27615	C	-1.44502	1.26787	-3.49902	H	-1.93422	1.30076	-2.52304	H	-2.22092	1.26687	-4.26834	H	-0.84740	2.17506	-3.60666	C	-1.80128	-0.01370	1.27579	C	-2.99676	-0.02488	2.25569	H	-3.00392	-0.91533	2.88583	H	-3.91322	-0.03013	1.66104	H	-3.01699	0.86226	2.89019	C	-1.97270	-1.33248	0.46920	H	-1.05977	-1.68827	0.00217	H	-2.73733	-1.21315	-0.30273	H	-2.30402	-2.11896	1.14988	C	-1.99155	1.30674	0.47603	H	-2.33652	2.08428	1.16016	H	-2.75252	1.17984	-0.29833	H	-1.08322	1.67917	0.01300
H	1.82471	0.65778	-3.60744																																																																																																																																																																																																																																																																																																																																																								
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C	1.41347	1.65255	-0.39014																																																																																																																																																																																																																																																																																																																																																								
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H	0.45065	-1.57978	-0.23606																																																																																																																																																																																																																																																																																																																																																								
C	0.64855	0.36923	1.62421																																																																																																																																																																																																																																																																																																																																																								
C	0.48075	0.12526	4.40453																																																																																																																																																																																																																																																																																																																																																								
C	1.78634	0.15035	2.40924																																																																																																																																																																																																																																																																																																																																																								
C	-0.61929	0.48203	2.24133																																																																																																																																																																																																																																																																																																																																																								
C	-0.65506	0.35099	3.63648																																																																																																																																																																																																																																																																																																																																																								
C	1.71862	0.02584	3.78924																																																																																																																																																																																																																																																																																																																																																								
H	2.74385	0.07360	1.90982																																																																																																																																																																																																																																																																																																																																																								
H	-1.59645	0.43174	4.15554																																																																																																																																																																																																																																																																																																																																																								
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H	1.24605	-1.55246	-3.90992																																																																																																																																																																																																																																																																																																																																																								
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H	1.56184	-3.28476	-1.41173																																																																																																																																																																																																																																																																																																																																																								
H	2.88787	-2.68273	-2.41352																																																																																																																																																																																																																																																																																																																																																								
H	1.72379	-3.84357	-3.08181																																																																																																																																																																																																																																																																																																																																																								
C	-0.52560	-2.27072	-2.94006																																																																																																																																																																																																																																																																																																																																																								
H	-0.86815	-2.55226	-1.94143																																																																																																																																																																																																																																																																																																																																																								
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C	-1.93100	0.73734	1.47067																																																																																																																																																																																																																																																																																																																																																								
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H	-2.94770	1.81635	3.08383																																																																																																																																																																																																																																																																																																																																																								
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C	1.16358	0.01063	-0.19283																																																																																																																																																																																																																																																																																																																																																								
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C	2.85089	0.02796	-1.98013																																																																																																																																																																																																																																																																																																																																																								
C	2.50693	0.02099	-0.36396																																																																																																																																																																																																																																																																																																																																																								
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H	-0.82713	0.00049	-1.02063																																																																																																																																																																																																																																																																																																																																																								
C	0.85488	0.00394	1.29718																																																																																																																																																																																																																																																																																																																																																								
C	0.70274	-0.00392	4.15429																																																																																																																																																																																																																																																																																																																																																								
C	1.98212	0.00845	2.14581																																																																																																																																																																																																																																																																																																																																																								
C	-0.42148	-0.00589	1.96202																																																																																																																																																																																																																																																																																																																																																								
C	-0.43413	-0.00915	3.36344																																																																																																																																																																																																																																																																																																																																																								
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H	2.85548	0.00889	4.09495																																																																																																																																																																																																																																																																																																																																																								
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H	-0.10096	0.01778	-4.60512																																																																																																																																																																																																																																																																																																																																																								
C	-1.43320	-1.25145	-3.50663																																																																																																																																																																																																																																																																																																																																																								
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H	-2.30402	-2.11896	1.14988																																																																																																																																																																																																																																																																																																																																																								
C	-1.99155	1.30674	0.47603																																																																																																																																																																																																																																																																																																																																																								
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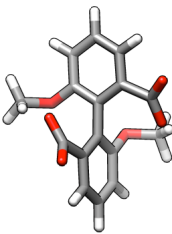
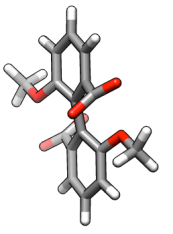
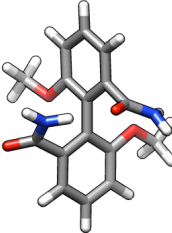
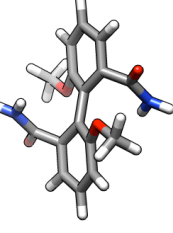
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<tr><td>C</td><td>-1.49252</td><td>0.44102</td><td>2.55688</td></tr> <tr><td>C</td><td>-1.78008</td><td>0.39362</td><td>3.91779</td></tr> <tr><td>C</td><td>0.54243</td><td>0.75937</td><td>4.41607</td></tr> <tr><td>H</td><td>1.83118</td><td>0.95125</td><td>2.71386</td></tr> <tr><td>H</td><td>-2.80183</td><td>0.24576</td><td>4.23759</td></tr> <tr><td>H</td><td>1.34423</td><td>0.88236</td><td>5.13191</td></tr> <tr><td>H</td><td>-0.99280</td><td>0.50897</td><td>5.90565</td></tr> <tr><td>C</td><td>-0.19254</td><td>-1.40970</td><td>-2.50478</td></tr> <tr><td>H</td><td>0.22925</td><td>-1.18376</td><td>-3.48822</td></tr> <tr><td>C</td><td>0.36310</td><td>-2.76513</td><td>-2.04860</td></tr> <tr><td>H</td><td>-0.04113</td><td>-3.03203</td><td>-1.06933</td></tr> <tr><td>H</td><td>1.45160</td><td>-2.73848</td><td>-1.96986</td></tr> <tr><td>H</td><td>0.08251</td><td>-3.54933</td><td>-2.75567</td></tr> <tr><td>C</td><td>-1.71948</td><td>-1.47614</td><td>-2.64335</td></tr> <tr><td>H</td><td>-2.17946</td><td>-1.69420</td><td>-1.67664</td></tr> <tr><td>H</td><td>-2.00550</td><td>-2.26526</td><td>-3.34289</td></tr> <tr><td>H</td><td>-2.12315</td><td>-0.52744</td><td>-3.00168</td></tr> <tr><td>Cl</td><td>-2.84704</td><td>0.29956</td><td>1.45339</td></tr> </tbody> </table>	H	1.29501	0.80972	-3.05546	C	0.99002	0.77591	-2.01645	C	0.19367	0.69249	0.65739	C	0.22148	-0.29628	-1.56652	C	1.36421	1.79531	-1.14613	C	0.97175	1.75473	0.18514	C	-0.16742	-0.32215	-0.22831	H	1.95828	2.62480	-1.50771	H	1.25241	2.55065	0.86244	H	-0.75915	-1.15092	0.13468	C	-0.18567	0.63908	2.08932	C	-0.76227	0.54892	4.84938	C	0.81575	0.80287	3.05663	C	-1.49252	0.44102	2.55688	C	-1.78008	0.39362	3.91779	C	0.54243	0.75937	4.41607	H	1.83118	0.95125	2.71386	H	-2.80183	0.24576	4.23759	H	1.34423	0.88236	5.13191	H	-0.99280	0.50897	5.90565	C	-0.19254	-1.40970	-2.50478	H	0.22925	-1.18376	-3.48822	C	0.36310	-2.76513	-2.04860	H	-0.04113	-3.03203	-1.06933	H	1.45160	-2.73848	-1.96986	H	0.08251	-3.54933	-2.75567	C	-1.71948	-1.47614	-2.64335	H	-2.17946	-1.69420	-1.67664	H	-2.00550	-2.26526	-3.34289	H	-2.12315	-0.52744	-3.00168	Cl	-2.84704	0.29956	1.45339	 <p>1e -1040.666360 -1040.646045 -1041.205174</p>	<table border="1"> <tbody> <tr><td>H</td><td>2.19014</td><td>-0.00129</td><td>-3.73445</td></tr> <tr><td>C</td><td>1.85182</td><td>-0.00084</td><td>-2.70535</td></tr> <tr><td>C</td><td>0.96759</td><td>0.00030</td><td>-0.00850</td></tr> <tr><td>C</td><td>0.49298</td><td>-0.00038</td><td>-2.42201</td></tr> <tr><td>C</td><td>2.76788</td><td>-0.00067</td><td>-1.65869</td></tr> <tr><td>C</td><td>2.33851</td><td>-0.00012</td><td>-0.34238</td></tr> <tr><td>C</td><td>0.07694</td><td>0.00020</td><td>-1.08966</td></tr> <tr><td>H</td><td>3.83016</td><td>-0.00101</td><td>-1.86678</td></tr> <tr><td>H</td><td>3.10283</td><td>-0.00009</td><td>0.41654</td></tr> <tr><td>H</td><td>-0.97976</td><td>0.00055</td><td>-0.91184</td></tr> <tr><td>C</td><td>0.53568</td><td>0.00061</td><td>1.42968</td></tr> <tr><td>C</td><td>-0.02935</td><td>0.00056</td><td>4.24462</td></tr> <tr><td>C</td><td>1.53525</td><td>0.00039</td><td>2.42842</td></tr> <tr><td>C</td><td>-0.78341</td><td>0.00095</td><td>1.94277</td></tr> 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</table>	H	2.19014	-0.00129	-3.73445	C	1.85182	-0.00084	-2.70535	C	0.96759	0.00030	-0.00850	C	0.49298	-0.00038	-2.42201	C	2.76788	-0.00067	-1.65869	C	2.33851	-0.00012	-0.34238	C	0.07694	0.00020	-1.08966	H	3.83016	-0.00101	-1.86678	H	3.10283	-0.00009	0.41654	H	-0.97976	0.00055	-0.91184	C	0.53568	0.00061	1.42968	C	-0.02935	0.00056	4.24462	C	1.53525	0.00039	2.42842	C	-0.78341	0.00095	1.94277	C	-1.05086	0.00088	3.31305	C	1.28134	0.00037	3.78736	H	2.57038	0.00013	2.13398	H	-2.08157	0.00113	3.63757	H	2.11033	0.00018	4.48238	H	-0.25787	0.00057	5.30178	C	-0.53944	-0.00010	-3.53002	H	0.00104	-0.00218	-4.48085	C	-1.41659	-1.25810	-3.47697	H	-1.97724	-1.29109	-2.53988	H	-0.81046	-2.16383	-3.54039	H	-2.13316	-1.25809	-4.30173	C	-1.41209	1.26118	-3.47991	H	-1.97208	1.29862	-2.54258	H	-2.12908	1.26158	-4.30430	H	-0.80273	2.16455	-3.54602	Cl	-2.26027	0.00152	0.98006
H	1.29501	0.80972	-3.05546																																																																																																																																																																																																																																																								
C	0.99002	0.77591	-2.01645																																																																																																																																																																																																																																																								
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C	1.85182	-0.00084	-2.70535																																																																																																																																																																																																																																																								
C	0.96759	0.00030	-0.00850																																																																																																																																																																																																																																																								
C	0.49298	-0.00038	-2.42201																																																																																																																																																																																																																																																								
C	2.76788	-0.00067	-1.65869																																																																																																																																																																																																																																																								
C	2.33851	-0.00012	-0.34238																																																																																																																																																																																																																																																								
C	0.07694	0.00020	-1.08966																																																																																																																																																																																																																																																								
H	3.83016	-0.00101	-1.86678																																																																																																																																																																																																																																																								
H	3.10283	-0.00009	0.41654																																																																																																																																																																																																																																																								
H	-0.97976	0.00055	-0.91184																																																																																																																																																																																																																																																								
C	0.53568	0.00061	1.42968																																																																																																																																																																																																																																																								
C	-0.02935	0.00056	4.24462																																																																																																																																																																																																																																																								
C	1.53525	0.00039	2.42842																																																																																																																																																																																																																																																								
C	-0.78341	0.00095	1.94277																																																																																																																																																																																																																																																								
C	-1.05086	0.00088	3.31305																																																																																																																																																																																																																																																								
C	1.28134	0.00037	3.78736																																																																																																																																																																																																																																																								
H	2.57038	0.00013	2.13398																																																																																																																																																																																																																																																								
H	-2.08157	0.00113	3.63757																																																																																																																																																																																																																																																								
H	2.11033	0.00018	4.48238																																																																																																																																																																																																																																																								
H	-0.25787	0.00057	5.30178																																																																																																																																																																																																																																																								
C	-0.53944	-0.00010	-3.53002																																																																																																																																																																																																																																																								
H	0.00104	-0.00218	-4.48085																																																																																																																																																																																																																																																								
C	-1.41659	-1.25810	-3.47697																																																																																																																																																																																																																																																								
H	-1.97724	-1.29109	-2.53988																																																																																																																																																																																																																																																								
H	-0.81046	-2.16383	-3.54039																																																																																																																																																																																																																																																								
H	-2.13316	-1.25809	-4.30173																																																																																																																																																																																																																																																								
C	-1.41209	1.26118	-3.47991																																																																																																																																																																																																																																																								
H	-1.97208	1.29862	-2.54258																																																																																																																																																																																																																																																								
H	-2.12908	1.26158	-4.30430																																																																																																																																																																																																																																																								
H	-0.80273	2.16455	-3.54602																																																																																																																																																																																																																																																								
Cl	-2.26027	0.00152	0.98006																																																																																																																																																																																																																																																								
 <p>1f -3154.558247 -3155.890169 -3155.043911</p>	<table border="1"> <tbody> <tr><td>H</td><td>1.54166</td><td>0.25908</td><td>-3.04118</td></tr> <tr><td>C</td><td>1.18916</td><td>0.39225</td><td>-2.02538</td></tr> <tr><td>C</td><td>0.26935</td><td>0.74118</td><td>0.58525</td></tr> <tr><td>C</td><td>0.30867</td><td>-0.54164</td><td>-1.48196</td></tr> <tr><td>C</td><td>1.61436</td><td>1.48621</td><td>-1.27756</td></tr> <tr><td>C</td><td>1.16041</td><td>1.66063</td><td>0.02317</td></tr> <tr><td>C</td><td>-0.13961</td><td>-0.35255</td><td>-0.17592</td></tr> <tr><td>H</td><td>2.29632</td><td>2.20620</td><td>-1.71144</td></tr> <tr><td>H</td><td>1.48055</td><td>2.51519</td><td>0.60477</td></tr> <tr><td>H</td><td>-0.81909</td><td>-1.07172</td><td>0.26006</td></tr> <tr><td>C</td><td>-0.18185</td><td>0.91515</td><td>1.98668</td></tr> <tr><td>C</td><td>-0.88187</td><td>1.23943</td><td>4.70012</td></tr> <tr><td>C</td><td>0.79038</td><td>1.07956</td><td>2.98397</td></tr> <tr><td>C</td><td>-1.52077</td><td>0.93383</td><td>2.39893</td></tr> <tr><td>C</td><td>-1.87122</td><td>1.09051</td><td>3.73650</td></tr> <tr><td>C</td><td>0.45584</td><td>1.23914</td><td>4.32068</td></tr> <tr><td>H</td><td>1.82992</td><td>1.06335</td><td>2.68438</td></tr> <tr><td>H</td><td>-2.91437</td><td>1.10691</td><td>4.01801</td></tr> <tr><td>H</td><td>1.23541</td><td>1.35603</td><td>5.06170</td></tr> <tr><td>H</td><td>-1.16095</td><td>1.35972</td><td>5.73851</td></tr> <tr><td>C</td><td>-0.16438</td><td>-1.73271</td><td>-2.28725</td></tr> <tr><td>H</td><td>0.32031</td><td>-1.68041</td><td>-3.26618</td></tr> <tr><td>C</td><td>0.24071</td><td>-3.05618</td><td>-1.62540</td></tr> <tr><td>H</td><td>-0.23059</td><td>-3.15105</td><td>-0.64432</td></tr> <tr><td>H</td><td>1.32227</td><td>-3.11368</td><td>-1.48867</td></tr> <tr><td>H</td><td>-0.07995</td><td>-3.90219</td><td>-2.23784</td></tr> <tr><td>C</td><td>-1.68323</td><td>-1.68395</td><td>-2.50182</td></tr> <tr><td>H</td><td>-2.20389</td><td>-1.72456</td><td>-1.54216</td></tr> <tr><td>H</td><td>-2.01134</td><td>-2.53416</td><td>-3.10459</td></tr> <tr><td>H</td><td>-1.97935</td><td>-0.76219</td><td>-3.00594</td></tr> <tr><td>Br</td><td>-2.96845</td><td>0.81870</td><td>1.14114</td></tr> </tbody> </table>	H	1.54166	0.25908	-3.04118	C	1.18916	0.39225	-2.02538	C	0.26935	0.74118	0.58525	C	0.30867	-0.54164	-1.48196	C	1.61436	1.48621	-1.27756	C	1.16041	1.66063	0.02317	C	-0.13961	-0.35255	-0.17592	H	2.29632	2.20620	-1.71144	H	1.48055	2.51519	0.60477	H	-0.81909	-1.07172	0.26006	C	-0.18185	0.91515	1.98668	C	-0.88187	1.23943	4.70012	C	0.79038	1.07956	2.98397	C	-1.52077	0.93383	2.39893	C	-1.87122	1.09051	3.73650	C	0.45584	1.23914	4.32068	H	1.82992	1.06335	2.68438	H	-2.91437	1.10691	4.01801	H	1.23541	1.35603	5.06170	H	-1.16095	1.35972	5.73851	C	-0.16438	-1.73271	-2.28725	H	0.32031	-1.68041	-3.26618	C	0.24071	-3.05618	-1.62540	H	-0.23059	-3.15105	-0.64432	H	1.32227	-3.11368	-1.48867	H	-0.07995	-3.90219	-2.23784	C	-1.68323	-1.68395	-2.50182	H	-2.20389	-1.72456	-1.54216	H	-2.01134	-2.53416	-3.10459	H	-1.97935	-0.76219	-3.00594	Br	-2.96845	0.81870	1.14114	 <p>1f -3154.545183 -3155.876934 -3155.032168</p>	<table border="1"> <tbody> <tr><td>H</td><td>2.13020</td><td>-0.00327</td><td>-4.16592</td></tr> <tr><td>C</td><td>1.91486</td><td>-0.00247</td><td>-3.10430</td></tr> <tr><td>C</td><td>1.35324</td><td>-0.00050</td><td>-0.32101</td></tr> <tr><td>C</td><td>0.59911</td><td>-0.00166</td><td>-2.66282</td></tr> <tr><td>C</td><td>2.94707</td><td>-0.00223</td><td>-2.17184</td></tr> <tr><td>C</td><td>2.67556</td><td>-0.00123</td><td>-0.81413</td></tr> <tr><td>C</td><td>0.34429</td><td>-0.00071</td><td>-1.29063</td></tr> <tr><td>H</td><td>3.97771</td><td>-0.00282</td><td>-2.50282</td></tr> <tr><td>H</td><td>3.52504</td><td>-0.00106</td><td>-0.15210</td></tr> <tr><td>H</td><td>-0.68469</td><td>-0.00008</td><td>-0.99204</td></tr> <tr><td>C</td><td>1.09058</td><td>0.00030</td><td>1.15872</td></tr> <tr><td>C</td><td>0.88549</td><td>0.00126</td><td>4.02413</td></tr> <tr><td>C</td><td>2.20705</td><td>0.00016</td><td>2.02635</td></tr> <tr><td>C</td><td>-0.15343</td><td>0.00112</td><td>1.83447</td></tr> <tr><td>C</td><td>-0.24536</td><td>0.00151</td><td>3.22792</td></tr> <tr><td>C</td><td>2.12751</td><td>0.00065</td><td>3.40599</td></tr> <tr><td>H</td><td>3.19694</td><td>-0.00029</td><td>1.60462</td></tr> <tr><td>H</td><td>-1.22232</td><td>0.00193</td><td>3.68875</td></tr> <tr><td>H</td><td>3.03800</td><td>0.00056</td><td>3.99029</td></tr> <tr><td>H</td><td>0.79018</td><td>0.00152</td><td>5.10155</td></tr> <tr><td>C</td><td>-0.55867</td><td>-0.00094</td><td>-3.63870</td></tr> <tr><td>H</td><td>-0.13694</td><td>-0.00463</td><td>-4.64783</td></tr> <tr><td>C</td><td>-1.42519</td><td>-1.25717</td><td>-3.47785</td></tr> <tr><td>H</td><td>-1.86910</td><td>-1.28690</td><td>-2.48001</td></tr> <tr><td>H</td><td>-0.83287</td><td>-2.16434</td><td>-3.61176</td></tr> <tr><td>H</td><td>-2.23575</td><td>-1.25726</td><td>-4.21048</td></tr> <tr><td>C</td><td>-1.41730</td><td>1.26150</td><td>-3.48377</td></tr> <tr><td>H</td><td>-1.86023</td><td>1.29886</td><td>-2.48574</td></tr> <tr><td>H</td><td>-2.22831</td><td>1.26303</td><td>-4.21591</td></tr> <tr><td>H</td><td>-0.81937</td><td>2.16424</td><td>-3.62254</td></tr> <tr><td>Br</td><td>-1.91588</td><td>0.00182</td><td>1.03173</td></tr> </tbody> </table>	H	2.13020	-0.00327	-4.16592	C	1.91486	-0.00247	-3.10430	C	1.35324	-0.00050	-0.32101	C	0.59911	-0.00166	-2.66282	C	2.94707	-0.00223	-2.17184	C	2.67556	-0.00123	-0.81413	C	0.34429	-0.00071	-1.29063	H	3.97771	-0.00282	-2.50282	H	3.52504	-0.00106	-0.15210	H	-0.68469	-0.00008	-0.99204	C	1.09058	0.00030	1.15872	C	0.88549	0.00126	4.02413	C	2.20705	0.00016	2.02635	C	-0.15343	0.00112	1.83447	C	-0.24536	0.00151	3.22792	C	2.12751	0.00065	3.40599	H	3.19694	-0.00029	1.60462	H	-1.22232	0.00193	3.68875	H	3.03800	0.00056	3.99029	H	0.79018	0.00152	5.10155	C	-0.55867	-0.00094	-3.63870	H	-0.13694	-0.00463	-4.64783	C	-1.42519	-1.25717	-3.47785	H	-1.86910	-1.28690	-2.48001	H	-0.83287	-2.16434	-3.61176	H	-2.23575	-1.25726	-4.21048	C	-1.41730	1.26150	-3.48377	H	-1.86023	1.29886	-2.48574	H	-2.22831	1.26303	-4.21591	H	-0.81937	2.16424	-3.62254	Br	-1.91588	0.00182	1.03173
H	1.54166	0.25908	-3.04118																																																																																																																																																																																																																																																								
C	1.18916	0.39225	-2.02538																																																																																																																																																																																																																																																								
C	0.26935	0.74118	0.58525																																																																																																																																																																																																																																																								
C	0.30867	-0.54164	-1.48196																																																																																																																																																																																																																																																								
C	1.61436	1.48621	-1.27756																																																																																																																																																																																																																																																								
C	1.16041	1.66063	0.02317																																																																																																																																																																																																																																																								
C	-0.13961	-0.35255	-0.17592																																																																																																																																																																																																																																																								
H	2.29632	2.20620	-1.71144																																																																																																																																																																																																																																																								
H	1.48055	2.51519	0.60477																																																																																																																																																																																																																																																								
H	-0.81909	-1.07172	0.26006																																																																																																																																																																																																																																																								
C	-0.18185	0.91515	1.98668																																																																																																																																																																																																																																																								
C	-0.88187	1.23943	4.70012																																																																																																																																																																																																																																																								
C	0.79038	1.07956	2.98397																																																																																																																																																																																																																																																								
C	-1.52077	0.93383	2.39893																																																																																																																																																																																																																																																								
C	-1.87122	1.09051	3.73650																																																																																																																																																																																																																																																								
C	0.45584	1.23914	4.32068																																																																																																																																																																																																																																																								
H	1.82992	1.06335	2.68438																																																																																																																																																																																																																																																								
H	-2.91437	1.10691	4.01801																																																																																																																																																																																																																																																								
H	1.23541	1.35603	5.06170																																																																																																																																																																																																																																																								
H	-1.16095	1.35972	5.73851																																																																																																																																																																																																																																																								
C	-0.16438	-1.73271	-2.28725																																																																																																																																																																																																																																																								
H	0.32031	-1.68041	-3.26618																																																																																																																																																																																																																																																								
C	0.24071	-3.05618	-1.62540																																																																																																																																																																																																																																																								
H	-0.23059	-3.15105	-0.64432																																																																																																																																																																																																																																																								
H	1.32227	-3.11368	-1.48867																																																																																																																																																																																																																																																								
H	-0.07995	-3.90219	-2.23784																																																																																																																																																																																																																																																								
C	-1.68323	-1.68395	-2.50182																																																																																																																																																																																																																																																								
H	-2.20389	-1.72456	-1.54216																																																																																																																																																																																																																																																								
H	-2.01134	-2.53416	-3.10459																																																																																																																																																																																																																																																								
H	-1.97935	-0.76219	-3.00594																																																																																																																																																																																																																																																								
Br	-2.96845	0.81870	1.14114																																																																																																																																																																																																																																																								
H	2.13020	-0.00327	-4.16592																																																																																																																																																																																																																																																								
C	1.91486	-0.00247	-3.10430																																																																																																																																																																																																																																																								
C	1.35324	-0.00050	-0.32101																																																																																																																																																																																																																																																								
C	0.59911	-0.00166	-2.66282																																																																																																																																																																																																																																																								
C	2.94707	-0.00223	-2.17184																																																																																																																																																																																																																																																								
C	2.67556	-0.00123	-0.81413																																																																																																																																																																																																																																																								
C	0.34429	-0.00071	-1.29063																																																																																																																																																																																																																																																								
H	3.97771	-0.00282	-2.50282																																																																																																																																																																																																																																																								
H	3.52504	-0.00106	-0.15210																																																																																																																																																																																																																																																								
H	-0.68469	-0.00008	-0.99204																																																																																																																																																																																																																																																								
C	1.09058	0.00030	1.15872																																																																																																																																																																																																																																																								
C	0.88549	0.00126	4.02413																																																																																																																																																																																																																																																								
C	2.20705	0.00016	2.02635																																																																																																																																																																																																																																																								
C	-0.15343	0.00112	1.83447																																																																																																																																																																																																																																																								
C	-0.24536	0.00151	3.22792																																																																																																																																																																																																																																																								
C	2.12751	0.00065	3.40599																																																																																																																																																																																																																																																								
H	3.19694	-0.00029	1.60462																																																																																																																																																																																																																																																								
H	-1.22232	0.00193	3.68875																																																																																																																																																																																																																																																								
H	3.03800	0.00056	3.99029																																																																																																																																																																																																																																																								
H	0.79018	0.00152	5.10155																																																																																																																																																																																																																																																								
C	-0.55867	-0.00094	-3.63870																																																																																																																																																																																																																																																								
H	-0.13694	-0.00463	-4.64783																																																																																																																																																																																																																																																								
C	-1.42519	-1.25717	-3.47785																																																																																																																																																																																																																																																								
H	-1.86910	-1.28690	-2.48001																																																																																																																																																																																																																																																								
H	-0.83287	-2.16434	-3.61176																																																																																																																																																																																																																																																								
H	-2.23575	-1.25726	-4.21048																																																																																																																																																																																																																																																								
C	-1.41730	1.26150	-3.48377																																																																																																																																																																																																																																																								
H	-1.86023	1.29886	-2.48574																																																																																																																																																																																																																																																								
H	-2.22831	1.26303	-4.21591																																																																																																																																																																																																																																																								
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 <p>1g -878.2216168 -878.6392616 -878.5762347</p>	<table border="1"> <tbody> <tr><td>H</td><td>1.52740</td><td>0.26900</td><td>-3.04889</td></tr> <tr><td>C</td><td>1.17913</td><td>0.40096</td><td>-2.03149</td></tr> <tr><td>C</td><td>0.26931</td><td>0.74834</td><td>0.58173</td></tr> <tr><td>C</td><td>0.31161</td><td>-0.54087</td><td>-1.48123</td></tr> <tr><td>C</td><td>1.59769</td><td>1.50100</td><td>-1.28864</td></tr> <tr><td>C</td><td>1.14871</td><td>1.67482</td><td>0.01408</td></tr> <tr><td>C</td><td>-0.13077</td><td>-0.35271</td><td>-0.17296</td></tr> <tr><td>H</td><td>2.27047</td><td>2.22619</td><td>-1.72812</td></tr> <tr><td>H</td><td>1.46302</td><td>2.53380</td><td>0.59237</td></tr> <tr><td>H</td><td>-0.79990</td><td>-1.07778</td><td>0.26998</td></tr> <tr><td>C</td><td>-0.18601</td><td>0.92169</td><td>1.98228</td></tr> <tr><td>C</td><td>-0.88257</td><td>1.22830</td><td>4.69573</td></tr> <tr><td>C</td><td>0.78924</td><td>1.03768</td><td>2.98339</td></tr> <tr><td>C</td><td>-1.52789</td><td>0.98129</td><td>2.38464</td></tr> <tr><td>C</td><td>-1.87345</td><td>1.12898</td><td>3.72655</td></tr> <tr><td>C</td><td>0.45556</td><td>1.18851</td><td>4.32129</td></tr> <tr><td>H</td><td>1.82865</td><td>0.99045</td><td>2.68612</td></tr> <tr><td>H</td><td>-2.91395</td><td>1.17838</td><td>4.01418</td></tr> <tr><td>H</td><td>1.23585</td><td>1.26806</td><td>5.06659</td></tr> <tr><td>H</td><td>-1.16175</td><td>1.34249</td><td>5.73489</td></tr> </tbody> </table>	H	1.52740	0.26900	-3.04889	C	1.17913	0.40096	-2.03149	C	0.26931	0.74834	0.58173	C	0.31161	-0.54087	-1.48123	C	1.59769	1.50100	-1.28864	C	1.14871	1.67482	0.01408	C	-0.13077	-0.35271	-0.17296	H	2.27047	2.22619	-1.72812	H	1.46302	2.53380	0.59237	H	-0.79990	-1.07778	0.26998	C	-0.18601	0.92169	1.98228	C	-0.88257	1.22830	4.69573	C	0.78924	1.03768	2.98339	C	-1.52789	0.98129	2.38464	C	-1.87345	1.12898	3.72655	C	0.45556	1.18851	4.32129	H	1.82865	0.99045	2.68612	H	-2.91395	1.17838	4.01418	H	1.23585	1.26806	5.06659	H	-1.16175	1.34249	5.73489	 <p>1g -878.2064202 -878.6240332 -878.5625896</p>	<table border="1"> <tbody> <tr><td>H</td><td>1.69176</td><td>0.00544</td><td>-4.68808</td></tr> <tr><td>C</td><td>1.66914</td><td>0.00386</td><td>-3.60510</td></tr> <tr><td>C</td><td>1.61342</td><td>-0.00023</td><td>-0.76473</td></tr> <tr><td>C</td><td>0.45369</td><td>0.00004</td><td>-2.93557</td></tr> <tr><td>C</td><td>2.85085</td><td>0.00562</td><td>-2.87107</td></tr> <tr><td>C</td><td>2.82656</td><td>0.00363</td><td>-1.48654</td></tr> <tr><td>C</td><td>0.45071</td><td>-0.00191</td><td>-1.54006</td></tr> <tr><td>H</td><td>3.80601</td><td>0.00861</td><td>-3.38039</td></tr> <tr><td>H</td><td>3.78119</td><td>0.00524</td><td>-0.98830</td></tr> <tr><td>H</td><td>-0.51026</td><td>-0.00484</td><td>-1.06572</td></tr> <tr><td>C</td><td>1.61323</td><td>-0.00214</td><td>0.73946</td></tr> <tr><td>C</td><td>1.93925</td><td>-0.00430</td><td>3.59168</td></tr> <tr><td>C</td><td>2.87012</td><td>0.00000</td><td>1.38749</td></tr> <tr><td>C</td><td>0.50756</td><td>-0.00575</td><td>1.62739</td></tr> <tr><td>C</td><td>0.68116</td><td>-0.00669</td><td>3.01576</td></tr> <tr><td>C</td><td>3.04667</td><td>-0.00099</td><td>2.75775</td></tr> <tr><td>H</td><td>3.76574</td><td>0.00263</td><td>0.79131</td></tr> <tr><td>H</td><td>-0.18577</td><td>-0.00937</td><td>3.66001</td></tr> <tr><td>H</td><td>4.04920</td><td>0.00086</td><td>3.16449</td></tr> <tr><td>H</td><td>2.04116</td><td>-0.00508</td><td>4.66859</td></tr> </tbody> </table>	H	1.69176	0.00544	-4.68808	C	1.66914	0.00386	-3.60510	C	1.61342	-0.00023	-0.76473	C	0.45369	0.00004	-2.93557	C	2.85085	0.00562	-2.87107	C	2.82656	0.00363	-1.48654	C	0.45071	-0.00191	-1.54006	H	3.80601	0.00861	-3.38039	H	3.78119	0.00524	-0.98830	H	-0.51026	-0.00484	-1.06572	C	1.61323	-0.00214	0.73946	C	1.93925	-0.00430	3.59168	C	2.87012	0.00000	1.38749	C	0.50756	-0.00575	1.62739	C	0.68116	-0.00669	3.01576	C	3.04667	-0.00099	2.75775	H	3.76574	0.00263	0.79131	H	-0.18577	-0.00937	3.66001	H	4.04920	0.00086	3.16449	H	2.04116	-0.00508	4.66859																																																																																								
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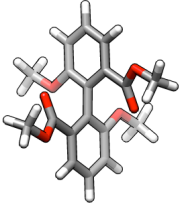
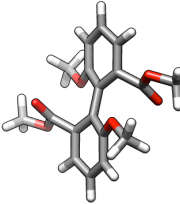
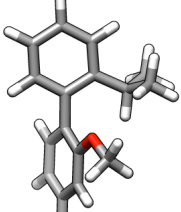
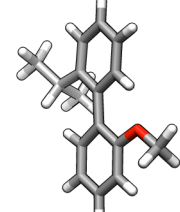
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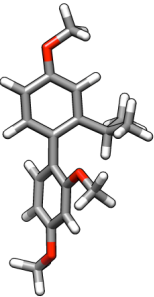
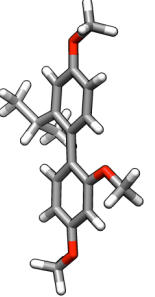
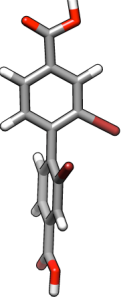
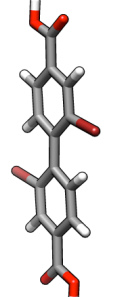
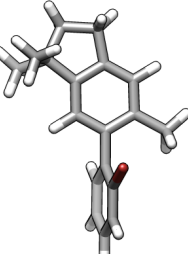
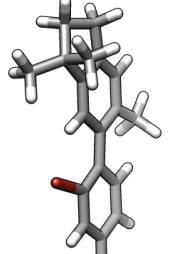
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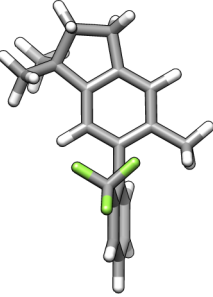
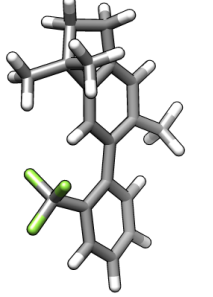
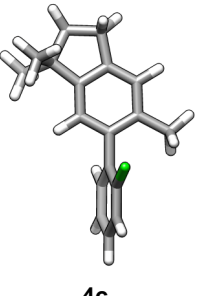
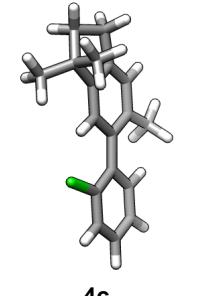
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<tr><td>C</td><td>1.32080</td><td>1.78093</td><td>3.66753</td></tr> <tr><td>H</td><td>-1.07517</td><td>4.07580</td><td>2.98542</td></tr> <tr><td>H</td><td>2.19961</td><td>1.64849</td><td>4.28553</td></tr> <tr><td>H</td><td>-0.97304</td><td>-0.39940</td><td>-2.35724</td></tr> <tr><td>H</td><td>-1.92928</td><td>-2.59011</td><td>-1.66584</td></tr> <tr><td>H</td><td>0.93145</td><td>3.75193</td><td>4.42069</td></tr> <tr><td>C</td><td>-1.37028</td><td>-1.70865</td><td>2.87556</td></tr> <tr><td>H</td><td>-1.77307</td><td>2.27081</td><td>1.44721</td></tr> <tr><td>C</td><td>1.78411</td><td>-0.50871</td><td>2.73740</td></tr> <tr><td>H</td><td>1.26302</td><td>-1.23660</td><td>2.11822</td></tr> <tr><td>C</td><td>2.00526</td><td>-1.14050</td><td>4.11640</td></tr> <tr><td>H</td><td>2.56701</td><td>-2.07201</td><td>4.01668</td></tr> <tr><td>H</td><td>1.05612</td><td>-1.36281</td><td>4.60559</td></tr> <tr><td>H</td><td>2.57586</td><td>-0.47302</td><td>4.76547</td></tr> <tr><td>C</td><td>3.12919</td><td>-0.20854</td><td>2.06080</td></tr> <tr><td>H</td><td>3.72878</td><td>-1.11886</td><td>1.98289</td></tr> <tr><td>H</td><td>3.69318</td><td>0.52474</td><td>2.64241</td></tr> <tr><td>H</td><td>2.97873</td><td>0.19599</td><td>1.05819</td></tr> <tr><td>H</td><td>-0.85502</td><td>-0.96642</td><td>3.48250</td></tr> <tr><td>C</td><td>-0.75631</td><td>-3.07749</td><td>3.18977</td></tr> <tr><td>H</td><td>0.29893</td><td>-3.10896</td><td>2.91588</td></tr> <tr><td>H</td><td>-1.27359</td><td>-3.87203</td><td>2.64796</td></tr> <tr><td>H</td><td>-0.84069</td><td>-3.29036</td><td>4.25786</td></tr> <tr><td>C</td><td>-2.85277</td><td>-1.67943</td><td>3.27369</td></tr> <tr><td>H</td><td>-3.41909</td><td>-2.40756</td><td>2.68795</td></tr> <tr><td>H</td><td>-3.28389</td><td>-0.69223</td><td>3.09730</td></tr> <tr><td>H</td><td>-2.96851</td><td>-1.92609</td><td>4.33202</td></tr> </tbody> </table>	C	-1.57601	-1.88694	-0.92257	C	-0.66838	-0.08937	1.02340	C	-1.65643	-2.20331	0.42690	C	-1.04320	-0.66192	-1.30964	C	-0.59850	0.22481	-0.33841	C	-1.20816	-1.32547	1.41679	H	-2.08330	-3.15276	0.72376	H	-0.18046	1.18029	-0.62873	C	-0.19624	0.93356	1.99970	C	0.61068	2.97160	3.74255	C	0.93736	0.74797	2.80881	C	-0.90132	2.13990	2.07562	C	-0.51004	3.15394	2.93933	C	1.32080	1.78093	3.66753	H	-1.07517	4.07580	2.98542	H	2.19961	1.64849	4.28553	H	-0.97304	-0.39940	-2.35724	H	-1.92928	-2.59011	-1.66584	H	0.93145	3.75193	4.42069	C	-1.37028	-1.70865	2.87556	H	-1.77307	2.27081	1.44721	C	1.78411	-0.50871	2.73740	H	1.26302	-1.23660	2.11822	C	2.00526	-1.14050	4.11640	H	2.56701	-2.07201	4.01668	H	1.05612	-1.36281	4.60559	H	2.57586	-0.47302	4.76547	C	3.12919	-0.20854	2.06080	H	3.72878	-1.11886	1.98289	H	3.69318	0.52474	2.64241	H	2.97873	0.19599	1.05819	H	-0.85502	-0.96642	3.48250	C	-0.75631	-3.07749	3.18977	H	0.29893	-3.10896	2.91588	H	-1.27359	-3.87203	2.64796	H	-0.84069	-3.29036	4.25786	C	-2.85277	-1.67943	3.27369	H	-3.41909	-2.40756	2.68795	H	-3.28389	-0.69223	3.09730	H	-2.96851	-1.92609	4.33202	 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<tr><td>H</td><td>0.86150</td><td>-4.65946</td><td>0.75847</td></tr> <tr><td>H</td><td>1.44226</td><td>-4.03681</td><td>2.29898</td></tr> <tr><td>H</td><td>-0.61384</td><td>1.83821</td><td>-1.94366</td></tr> <tr><td>C</td><td>-1.20249</td><td>3.73539</td><td>-1.29667</td></tr> <tr><td>H</td><td>-0.83063</td><td>4.62707</td><td>-0.79018</td></tr> <tr><td>H</td><td>-2.14114</td><td>3.44008</td><td>-0.82523</td></tr> <tr><td>H</td><td>-1.40545</td><td>4.00890</td><td>-2.33477</td></tr> <tr><td>C</td><td>1.15653</td><td>3.06861</td><td>-1.83901</td></tr> <tr><td>H</td><td>1.54715</td><td>3.86603</td><td>-1.20229</td></tr> <tr><td>H</td><td>1.03063</td><td>3.46884</td><td>-2.84815</td></tr> <tr><td>H</td><td>1.90627</td><td>2.27585</td><td>-1.86866</td></tr> <tr><td>C</td><td>0.22024</td><td>-2.60915</td><td>1.24085</td></tr> <tr><td>H</td><td>0.64887</td><td>-1.86825</td><td>1.90652</td></tr> </tbody> 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C	-1.20816	-1.32547	1.41679																																																																																																																																																																																																																																																																																																																																																								
H	-2.08330	-3.15276	0.72376																																																																																																																																																																																																																																																																																																																																																								
H	-0.18046	1.18029	-0.62873																																																																																																																																																																																																																																																																																																																																																								
C	-0.19624	0.93356	1.99970																																																																																																																																																																																																																																																																																																																																																								
C	0.61068	2.97160	3.74255																																																																																																																																																																																																																																																																																																																																																								
C	0.93736	0.74797	2.80881																																																																																																																																																																																																																																																																																																																																																								
C	-0.90132	2.13990	2.07562																																																																																																																																																																																																																																																																																																																																																								
C	-0.51004	3.15394	2.93933																																																																																																																																																																																																																																																																																																																																																								
C	1.32080	1.78093	3.66753																																																																																																																																																																																																																																																																																																																																																								
H	-1.07517	4.07580	2.98542																																																																																																																																																																																																																																																																																																																																																								
H	2.19961	1.64849	4.28553																																																																																																																																																																																																																																																																																																																																																								
H	-0.97304	-0.39940	-2.35724																																																																																																																																																																																																																																																																																																																																																								
H	-1.92928	-2.59011	-1.66584																																																																																																																																																																																																																																																																																																																																																								
H	0.93145	3.75193	4.42069																																																																																																																																																																																																																																																																																																																																																								
C	-1.37028	-1.70865	2.87556																																																																																																																																																																																																																																																																																																																																																								
H	-1.77307	2.27081	1.44721																																																																																																																																																																																																																																																																																																																																																								
C	1.78411	-0.50871	2.73740																																																																																																																																																																																																																																																																																																																																																								
H	1.26302	-1.23660	2.11822																																																																																																																																																																																																																																																																																																																																																								
C	2.00526	-1.14050	4.11640																																																																																																																																																																																																																																																																																																																																																								
H	2.56701	-2.07201	4.01668																																																																																																																																																																																																																																																																																																																																																								
H	1.05612	-1.36281	4.60559																																																																																																																																																																																																																																																																																																																																																								
H	2.57586	-0.47302	4.76547																																																																																																																																																																																																																																																																																																																																																								
C	3.12919	-0.20854	2.06080																																																																																																																																																																																																																																																																																																																																																								
H	3.72878	-1.11886	1.98289																																																																																																																																																																																																																																																																																																																																																								
H	3.69318	0.52474	2.64241																																																																																																																																																																																																																																																																																																																																																								
H	2.97873	0.19599	1.05819																																																																																																																																																																																																																																																																																																																																																								
H	-0.85502	-0.96642	3.48250																																																																																																																																																																																																																																																																																																																																																								
C	-0.75631	-3.07749	3.18977																																																																																																																																																																																																																																																																																																																																																								
H	0.29893	-3.10896	2.91588																																																																																																																																																																																																																																																																																																																																																								
H	-1.27359	-3.87203	2.64796																																																																																																																																																																																																																																																																																																																																																								
H	-0.84069	-3.29036	4.25786																																																																																																																																																																																																																																																																																																																																																								
C	-2.85277	-1.67943	3.27369																																																																																																																																																																																																																																																																																																																																																								
H	-3.41909	-2.40756	2.68795																																																																																																																																																																																																																																																																																																																																																								
H	-3.28389	-0.69223	3.09730																																																																																																																																																																																																																																																																																																																																																								
H	-2.96851	-1.92609	4.33202																																																																																																																																																																																																																																																																																																																																																								
C	0.09409	-2.60939	-2.52548																																																																																																																																																																																																																																																																																																																																																								
C	0.10921	-0.59489	-0.49398																																																																																																																																																																																																																																																																																																																																																								
C	-0.01768	-2.92844	-1.18364																																																																																																																																																																																																																																																																																																																																																								
C	0.38217	-1.29436	-2.85106																																																																																																																																																																																																																																																																																																																																																								
C	0.39252	-0.33586	-1.85237																																																																																																																																																																																																																																																																																																																																																								
C	0.06601	-1.98690	-0.15059																																																																																																																																																																																																																																																																																																																																																								
H	-0.13268	-3.96920	-0.91563																																																																																																																																																																																																																																																																																																																																																								
C	-0.07681	0.56386	0.45743																																																																																																																																																																																																																																																																																																																																																								
C	-0.05556	2.57798	2.48912																																																																																																																																																																																																																																																																																																																																																								
C	-0.03227	1.95583	0.11412																																																																																																																																																																																																																																																																																																																																																								
C	-0.35903	0.30509	1.81609																																																																																																																																																																																																																																																																																																																																																								
C	-0.34563	1.26344	2.81490																																																																																																																																																																																																																																																																																																																																																								
C	0.05442	2.89710	1.14715																																																																																																																																																																																																																																																																																																																																																								
H	-0.55829	0.97187	3.83519																																																																																																																																																																																																																																																																																																																																																								
H	0.17126	3.93767	0.87914																																																																																																																																																																																																																																																																																																																																																								
H	0.59562	-1.00256	-3.87112																																																																																																																																																																																																																																																																																																																																																								
H	0.02251	-3.37878	-3.28300																																																																																																																																																																																																																																																																																																																																																								
H	0.01871	3.34707	3.24669																																																																																																																																																																																																																																																																																																																																																								
H	0.66208	0.65237	-2.15473																																																																																																																																																																																																																																																																																																																																																								
H	-0.62938	-0.68283	2.11866																																																																																																																																																																																																																																																																																																																																																								
C	-0.18612	2.57871	-1.27705																																																																																																																																																																																																																																																																																																																																																								
C	-1.12203	-3.09821	1.80435																																																																																																																																																																																																																																																																																																																																																								
H	-0.99507	-3.49877	2.81323																																																																																																																																																																																																																																																																																																																																																								
H	-1.51395	-3.89524	1.16796																																																																																																																																																																																																																																																																																																																																																								
H	-1.87130	-2.30508	1.83521																																																																																																																																																																																																																																																																																																																																																								
C	1.23597	-3.76647	1.26073																																																																																																																																																																																																																																																																																																																																																								
H	2.17327	-3.47363	0.78507																																																																																																																																																																																																																																																																																																																																																								
H	0.86150	-4.65946	0.75847																																																																																																																																																																																																																																																																																																																																																								
H	1.44226	-4.03681	2.29898																																																																																																																																																																																																																																																																																																																																																								
H	-0.61384	1.83821	-1.94366																																																																																																																																																																																																																																																																																																																																																								
C	-1.20249	3.73539	-1.29667																																																																																																																																																																																																																																																																																																																																																								
H	-0.83063	4.62707	-0.79018																																																																																																																																																																																																																																																																																																																																																								
H	-2.14114	3.44008	-0.82523																																																																																																																																																																																																																																																																																																																																																								
H	-1.40545	4.00890	-2.33477																																																																																																																																																																																																																																																																																																																																																								
C	1.15653	3.06861	-1.83901																																																																																																																																																																																																																																																																																																																																																								
H	1.54715	3.86603	-1.20229																																																																																																																																																																																																																																																																																																																																																								
H	1.03063	3.46884	-2.84815																																																																																																																																																																																																																																																																																																																																																								
H	1.90627	2.27585	-1.86866																																																																																																																																																																																																																																																																																																																																																								
C	0.22024	-2.60915	1.24085																																																																																																																																																																																																																																																																																																																																																								
H	0.64887	-1.86825	1.90652																																																																																																																																																																																																																																																																																																																																																								
 <p>2d -738.3279895 -738.2173119 -738.9191202</p>	<table border="1"> <tbody> <tr><td>C</td><td>-2.12159</td><td>-1.61004</td><td>-2.79661</td></tr> <tr><td>C</td><td>-0.76829</td><td>0.21581</td><td>-1.17311</td></tr> <tr><td>C</td><td>-2.15989</td><td>-1.73119</td><td>-1.41206</td></tr> <tr><td>C</td><td>-1.40995</td><td>-0.56716</td><td>-3.37754</td></tr> <tr><td>C</td><td>-0.74580</td><td>0.34138</td><td>-2.56225</td></tr> <tr><td>C</td><td>-1.49035</td><td>-0.83234</td><td>-0.58130</td></tr> <tr><td>H</td><td>-2.71807</td><td>-2.54582</td><td>-0.97084</td></tr> <tr><td>H</td><td>-0.18951</td><td>1.15932</td><td>-3.00256</td></tr> <tr><td>C</td><td>-0.09856</td><td>1.26602</td><td>-0.34724</td></tr> <tr><td>C</td><td>0.83083</td><td>3.41534</td><td>1.19241</td></tr> <tr><td>C</td><td>1.14665</td><td>1.15143</td><td>0.29966</td></tr> <tr><td>C</td><td>-0.83342</td><td>2.45574</td><td>-0.22277</td></tr> <tr><td>C</td><td>-0.38646</td><td>3.52705</td><td>0.53143</td></tr> <tr><td>C</td><td>1.56832</td><td>2.25010</td><td>1.06712</td></tr> <tr><td>H</td><td>-0.98035</td><td>4.42861</td><td>0.60674</td></tr> <tr><td>H</td><td>2.51475</td><td>2.18909</td><td>1.58519</td></tr> <tr><td>H</td><td>-1.37189</td><td>-0.46017</td><td>-4.45389</td></tr> <tr><td>H</td><td>-2.64624</td><td>-2.32610</td><td>-3.41601</td></tr> <tr><td>H</td><td>1.20748</td><td>4.22932</td><td>1.79831</td></tr> <tr><td>C</td><td>-1.56355</td><td>-0.96369</td><td>0.92848</td></tr> <tr><td>H</td><td>-1.78576</td><td>2.51921</td><td>-0.73354</td></tr> <tr><td>C</td><td>2.11898</td><td>-0.04698</td><td>0.25607</td></tr> <tr><td>C</td><td>1.70124</td><td>-1.23984</td><td>-0.61433</td></tr> <tr><td>H</td><td>2.52002</td><td>-1.96330</td><td>-0.60413</td></tr> <tr><td>H</td><td>1.51346</td><td>-0.95126</td><td>-1.64703</td></tr> <tr><td>H</td><td>0.81347</td><td>-1.73694</td><td>-0.23254</td></tr> <tr><td>C</td><td>2.32006</td><td>-0.58343</td><td>1.68789</td></tr> <tr><td>H</td><td>3.03228</td><td>-1.41205</td><td>1.67140</td></tr> <tr><td>H</td><td>1.37584</td><td>-0.95179</td><td>2.09448</td></tr> <tr><td>H</td><td>2.70485</td><td>0.18452</td><td>2.35921</td></tr> <tr><td>H</td><td>-0.67761</td><td>-0.48226</td><td>1.34326</td></tr> <tr><td>C</td><td>-1.56733</td><td>-2.41384</td><td>1.41864</td></tr> <tr><td>H</td><td>-0.72028</td><td>-2.97176</td><td>1.01402</td></tr> <tr><td>H</td><td>-2.48453</td><td>-2.93126</td><td>1.12963</td></tr> <tr><td>H</td><td>-1.50714</td><td>-2.43492</td><td>2.50880</td></tr> <tr><td>C</td><td>-2.78765</td><td>-0.20732</td><td>1.46462</td></tr> <tr><td>H</td><td>-3.70545</td><td>-0.64275</td><td>1.06128</td></tr> <tr><td>H</td><td>-2.74904</td><td>0.84400</td><td>1.17588</td></tr> <tr><td>H</td><td>-2.82744</td><td>-0.26714</td><td>2.55523</td></tr> <tr><td>C</td><td>3.47710</td><td>0.44011</td><td>-0.29359</td></tr> <tr><td>H</td><td>4.18444</td><td>-0.39256</td><td>-0.30423</td></tr> <tr><td>H</td><td>3.90348</td><td>1.24017</td><td>0.31107</td></tr> <tr><td>H</td><td>3.36287</td><td>0.80871</td><td>-1.31524</td></tr> </tbody> </table>	C	-2.12159	-1.61004	-2.79661	C	-0.76829	0.21581	-1.17311	C	-2.15989	-1.73119	-1.41206	C	-1.40995	-0.56716	-3.37754	C	-0.74580	0.34138	-2.56225	C	-1.49035	-0.83234	-0.58130	H	-2.71807	-2.54582	-0.97084	H	-0.18951	1.15932	-3.00256	C	-0.09856	1.26602	-0.34724	C	0.83083	3.41534	1.19241	C	1.14665	1.15143	0.29966	C	-0.83342	2.45574	-0.22277	C	-0.38646	3.52705	0.53143	C	1.56832	2.25010	1.06712	H	-0.98035	4.42861	0.60674	H	2.51475	2.18909	1.58519	H	-1.37189	-0.46017	-4.45389	H	-2.64624	-2.32610	-3.41601	H	1.20748	4.22932	1.79831	C	-1.56355	-0.96369	0.92848	H	-1.78576	2.51921	-0.73354	C	2.11898	-0.04698	0.25607	C	1.70124	-1.23984	-0.61433	H	2.52002	-1.96330	-0.60413	H	1.51346	-0.95126	-1.64703	H	0.81347	-1.73694	-0.23254	C	2.32006	-0.58343	1.68789	H	3.03228	-1.41205	1.67140	H	1.37584	-0.95179	2.09448	H	2.70485	0.18452	2.35921	H	-0.67761	-0.48226	1.34326	C	-1.56733	-2.41384	1.41864	H	-0.72028	-2.97176	1.01402	H	-2.48453	-2.93126	1.12963	H	-1.50714	-2.43492	2.50880	C	-2.78765	-0.20732	1.46462	H	-3.70545	-0.64275	1.06128	H	-2.74904	0.84400	1.17588	H	-2.82744	-0.26714	2.55523	C	3.47710	0.44011	-0.29359	H	4.18444	-0.39256	-0.30423	H	3.90348	1.24017	0.31107	H	3.36287	0.80871	-1.31524	 <p>2d -738.2779511 -738.1679929 -738.8726330</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.57142</td><td>-2.24432</td><td>-2.68543</td></tr> <tr><td>C</td><td>-0.03202</td><td>-0.42580</td><td>-0.56201</td></tr> <tr><td>C</td><td>-0.64379</td><td>-2.62960</td><td>-1.35577</td></tr> <tr><td>C</td><td>-0.00499</td><td>-1.01481</td><td>-2.96625</td></tr> <tr><td>C</td><td>0.24864</td><td>-0.14980</td><td>-1.91604</td></tr> <tr><td>C</td><td>-0.27239</td><td>-1.82291</td><td>-0.27085</td></tr> <tr><td>H</td><td>-0.95281</td><td>-3.64363</td><td>-1.16216</td></tr> <tr><td>C</td><td>-0.09353</td><td>0.73603</td><td>0.39896</td></tr> <tr><td>C</td><td>-0.01308</td><td>2.70967</td><td>2.46705</td></tr> <tr><td>C</td><td>0.05639</td><td>2.12804</td><td>0.07990</td></tr> <tr><td>C</td><td>-0.41797</td><td>0.47464</td><td>1.74183</td></tr> <tr><td>C</td><td>-0.38219</td><td>1.40772</td><td>2.76174</td></tr> <tr><td>C</td><td>0.16552</td><td>3.04251</td><td>1.13554</td></tr> <tr><td>H</td><td>-0.63124</td><td>1.10712</td><td>3.77117</td></tr> <tr><td>H</td><td>0.35870</td><td>0.07795</td><td>0.89451</td></tr> <tr><td>H</td><td>0.22152</td><td>-0.71149</td><td>-3.98000</td></tr> <tr><td>H</td><td>-0.87110</td><td>-2.92774</td><td>-3.46893</td></tr> <tr><td>H</td><td>0.07868</td><td>3.46217</td><td>3.23927</td></tr> <tr><td>H</td><td>0.69779</td><td>0.78597</td><td>-2.16854</td></tr> <tr><td>H</td><td>-0.71428</td><td>-0.51304</td><td>2.00641</td></tr> <tr><td>C</td><td>0.01200</td><td>-2.61937</td><td>1.04443</td></tr> <tr><td>C</td><td>0.01155</td><td>2.78597</td><td>-1.30298</td></tr> <tr><td>C</td><td>0.43425</td><td>-4.08142</td><td>0.71942</td></tr> <tr><td>H</td><td>0.82496</td><td>-4.53173</td><td>1.63392</td></tr> <tr><td>H</td><td>1.21554</td><td>-4.10662</td><td>-0.04064</td></tr> <tr><td>H</td><td>-0.39813</td><td>-4.70307</td><td>0.39042</td></tr> <tr><td>C</td><td>1.26100</td><td>-2.07077</td><td>1.77648</td></tr> <tr><td>H</td><td>1.24017</td><td>-1.01396</td><td>2.00928</td></tr> <tr><td>H</td><td>2.14014</td><td>-2.25002</td><td>1.15355</td></tr> <tr><td>H</td><td>1.39364</td><td>-6.22282</td><td>2.71003</td></tr> <tr><td>H</td><td>-0.47187</td><td>2.10423</td><td>-1.99381</td></tr> <tr><td>C</td><td>-0.86872</td><td>4.04876</td><td>-1.34043</td></tr> <tr><td>H</td><td>-0.40964</td><td>4.89511</td><td>-0.82758</td></tr> <tr><td>H</td><td>-1.84386</td><td>3.86150</td><td>-0.88822</td></tr> <tr><td>H</td><td>-1.01888</td><td>4.34127</td><td>-2.38225</td></tr> <tr><td>C</td><td>1.41758</td><td>3.13178</td><td>-1.81628</td></tr> <tr><td>H</td><td>1.87092</td><td>3.87502</td><td>-1.15596</td></tr> <tr><td>H</td><td>1.36895</td><td>3.55407</td><td>-2.82310</td></tr> <tr><td>H</td><td>2.07886</td><td>2.26339</td><td>-1.83363</td></tr> <tr><td>C</td><td>-1.23112</td><td>-2.78812</td><td>1.94957</td></tr> <tr><td>H</td><td>-1.69925</td><td>-1.86512</td><td>2.28276</td></tr> <tr><td>H</td><td>-0.95650</td><td>-3.36478</td><td>2.83665</td></tr> <tr><td>H</td><td>-1.99137</td><td>-3.34987</td><td>1.40261</td></tr> </tbody> </table>	C	-0.57142	-2.24432	-2.68543	C	-0.03202	-0.42580	-0.56201	C	-0.64379	-2.62960	-1.35577	C	-0.00499	-1.01481	-2.96625	C	0.24864	-0.14980	-1.91604	C	-0.27239	-1.82291	-0.27085	H	-0.95281	-3.64363	-1.16216	C	-0.09353	0.73603	0.39896	C	-0.01308	2.70967	2.46705	C	0.05639	2.12804	0.07990	C	-0.41797	0.47464	1.74183	C	-0.38219	1.40772	2.76174	C	0.16552	3.04251	1.13554	H	-0.63124	1.10712	3.77117	H	0.35870	0.07795	0.89451	H	0.22152	-0.71149	-3.98000	H	-0.87110	-2.92774	-3.46893	H	0.07868	3.46217	3.23927	H	0.69779	0.78597	-2.16854	H	-0.71428	-0.51304	2.00641	C	0.01200	-2.61937	1.04443	C	0.01155	2.78597	-1.30298	C	0.43425	-4.08142	0.71942	H	0.82496	-4.53173	1.63392	H	1.21554	-4.10662	-0.04064	H	-0.39813	-4.70307	0.39042	C	1.26100	-2.07077	1.77648	H	1.24017	-1.01396	2.00928	H	2.14014	-2.25002	1.15355	H	1.39364	-6.22282	2.71003	H	-0.47187	2.10423	-1.99381	C	-0.86872	4.04876	-1.34043	H	-0.40964	4.89511	-0.82758	H	-1.84386	3.86150	-0.88822	H	-1.01888	4.34127	-2.38225	C	1.41758	3.13178	-1.81628	H	1.87092	3.87502	-1.15596	H	1.36895	3.55407	-2.82310	H	2.07886	2.26339	-1.83363	C	-1.23112	-2.78812	1.94957	H	-1.69925	-1.86512	2.28276	H	-0.95650	-3.36478	2.83665	H	-1.99137	-3.34987	1.40261
C	-2.12159	-1.61004	-2.79661																																																																																																																																																																																																																																																																																																																																																								
C	-0.76829	0.21581	-1.17311																																																																																																																																																																																																																																																																																																																																																								
C	-2.15989	-1.73119	-1.41206																																																																																																																																																																																																																																																																																																																																																								
C	-1.40995	-0.56716	-3.37754																																																																																																																																																																																																																																																																																																																																																								
C	-0.74580	0.34138	-2.56225																																																																																																																																																																																																																																																																																																																																																								
C	-1.49035	-0.83234	-0.58130																																																																																																																																																																																																																																																																																																																																																								
H	-2.71807	-2.54582	-0.97084																																																																																																																																																																																																																																																																																																																																																								
H	-0.18951	1.15932	-3.00256																																																																																																																																																																																																																																																																																																																																																								
C	-0.09856	1.26602	-0.34724																																																																																																																																																																																																																																																																																																																																																								
C	0.83083	3.41534	1.19241																																																																																																																																																																																																																																																																																																																																																								
C	1.14665	1.15143	0.29966																																																																																																																																																																																																																																																																																																																																																								
C	-0.83342	2.45574	-0.22277																																																																																																																																																																																																																																																																																																																																																								
C	-0.38646	3.52705	0.53143																																																																																																																																																																																																																																																																																																																																																								
C	1.56832	2.25010	1.06712																																																																																																																																																																																																																																																																																																																																																								
H	-0.98035	4.42861	0.60674																																																																																																																																																																																																																																																																																																																																																								
H	2.51475	2.18909	1.58519																																																																																																																																																																																																																																																																																																																																																								
H	-1.37189	-0.46017	-4.45389																																																																																																																																																																																																																																																																																																																																																								
H	-2.64624	-2.32610	-3.41601																																																																																																																																																																																																																																																																																																																																																								
H	1.20748	4.22932	1.79831																																																																																																																																																																																																																																																																																																																																																								
C	-1.56355	-0.96369	0.92848																																																																																																																																																																																																																																																																																																																																																								
H	-1.78576	2.51921	-0.73354																																																																																																																																																																																																																																																																																																																																																								
C	2.11898	-0.04698	0.25607																																																																																																																																																																																																																																																																																																																																																								
C	1.70124	-1.23984	-0.61433																																																																																																																																																																																																																																																																																																																																																								
H	2.52002	-1.96330	-0.60413																																																																																																																																																																																																																																																																																																																																																								
H	1.51346	-0.95126	-1.64703																																																																																																																																																																																																																																																																																																																																																								
H	0.81347	-1.73694	-0.23254																																																																																																																																																																																																																																																																																																																																																								
C	2.32006	-0.58343	1.68789																																																																																																																																																																																																																																																																																																																																																								
H	3.03228	-1.41205	1.67140																																																																																																																																																																																																																																																																																																																																																								
H	1.37584	-0.95179	2.09448																																																																																																																																																																																																																																																																																																																																																								
H	2.70485	0.18452	2.35921																																																																																																																																																																																																																																																																																																																																																								
H	-0.67761	-0.48226	1.34326																																																																																																																																																																																																																																																																																																																																																								
C	-1.56733	-2.41384	1.41864																																																																																																																																																																																																																																																																																																																																																								
H	-0.72028	-2.97176	1.01402																																																																																																																																																																																																																																																																																																																																																								
H	-2.48453	-2.93126	1.12963																																																																																																																																																																																																																																																																																																																																																								
H	-1.50714	-2.43492	2.50880																																																																																																																																																																																																																																																																																																																																																								
C	-2.78765	-0.20732	1.46462																																																																																																																																																																																																																																																																																																																																																								
H	-3.70545	-0.64275	1.06128																																																																																																																																																																																																																																																																																																																																																								
H	-2.74904	0.84400	1.17588																																																																																																																																																																																																																																																																																																																																																								
H	-2.82744	-0.26714	2.55523																																																																																																																																																																																																																																																																																																																																																								
C	3.47710	0.44011	-0.29359																																																																																																																																																																																																																																																																																																																																																								
H	4.18444	-0.39256	-0.30423																																																																																																																																																																																																																																																																																																																																																								
H	3.90348	1.24017	0.31107																																																																																																																																																																																																																																																																																																																																																								
H	3.36287	0.80871	-1.31524																																																																																																																																																																																																																																																																																																																																																								
C	-0.57142	-2.24432	-2.68543																																																																																																																																																																																																																																																																																																																																																								
C	-0.03202	-0.42580	-0.56201																																																																																																																																																																																																																																																																																																																																																								
C	-0.64379	-2.62960	-1.35577																																																																																																																																																																																																																																																																																																																																																								
C	-0.00499	-1.01481	-2.96625																																																																																																																																																																																																																																																																																																																																																								
C	0.24864	-0.14980	-1.91604																																																																																																																																																																																																																																																																																																																																																								
C	-0.27239	-1.82291	-0.27085																																																																																																																																																																																																																																																																																																																																																								
H	-0.95281	-3.64363	-1.16216																																																																																																																																																																																																																																																																																																																																																								
C	-0.09353	0.73603	0.39896																																																																																																																																																																																																																																																																																																																																																								
C	-0.01308	2.70967	2.46705																																																																																																																																																																																																																																																																																																																																																								
C	0.05639	2.12804	0.07990																																																																																																																																																																																																																																																																																																																																																								
C	-0.41797	0.47464	1.74183																																																																																																																																																																																																																																																																																																																																																								
C	-0.38219	1.40772	2.76174																																																																																																																																																																																																																																																																																																																																																								
C	0.16552	3.04251	1.13554																																																																																																																																																																																																																																																																																																																																																								
H	-0.63124	1.10712	3.77117																																																																																																																																																																																																																																																																																																																																																								
H	0.35870	0.07795	0.89451																																																																																																																																																																																																																																																																																																																																																								
H	0.22152	-0.71149	-3.98000																																																																																																																																																																																																																																																																																																																																																								
H	-0.87110	-2.92774	-3.46893																																																																																																																																																																																																																																																																																																																																																								
H	0.07868	3.46217	3.23927																																																																																																																																																																																																																																																																																																																																																								
H	0.69779	0.78597	-2.16854																																																																																																																																																																																																																																																																																																																																																								
H	-0.71428	-0.51304	2.00641																																																																																																																																																																																																																																																																																																																																																								
C	0.01200	-2.61937	1.04443																																																																																																																																																																																																																																																																																																																																																								
C	0.01155	2.78597	-1.30298																																																																																																																																																																																																																																																																																																																																																								
C	0.43425	-4.08142	0.71942																																																																																																																																																																																																																																																																																																																																																								
H	0.82496	-4.53173	1.63392																																																																																																																																																																																																																																																																																																																																																								
H	1.21554	-4.10662	-0.04064																																																																																																																																																																																																																																																																																																																																																								
H	-0.39813	-4.70307	0.39042																																																																																																																																																																																																																																																																																																																																																								
C	1.26100	-2.07077	1.77648																																																																																																																																																																																																																																																																																																																																																								
H	1.24017	-1.01396	2.00928																																																																																																																																																																																																																																																																																																																																																								
H	2.14014	-2.25002	1.15355																																																																																																																																																																																																																																																																																																																																																								
H	1.39364	-6.22282	2.71003																																																																																																																																																																																																																																																																																																																																																								
H	-0.47187	2.10423	-1.99381																																																																																																																																																																																																																																																																																																																																																								
C	-0.86872	4.04876	-1.34043																																																																																																																																																																																																																																																																																																																																																								
H	-0.40964	4.89511	-0.82758																																																																																																																																																																																																																																																																																																																																																								
H	-1.84386	3.86150	-0.88822																																																																																																																																																																																																																																																																																																																																																								
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H	1.36895	3.55407	-2.82310																																																																																																																																																																																																																																																																																																																																																								
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C	-1.23112	-2.78812	1.94957																																																																																																																																																																																																																																																																																																																																																								
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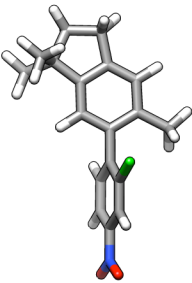
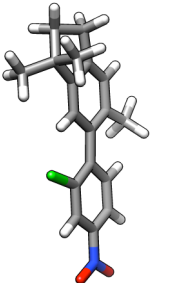
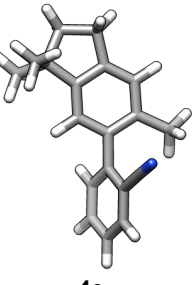
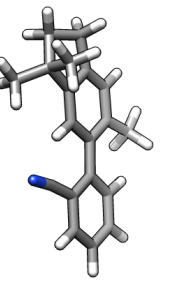
 <p>2e -970.7906701 -970.6285558 -971.4596677</p>	<table border="1"> <tbody> <tr><td>C</td><td>1.79345</td><td>6.41208</td><td>0.15526</td></tr> <tr><td>C</td><td>1.17261</td><td>4.19394</td><td>1.72996</td></tr> <tr><td>C</td><td>2.03560</td><td>5.12936</td><td>-0.33158</td></tr> <tr><td>C</td><td>1.24527</td><td>6.59643</td><td>1.41619</td></tr> <tr><td>C</td><td>0.94313</td><td>5.48398</td><td>2.19445</td></tr> <tr><td>C</td><td>1.72392</td><td>4.01984</td><td>0.44973</td></tr> <tr><td>H</td><td>2.46863</td><td>5.00254</td><td>-1.31222</td></tr> <tr><td>H</td><td>0.51677</td><td>5.61478</td><td>3.18084</td></tr> <tr><td>C</td><td>0.85086</td><td>3.02846</td><td>2.58819</td></tr> <tr><td>C</td><td>0.26248</td><td>0.86969</td><td>4.33107</td></tr> <tr><td>C</td><td>1.41050</td><td>2.91036</td><td>3.86356</td></tr> <tr><td>C</td><td>-0.02780</td><td>1.99648</td><td>2.20515</td></tr> <tr><td>C</td><td>-0.28725</td><td>0.92349</td><td>3.05836</td></tr> <tr><td>C</td><td>1.11122</td><td>1.88336</td><td>4.74627</td></tr> <tr><td>H</td><td>-0.94265</td><td>0.13870</td><td>2.70767</td></tr> <tr><td>H</td><td>1.56182</td><td>1.88222</td><td>5.72839</td></tr> <tr><td>H</td><td>1.05631</td><td>7.59115</td><td>1.79509</td></tr> <tr><td>H</td><td>2.04034</td><td>7.26616</td><td>-0.46172</td></tr> <tr><td>H</td><td>0.03555</td><td>0.04459</td><td>4.99161</td></tr> <tr><td>O</td><td>1.91722</td><td>2.73420</td><td>0.05451</td></tr> <tr><td>C</td><td>2.43543</td><td>2.49476</td><td>-1.24476</td></tr> <tr><td>H</td><td>1.78191</td><td>2.92210</td><td>-2.01160</td></tr> <tr><td>H</td><td>2.47611</td><td>1.41393</td><td>-1.35610</td></tr> <tr><td>H</td><td>3.43837</td><td>2.91902</td><td>-1.34926</td></tr> <tr><td>N</td><td>2.42574</td><td>3.87950</td><td>4.33132</td></tr> <tr><td>O</td><td>3.39809</td><td>4.06395</td><td>3.62350</td></tr> <tr><td>O</td><td>2.23106</td><td>4.39968</td><td>5.41976</td></tr> 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</table>	C	1.79345	6.41208	0.15526	C	1.17261	4.19394	1.72996	C	2.03560	5.12936	-0.33158	C	1.24527	6.59643	1.41619	C	0.94313	5.48398	2.19445	C	1.72392	4.01984	0.44973	H	2.46863	5.00254	-1.31222	H	0.51677	5.61478	3.18084	C	0.85086	3.02846	2.58819	C	0.26248	0.86969	4.33107	C	1.41050	2.91036	3.86356	C	-0.02780	1.99648	2.20515	C	-0.28725	0.92349	3.05836	C	1.11122	1.88336	4.74627	H	-0.94265	0.13870	2.70767	H	1.56182	1.88222	5.72839	H	1.05631	7.59115	1.79509	H	2.04034	7.26616	-0.46172	H	0.03555	0.04459	4.99161	O	1.91722	2.73420	0.05451	C	2.43543	2.49476	-1.24476	H	1.78191	2.92210	-2.01160	H	2.47611	1.41393	-1.35610	H	3.43837	2.91902	-1.34926	N	2.42574	3.87950	4.33132	O	3.39809	4.06395	3.62350	O	2.23106	4.39968	5.41976	C	-0.74118	1.94953	0.89107	O	-0.97969	0.92698	0.29845	O	-1.15897	3.15611	0.45772	H	-1.61247	3.01438	-0.38529	 <p>2e -970.7581536 -970.5962381 -971.4289190</p>	<table border="1"> <tbody> <tr><td>C</td><td>0.38989</td><td>-1.63142</td><td>-3.38514</td></tr> <tr><td>C</td><td>0.22305</td><td>-0.26435</td><td>-0.88930</td></tr> <tr><td>C</td><td>0.28289</td><td>-2.34220</td><td>-2.20228</td></tr> <tr><td>C</td><td>0.52235</td><td>-0.24982</td><td>-3.33505</td></tr> <tr><td>C</td><td>0.45616</td><td>0.39502</td><td>-2.11341</td></tr> <tr><td>C</td><td>0.25984</td><td>-1.68403</td><td>-0.96825</td></tr> <tr><td>H</td><td>0.25197</td><td>-3.42042</td><td>-2.22582</td></tr> <tr><td>H</td><td>0.63780</td><td>1.45614</td><td>-2.12340</td></tr> <tr><td>C</td><td>0.10692</td><td>0.55189</td><td>0.35390</td></tr> <tr><td>C</td><td>0.71451</td><td>2.30149</td><td>2.55323</td></tr> <tr><td>C</td><td>0.02490</td><td>1.97534</td><td>0.25798</td></tr> <tr><td>C</td><td>0.20861</td><td>0.10705</td><td>1.69848</td></tr> <tr><td>C</td><td>0.56216</td><td>0.94184</td><td>2.75275</td></tr> <tr><td>C</td><td>0.37333</td><td>2.81503</td><td>1.31290</td></tr> <tr><td>H</td><td>0.67853</td><td>0.50323</td><td>3.73337</td></tr> <tr><td>H</td><td>0.33783</td><td>3.88255</td><td>1.14562</td></tr> <tr><td>H</td><td>0.69492</td><td>0.32547</td><td>-4.23391</td></tr> <tr><td>H</td><td>0.41698</td><td>-2.15851</td><td>-4.32969</td></tr> <tr><td>H</td><td>1.00594</td><td>2.95061</td><td>3.36658</td></tr> <tr><td>C</td><td>-0.59717</td><td>2.71820</td><td>-0.88450</td></tr> <tr><td>O</td><td>-1.76117</td><td>2.15440</td><td>-1.27520</td></tr> <tr><td>O</td><td>-0.19027</td><td>3.75816</td><td>-1.34085</td></tr> <tr><td>N</td><td>-0.27169</td><td>-1.20405</td><td>2.19415</td></tr> <tr><td>O</td><td>-1.43163</td><td>-1.47067</td><td>1.93358</td></tr> <tr><td>O</td><td>0.45547</td><td>-1.85954</td><td>2.92088</td></tr> <tr><td>O</td><td>0.34043</td><td>-2.36720</td><td>0.18131</td></tr> <tr><td>C</td><td>0.24063</td><td>-3.78296</td><td>0.21264</td></tr> <tr><td>H</td><td>1.08278</td><td>-4.24335</td><td>-0.31122</td></tr> <tr><td>H</td><td>-0.69912</td><td>-4.11370</td><td>-0.23635</td></tr> <tr><td>H</td><td>0.26341</td><td>-4.04693</td><td>1.26736</td></tr> <tr><td>H</td><td>-2.12054</td><td>2.70042</td><td>-1.98885</td></tr> </tbody> </table>	C	0.38989	-1.63142	-3.38514	C	0.22305	-0.26435	-0.88930	C	0.28289	-2.34220	-2.20228	C	0.52235	-0.24982	-3.33505	C	0.45616	0.39502	-2.11341	C	0.25984	-1.68403	-0.96825	H	0.25197	-3.42042	-2.22582	H	0.63780	1.45614	-2.12340	C	0.10692	0.55189	0.35390	C	0.71451	2.30149	2.55323	C	0.02490	1.97534	0.25798	C	0.20861	0.10705	1.69848	C	0.56216	0.94184	2.75275	C	0.37333	2.81503	1.31290	H	0.67853	0.50323	3.73337	H	0.33783	3.88255	1.14562	H	0.69492	0.32547	-4.23391	H	0.41698	-2.15851	-4.32969	H	1.00594	2.95061	3.36658	C	-0.59717	2.71820	-0.88450	O	-1.76117	2.15440	-1.27520	O	-0.19027	3.75816	-1.34085	N	-0.27169	-1.20405	2.19415	O	-1.43163	-1.47067	1.93358	O	0.45547	-1.85954	2.92088	O	0.34043	-2.36720	0.18131	C	0.24063	-3.78296	0.21264	H	1.08278	-4.24335	-0.31122	H	-0.69912	-4.11370	-0.23635	H	0.26341	-4.04693	1.26736	H	-2.12054	2.70042	-1.98885																																																																																								
C	1.79345	6.41208	0.15526																																																																																																																																																																																																																																																																																																																																																
C	1.17261	4.19394	1.72996																																																																																																																																																																																																																																																																																																																																																
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C	1.24527	6.59643	1.41619																																																																																																																																																																																																																																																																																																																																																
C	0.94313	5.48398	2.19445																																																																																																																																																																																																																																																																																																																																																
C	1.72392	4.01984	0.44973																																																																																																																																																																																																																																																																																																																																																
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C	0.26248	0.86969	4.33107																																																																																																																																																																																																																																																																																																																																																
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H	1.05631	7.59115	1.79509																																																																																																																																																																																																																																																																																																																																																
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O	1.91722	2.73420	0.05451																																																																																																																																																																																																																																																																																																																																																
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H	1.78191	2.92210	-2.01160																																																																																																																																																																																																																																																																																																																																																
H	2.47611	1.41393	-1.35610																																																																																																																																																																																																																																																																																																																																																
H	3.43837	2.91902	-1.34926																																																																																																																																																																																																																																																																																																																																																
N	2.42574	3.87950	4.33132																																																																																																																																																																																																																																																																																																																																																
O	3.39809	4.06395	3.62350																																																																																																																																																																																																																																																																																																																																																
O	2.23106	4.39968	5.41976																																																																																																																																																																																																																																																																																																																																																
C	-0.74118	1.94953	0.89107																																																																																																																																																																																																																																																																																																																																																
O	-0.97969	0.92698	0.29845																																																																																																																																																																																																																																																																																																																																																
O	-1.15897	3.15611	0.45772																																																																																																																																																																																																																																																																																																																																																
H	-1.61247	3.01438	-0.38529																																																																																																																																																																																																																																																																																																																																																
C	0.38989	-1.63142	-3.38514																																																																																																																																																																																																																																																																																																																																																
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C	0.10692	0.55189	0.35390																																																																																																																																																																																																																																																																																																																																																
C	0.71451	2.30149	2.55323																																																																																																																																																																																																																																																																																																																																																
C	0.02490	1.97534	0.25798																																																																																																																																																																																																																																																																																																																																																
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H	0.69492	0.32547	-4.23391																																																																																																																																																																																																																																																																																																																																																
H	0.41698	-2.15851	-4.32969																																																																																																																																																																																																																																																																																																																																																
H	1.00594	2.95061	3.36658																																																																																																																																																																																																																																																																																																																																																
C	-0.59717	2.71820	-0.88450																																																																																																																																																																																																																																																																																																																																																
O	-1.76117	2.15440	-1.27520																																																																																																																																																																																																																																																																																																																																																
O	-0.19027	3.75816	-1.34085																																																																																																																																																																																																																																																																																																																																																
N	-0.27169	-1.20405	2.19415																																																																																																																																																																																																																																																																																																																																																
O	-1.43163	-1.47067	1.93358																																																																																																																																																																																																																																																																																																																																																
O	0.45547	-1.85954	2.92088																																																																																																																																																																																																																																																																																																																																																
O	0.34043	-2.36720	0.18131																																																																																																																																																																																																																																																																																																																																																
C	0.24063	-3.78296	0.21264																																																																																																																																																																																																																																																																																																																																																
H	1.08278	-4.24335	-0.31122																																																																																																																																																																																																																																																																																																																																																
H	-0.69912	-4.11370	-0.23635																																																																																																																																																																																																																																																																																																																																																
H	0.26341	-4.04693	1.26736																																																																																																																																																																																																																																																																																																																																																
H	-2.12054	2.70042	-1.98885																																																																																																																																																																																																																																																																																																																																																
 <p>2f -770.7593707 -770.6420523 -771.3656017</p>	<table border="1"> <tbody> <tr><td>C</td><td>-1.70007</td><td>0.83189</td><td>-3.30666</td></tr> <tr><td>C</td><td>-1.06162</td><td>0.62193</td><td>-0.59446</td></tr> <tr><td>C</td><td>-1.35952</td><td>-0.39881</td><td>-2.75983</td></tr> <tr><td>C</td><td>-1.77053</td><td>1.95939</td><td>-2.49840</td></tr> <tr><td>C</td><td>-1.46036</td><td>1.83974</td><td>-1.15093</td></tr> <tr><td>C</td><td>-1.05099</td><td>-0.53758</td><td>-1.40003</td></tr> <tr><td>H</td><td>-1.35312</td><td>-1.26867</td><td>-3.39884</td></tr> <tr><td>H</td><td>-1.49282</td><td>2.71356</td><td>-0.51260</td></tr> <tr><td>C</td><td>-0.69469</td><td>0.64762</td><td>0.85506</td></tr> <tr><td>C</td><td>-0.35452</td><td>0.79971</td><td>3.65316</td></tr> <tr><td>C</td><td>0.59130</td><td>0.64296</td><td>1.42695</td></tr> <tr><td>C</td><td>-1.77797</td><td>0.77879</td><td>1.73662</td></tr> <tr><td>C</td><td>-1.62870</td><td>0.85470</td><td>3.11095</td></tr> <tr><td>C</td><td>0.74417</td><td>0.69903</td><td>2.81216</td></tr> <tr><td>H</td><td>-2.76809</td><td>0.81026</td><td>1.30286</td></tr> <tr><td>H</td><td>-2.49747</td><td>0.95204</td><td>3.74719</td></tr> <tr><td>H</td><td>1.71505</td><td>0.67953</td><td>3.27537</td></tr> <tr><td>H</td><td>-2.05868</td><td>2.91739</td><td>-2.90817</td></tr> <tr><td>H</td><td>-1.93401</td><td>0.89929</td><td>-4.36061</td></tr> <tr><td>H</td><td>-0.20111</td><td>0.84677</td><td>4.72202</td></tr> <tr><td>N</td><td>1.85925</td><td>0.54240</td><td>0.59645</td></tr> <tr><td>C</td><td>2.11434</td><td>-0.90674</td><td>0.26504</td></tr> <tr><td>H</td><td>2.98793</td><td>-0.95638</td><td>-0.38295</td></tr> <tr><td>H</td><td>1.22014</td><td>-1.30619</td><td>-0.21446</td></tr> <tr><td>H</td><td>2.30340</td><td>-1.42989</td><td>1.19947</td></tr> <tr><td>C</td><td>3.07107</td><td>1.06170</td><td>1.33001</td></tr> <tr><td>H</td><td>3.90165</td><td>1.04606</td><td>0.63009</td></tr> <tr><td>H</td><td>3.30556</td><td>0.41054</td><td>2.16393</td></tr> <tr><td>H</td><td>2.87324</td><td>2.07474</td><td>1.66886</td></tr> <tr><td>C</td><td>1.78831</td><td>1.34347</td><td>-0.68354</td></tr> <tr><td>H</td><td>2.77742</td><td>1.32463</td><td>-1.13381</td></tr> <tr><td>H</td><td>1.49716</td><td>2.35975</td><td>-0.43390</td></tr> <tr><td>H</td><td>1.06560</td><td>0.90034</td><td>-1.35293</td></tr> <tr><td>N</td><td>-0.68980</td><td>-1.79204</td><td>-0.85023</td></tr> <tr><td>C</td><td>-1.61652</td><td>-2.34340</td><td>0.14446</td></tr> <tr><td>H</td><td>-2.53821</td><td>-2.70327</td><td>-0.33180</td></tr> <tr><td>H</td><td>-1.87662</td><td>-1.59977</td><td>0.89030</td></tr> <tr><td>H</td><td>-1.13602</td><td>-3.18457</td><td>0.64638</td></tr> <tr><td>C</td><td>-0.28390</td><td>-2.82545</td><td>-1.79720</td></tr> <tr><td>H</td><td>0.16179</td><td>-3.64876</td><td>-1.23744</td></tr> <tr><td>H</td><td>0.45500</td><td>-2.42923</td><td>-2.49404</td></tr> <tr><td>H</td><td>-1.12702</td><td>-3.22748</td><td>-2.37450</td></tr> </tbody> </table>	C	-1.70007	0.83189	-3.30666	C	-1.06162	0.62193	-0.59446	C	-1.35952	-0.39881	-2.75983	C	-1.77053	1.95939	-2.49840	C	-1.46036	1.83974	-1.15093	C	-1.05099	-0.53758	-1.40003	H	-1.35312	-1.26867	-3.39884	H	-1.49282	2.71356	-0.51260	C	-0.69469	0.64762	0.85506	C	-0.35452	0.79971	3.65316	C	0.59130	0.64296	1.42695	C	-1.77797	0.77879	1.73662	C	-1.62870	0.85470	3.11095	C	0.74417	0.69903	2.81216	H	-2.76809	0.81026	1.30286	H	-2.49747	0.95204	3.74719	H	1.71505	0.67953	3.27537	H	-2.05868	2.91739	-2.90817	H	-1.93401	0.89929	-4.36061	H	-0.20111	0.84677	4.72202	N	1.85925	0.54240	0.59645	C	2.11434	-0.90674	0.26504	H	2.98793	-0.95638	-0.38295	H	1.22014	-1.30619	-0.21446	H	2.30340	-1.42989	1.19947	C	3.07107	1.06170	1.33001	H	3.90165	1.04606	0.63009	H	3.30556	0.41054	2.16393	H	2.87324	2.07474	1.66886	C	1.78831	1.34347	-0.68354	H	2.77742	1.32463	-1.13381	H	1.49716	2.35975	-0.43390	H	1.06560	0.90034	-1.35293	N	-0.68980	-1.79204	-0.85023	C	-1.61652	-2.34340	0.14446	H	-2.53821	-2.70327	-0.33180	H	-1.87662	-1.59977	0.89030	H	-1.13602	-3.18457	0.64638	C	-0.28390	-2.82545	-1.79720	H	0.16179	-3.64876	-1.23744	H	0.45500	-2.42923	-2.49404	H	-1.12702	-3.22748	-2.37450	 <p>2f -770.7139419 -770.5973848 -771.3226472</p>	<table border="1"> <tbody> <tr><td>C</td><td>-2.63282</td><td>-0.12744</td><td>-2.59600</td></tr> <tr><td>C</td><td>-0.69935</td><td>0.11749</td><td>-0.47358</td></tr> <tr><td>C</td><td>-2.99277</td><td>-0.28997</td><td>-1.27141</td></tr> <tr><td>C</td><td>-1.33491</td><td>0.26285</td><td>-2.87186</td></tr> <tr><td>C</td><td>-0.42544</td><td>0.37100</td><td>-1.83334</td></tr> <tr><td>C</td><td>-2.10261</td><td>-0.11506</td><td>-0.20426</td></tr> <tr><td>H</td><td>-4.02453</td><td>-0.50786</td><td>-1.04350</td></tr> <tr><td>H</td><td>0.55211</td><td>0.65458</td><td>-2.14654</td></tr> <tr><td>C</td><td>0.40570</td><td>0.04780</td><td>0.57033</td></tr> <tr><td>C</td><td>2.19859</td><td>0.00150</td><td>2.85105</td></tr> <tr><td>C</td><td>1.84366</td><td>0.02598</td><td>0.43742</td></tr> <tr><td>C</td><td>0.00202</td><td>-0.06431</td><td>1.91943</td></tr> <tr><td>C</td><td>0.83458</td><td>-0.09339</td><td>3.02337</td></tr> <tr><td>C</td><td>2.67748</td><td>0.03800</td><td>1.55282</td></tr> <tr><td>H</td><td>-1.05045</td><td>-0.17230</td><td>2.09261</td></tr> <tr><td>H</td><td>0.39896</td><td>-0.18193</td><td>4.00924</td></tr> <tr><td>H</td><td>3.74524</td><td>0.06230</td><td>1.44079</td></tr> <tr><td>H</td><td>-1.01537</td><td>0.47439</td><td>-3.88305</td></tr> <tr><td>H</td><td>-3.36482</td><td>-0.25228</td><td>-3.38223</td></tr> <tr><td>H</td><td>2.88749</td><td>0.02063</td><td>3.68352</td></tr> <tr><td>N</td><td>2.60114</td><td>-0.02285</td><td>-0.88353</td></tr> <tr><td>C</td><td>2.10402</td><td>-1.19470</td><td>-1.72150</td></tr> <tr><td>H</td><td>2.43923</td><td>-1.04499</td><td>-2.74519</td></tr> <tr><td>H</td><td>1.03038</td><td>-1.28017</td><td>-1.68055</td></tr> <tr><td>H</td><td>2.55241</td><td>-2.09093</td><td>-1.30221</td></tr> <tr><td>C</td><td>4.08589</td><td>-0.32115</td><td>-0.76457</td></tr> <tr><td>H</td><td>4.45598</td><td>-0.41953</td><td>-1.78266</td></tr> <tr><td>H</td><td>4.22491</td><td>-1.24987</td><td>-0.22123</td></tr> <tr><td>H</td><td>4.60213</td><td>0.49654</td><td>-0.27492</td></tr> <tr><td>C</td><td>2.55341</td><td>1.34907</td><td>-1.54264</td></tr> <tr><td>H</td><td>2.72240</td><td>1.23447</td><td>-2.61134</td></tr> <tr><td>H</td><td>3.34311</td><td>1.94822</td><td>-1.09832</td></tr> <tr><td>H</td><td>1.60894</td><td>1.83491</td><td>-1.34310</td></tr> <tr><td>N</td><td>-2.66432</td><td>-0.11239</td><td>1.09615</td></tr> <tr><td>C</td><td>-2.81865</td><td>1.24069</td><td>1.64107</td></tr> <tr><td>H</td><td>-3.62248</td><td>1.78409</td><td>1.12750</td></tr> <tr><td>H</td><td>-1.89107</td><td>1.80081</td><td>1.52923</td></tr> <tr><td>H</td><td>-3.06031</td><td>1.17437</td><td>2.70337</td></tr> <tr><td>C</td><td>-3.85169</td><td>-0.92273</td><td>1.33750</td></tr> <tr><td>H</td><td>-3.97765</td><td>-1.02678</td><td>2.41618</td></tr> <tr><td>H</td><td>-3.72231</td><td>-1.91184</td><td>0.90089</td></tr> <tr><td>H</td><td>-4.77060</td><td>-0.47296</td><td>0.93621</td></tr> </tbody> </table>	C	-2.63282	-0.12744	-2.59600	C	-0.69935	0.11749	-0.47358	C	-2.99277	-0.28997	-1.27141	C	-1.33491	0.26285	-2.87186	C	-0.42544	0.37100	-1.83334	C	-2.10261	-0.11506	-0.20426	H	-4.02453	-0.50786	-1.04350	H	0.55211	0.65458	-2.14654	C	0.40570	0.04780	0.57033	C	2.19859	0.00150	2.85105	C	1.84366	0.02598	0.43742	C	0.00202	-0.06431	1.91943	C	0.83458	-0.09339	3.02337	C	2.67748	0.03800	1.55282	H	-1.05045	-0.17230	2.09261	H	0.39896	-0.18193	4.00924	H	3.74524	0.06230	1.44079	H	-1.01537	0.47439	-3.88305	H	-3.36482	-0.25228	-3.38223	H	2.88749	0.02063	3.68352	N	2.60114	-0.02285	-0.88353	C	2.10402	-1.19470	-1.72150	H	2.43923	-1.04499	-2.74519	H	1.03038	-1.28017	-1.68055	H	2.55241	-2.09093	-1.30221	C	4.08589	-0.32115	-0.76457	H	4.45598	-0.41953	-1.78266	H	4.22491	-1.24987	-0.22123	H	4.60213	0.49654	-0.27492	C	2.55341	1.34907	-1.54264	H	2.72240	1.23447	-2.61134	H	3.34311	1.94822	-1.09832	H	1.60894	1.83491	-1.34310	N	-2.66432	-0.11239	1.09615	C	-2.81865	1.24069	1.64107	H	-3.62248	1.78409	1.12750	H	-1.89107	1.80081	1.52923	H	-3.06031	1.17437	2.70337	C	-3.85169	-0.92273	1.33750	H	-3.97765	-1.02678	2.41618	H	-3.72231	-1.91184	0.90089	H	-4.77060	-0.47296	0.93621
C	-1.70007	0.83189	-3.30666																																																																																																																																																																																																																																																																																																																																																
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C	0.74417	0.69903	2.81216																																																																																																																																																																																																																																																																																																																																																
H	-2.76809	0.81026	1.30286																																																																																																																																																																																																																																																																																																																																																
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H	3.90165	1.04606	0.63009																																																																																																																																																																																																																																																																																																																																																
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H	2.87324	2.07474	1.66886																																																																																																																																																																																																																																																																																																																																																
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H	1.06560	0.90034	-1.35293																																																																																																																																																																																																																																																																																																																																																
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C	-2.99277	-0.28997	-1.27141																																																																																																																																																																																																																																																																																																																																																
C	-1.33491	0.26285	-2.87186																																																																																																																																																																																																																																																																																																																																																
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C	0.40570	0.04780	0.57033																																																																																																																																																																																																																																																																																																																																																
C	2.19859	0.00150	2.85105																																																																																																																																																																																																																																																																																																																																																
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C	0.00202	-0.06431	1.91943																																																																																																																																																																																																																																																																																																																																																
C	0.83458	-0.09339	3.02337																																																																																																																																																																																																																																																																																																																																																
C	2.67748	0.03800	1.55282																																																																																																																																																																																																																																																																																																																																																
H	-1.05045	-0.17230	2.09261																																																																																																																																																																																																																																																																																																																																																
H	0.39896	-0.18193	4.00924																																																																																																																																																																																																																																																																																																																																																
H	3.74524	0.06230	1.44079																																																																																																																																																																																																																																																																																																																																																
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H	-3.36482	-0.25228	-3.38223																																																																																																																																																																																																																																																																																																																																																
H	2.88749	0.02063	3.68352																																																																																																																																																																																																																																																																																																																																																
N	2.60114	-0.02285	-0.88353																																																																																																																																																																																																																																																																																																																																																
C	2.10402	-1.19470	-1.72150																																																																																																																																																																																																																																																																																																																																																
H	2.43923	-1.04499	-2.74519																																																																																																																																																																																																																																																																																																																																																
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H	4.22491	-1.24987	-0.22123																																																																																																																																																																																																																																																																																																																																																
H	4.60213	0.49654	-0.27492																																																																																																																																																																																																																																																																																																																																																
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H	-1.89107	1.80081	1.52923																																																																																																																																																																																																																																																																																																																																																
H	-3.06031	1.17437	2.70337																																																																																																																																																																																																																																																																																																																																																
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H	-3.97765	-1.02678	2.41618																																																																																																																																																																																																																																																																																																																																																
H	-3.72231	-1.91184	0.90089																																																																																																																																																																																																																																																																																																																																																
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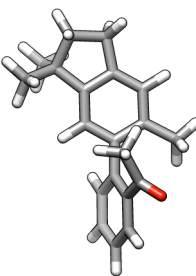
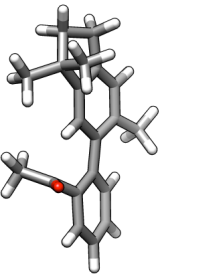
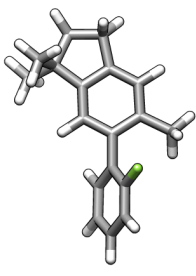
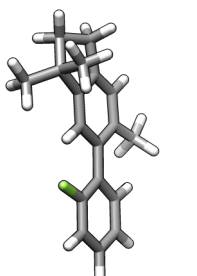
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<tr><td>H</td><td>-1.17462</td><td>-1.35409</td><td>4.46539</td></tr> <tr><td>H</td><td>-0.91273</td><td>3.83342</td><td>-2.03110</td></tr> <tr><td>H</td><td>0.61532</td><td>0.26989</td><td>3.83836</td></tr> <tr><td>H</td><td>-1.21820</td><td>-0.09294</td><td>-3.75076</td></tr> <tr><td>H</td><td>-2.98891</td><td>-1.84154</td><td>2.82909</td></tr> <tr><td>C</td><td>-1.31534</td><td>-1.56931</td><td>-1.60206</td></tr> <tr><td>O</td><td>-0.67772</td><td>-2.19488</td><td>-0.72998</td></tr> <tr><td>O</td><td>-2.08110</td><td>-2.03975</td><td>-2.48322</td></tr> <tr><td>C</td><td>1.08714</td><td>1.53999</td><td>1.60927</td></tr> <tr><td>O</td><td>1.38382</td><td>2.26780</td><td>2.59230</td></tr> <tr><td>O</td><td>1.62589</td><td>1.51900</td><td>0.48328</td></tr> <tr><td>O</td><td>-1.10410</td><td>2.98289</td><td>0.45270</td></tr> <tr><td>O</td><td>-3.17999</td><td>-0.78143</td><td>0.42753</td></tr> <tr><td>C</td><td>-3.66302</td><td>-2.10933</td><td>0.29270</td></tr> <tr><td>H</td><td>-2.82421</td><td>-2.80636</td><td>0.22335</td></tr> <tr><td>H</td><td>-4.21239</td><td>-2.13684</td><td>-0.64755</td></tr> <tr><td>H</td><td>-4.32582</td><td>-2.38072</td><td>1.12880</td></tr> <tr><td>C</td><td>-0.21174</td><td>4.08571</td><td>0.49946</td></tr> <tr><td>H</td><td>-0.57674</td><td>4.92213</td><td>-0.11635</td></tr> <tr><td>H</td><td>0.78428</td><td>3.77392</td><td>0.17542</td></tr> <tr><td>H</td><td>-0.15591</td><td>4.38484</td><td>1.54542</td></tr> </tbody> </table>	C	-1.01081	1.93557	-3.05517	C	-1.08994	0.79221	-0.48317	C	-1.13261	0.56475	-2.89594	C	-0.98089	2.75754	-1.93321	C	-1.04250	2.18559	-0.66721	C	-1.17230	-0.02694	-1.62805	C	-1.08774	0.25091	0.90988	C	-1.16131	-0.89524	3.48081	C	-0.09384	0.56861	1.85849	C	-2.14258	-0.58829	1.31083	C	-2.17535	-1.17587	2.57073	C	-0.15270	-0.01243	3.13055	H	-0.95702	2.37228	-4.04840	H	-1.17462	-1.35409	4.46539	H	-0.91273	3.83342	-2.03110	H	0.61532	0.26989	3.83836	H	-1.21820	-0.09294	-3.75076	H	-2.98891	-1.84154	2.82909	C	-1.31534	-1.56931	-1.60206	O	-0.67772	-2.19488	-0.72998	O	-2.08110	-2.03975	-2.48322	C	1.08714	1.53999	1.60927	O	1.38382	2.26780	2.59230	O	1.62589	1.51900	0.48328	O	-1.10410	2.98289	0.45270	O	-3.17999	-0.78143	0.42753	C	-3.66302	-2.10933	0.29270	H	-2.82421	-2.80636	0.22335	H	-4.21239	-2.13684	-0.64755	H	-4.32582	-2.38072	1.12880	C	-0.21174	4.08571	0.49946	H	-0.57674	4.92213	-0.11635	H	0.78428	3.77392	0.17542	H	-0.15591	4.38484	1.54542	 <p>2g -1068.138459 -1067.946502 -1068.863514</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.46295</td><td>0.60050</td><td>-3.51715</td></tr> <tr><td>C</td><td>0.01424</td><td>0.16357</td><td>-0.73328</td></tr> <tr><td>C</td><td>-0.12185</td><td>-0.66433</td><td>-3.06279</td></tr> <tr><td>C</td><td>-0.36233</td><td>1.66458</td><td>-2.63833</td></tr> <tr><td>C</td><td>-0.05262</td><td>1.48597</td><td>-1.28431</td></tr> <tr><td>C</td><td>0.19283</td><td>-0.85690</td><td>-1.71588</td></tr> <tr><td>C</td><td>-0.01393</td><td>-0.16457</td><td>0.73239</td></tr> <tr><td>C</td><td>0.46643</td><td>-0.60063</td><td>3.51575</td></tr> <tr><td>C</td><td>-0.19213</td><td>0.85598</td><td>1.71492</td></tr> <tr><td>C</td><td>0.05305</td><td>-1.48678</td><td>1.28372</td></tr> <tr><td>C</td><td>0.36440</td><td>-1.66501</td><td>2.63744</td></tr> <tr><td>C</td><td>0.12446</td><td>0.66401</td><td>3.06147</td></tr> <tr><td>H</td><td>-0.73550</td><td>0.75632</td><td>-4.55693</td></tr> 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<tr><td>H</td><td>0.44863</td><td>3.33360</td><td>2.29524</td></tr> <tr><td>H</td><td>-1.18261</td><td>3.14389</td><td>3.03150</td></tr> <tr><td>H</td><td>-0.96220</td><td>3.99395</td><td>1.45138</td></tr> <tr><td>C</td><td>0.60925</td><td>-3.18688</td><td>-2.09033</td></tr> <tr><td>H</td><td>1.17704</td><td>-3.14950</td><td>-3.03139</td></tr> <tr><td>H</td><td>-0.45455</td><td>-3.33240</td><td>-2.29398</td></tr> <tr><td>H</td><td>0.95426</td><td>-3.99673</td><td>-1.45015</td></tr> </tbody> </table>	C	-0.46295	0.60050	-3.51715	C	0.01424	0.16357	-0.73328	C	-0.12185	-0.66433	-3.06279	C	-0.36233	1.66458	-2.63833	C	-0.05262	1.48597	-1.28431	C	0.19283	-0.85690	-1.71588	C	-0.01393	-0.16457	0.73239	C	0.46643	-0.60063	3.51575	C	-0.19213	0.85598	1.71492	C	0.05305	-1.48678	1.28372	C	0.36440	-1.66501	2.63744	C	0.12446	0.66401	3.06147	H	-0.73550	0.75632	-4.55693	H	0.74058	-0.75599	4.55517	H	0.49425	-2.68507	2.97381	H	-0.49217	2.68467	-2.97462	H	-0.05954	-1.49732	-3.74757	H	0.06310	1.49716	3.74611	C	-0.42826	-2.81306	0.62965	O	0.25471	-3.84204	0.85360	O	-1.53011	-2.73294	0.04229	C	0.42674	2.81256	-0.62954	O	1.52936	2.73399	-0.04373	O	-0.25846	3.84049	-0.85165	O	0.80428	-2.00947	-1.33349	O	-0.80507	2.00758	1.33250	C	-0.61452	3.18459	2.09075	H	0.44863	3.33360	2.29524	H	-1.18261	3.14389	3.03150	H	-0.96220	3.99395	1.45138	C	0.60925	-3.18688	-2.09033	H	1.17704	-3.14950	-3.03139	H	-0.45455	-3.33240	-2.29398	H	0.95426	-3.99673	-1.45015																																
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H	0.61532	0.26989	3.83836																																																																																																																																																																																																																																																																																																																
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C	1.08714	1.53999	1.60927																																																																																																																																																																																																																																																																																																																
O	1.38382	2.26780	2.59230																																																																																																																																																																																																																																																																																																																
O	1.62589	1.51900	0.48328																																																																																																																																																																																																																																																																																																																
O	-1.10410	2.98289	0.45270																																																																																																																																																																																																																																																																																																																
O	-3.17999	-0.78143	0.42753																																																																																																																																																																																																																																																																																																																
C	-3.66302	-2.10933	0.29270																																																																																																																																																																																																																																																																																																																
H	-2.82421	-2.80636	0.22335																																																																																																																																																																																																																																																																																																																
H	-4.21239	-2.13684	-0.64755																																																																																																																																																																																																																																																																																																																
H	-4.32582	-2.38072	1.12880																																																																																																																																																																																																																																																																																																																
C	-0.21174	4.08571	0.49946																																																																																																																																																																																																																																																																																																																
H	-0.57674	4.92213	-0.11635																																																																																																																																																																																																																																																																																																																
H	0.78428	3.77392	0.17542																																																																																																																																																																																																																																																																																																																
H	-0.15591	4.38484	1.54542																																																																																																																																																																																																																																																																																																																
C	-0.46295	0.60050	-3.51715																																																																																																																																																																																																																																																																																																																
C	0.01424	0.16357	-0.73328																																																																																																																																																																																																																																																																																																																
C	-0.12185	-0.66433	-3.06279																																																																																																																																																																																																																																																																																																																
C	-0.36233	1.66458	-2.63833																																																																																																																																																																																																																																																																																																																
C	-0.05262	1.48597	-1.28431																																																																																																																																																																																																																																																																																																																
C	0.19283	-0.85690	-1.71588																																																																																																																																																																																																																																																																																																																
C	-0.01393	-0.16457	0.73239																																																																																																																																																																																																																																																																																																																
C	0.46643	-0.60063	3.51575																																																																																																																																																																																																																																																																																																																
C	-0.19213	0.85598	1.71492																																																																																																																																																																																																																																																																																																																
C	0.05305	-1.48678	1.28372																																																																																																																																																																																																																																																																																																																
C	0.36440	-1.66501	2.63744																																																																																																																																																																																																																																																																																																																
C	0.12446	0.66401	3.06147																																																																																																																																																																																																																																																																																																																
H	-0.73550	0.75632	-4.55693																																																																																																																																																																																																																																																																																																																
H	0.74058	-0.75599	4.55517																																																																																																																																																																																																																																																																																																																
H	0.49425	-2.68507	2.97381																																																																																																																																																																																																																																																																																																																
H	-0.49217	2.68467	-2.97462																																																																																																																																																																																																																																																																																																																
H	-0.05954	-1.49732	-3.74757																																																																																																																																																																																																																																																																																																																
H	0.06310	1.49716	3.74611																																																																																																																																																																																																																																																																																																																
C	-0.42826	-2.81306	0.62965																																																																																																																																																																																																																																																																																																																
O	0.25471	-3.84204	0.85360																																																																																																																																																																																																																																																																																																																
O	-1.53011	-2.73294	0.04229																																																																																																																																																																																																																																																																																																																
C	0.42674	2.81256	-0.62954																																																																																																																																																																																																																																																																																																																
O	1.52936	2.73399	-0.04373																																																																																																																																																																																																																																																																																																																
O	-0.25846	3.84049	-0.85165																																																																																																																																																																																																																																																																																																																
O	0.80428	-2.00947	-1.33349																																																																																																																																																																																																																																																																																																																
O	-0.80507	2.00758	1.33250																																																																																																																																																																																																																																																																																																																
C	-0.61452	3.18459	2.09075																																																																																																																																																																																																																																																																																																																
H	0.44863	3.33360	2.29524																																																																																																																																																																																																																																																																																																																
H	-1.18261	3.14389	3.03150																																																																																																																																																																																																																																																																																																																
H	-0.96220	3.99395	1.45138																																																																																																																																																																																																																																																																																																																
C	0.60925	-3.18688	-2.09033																																																																																																																																																																																																																																																																																																																
H	1.17704	-3.14950	-3.03139																																																																																																																																																																																																																																																																																																																
H	-0.45455	-3.33240	-2.29398																																																																																																																																																																																																																																																																																																																
H	0.95426	-3.99673	-1.45015																																																																																																																																																																																																																																																																																																																
 <p>2h -1029.637239 -1029.459687 -1030.354784</p>	<table border="1"> <tbody> <tr><td>H</td><td>0.30704</td><td>0.54202</td><td>-4.58149</td></tr> <tr><td>C</td><td>0.23196</td><td>0.45627</td><td>-3.50541</td></tr> <tr><td>C</td><td>0.03554</td><td>0.22191</td><td>-0.72567</td></tr> <tr><td>C</td><td>-0.53612</td><td>-0.56662</td><td>-2.95372</td></tr> <tr><td>C</td><td>0.89859</td><td>1.35244</td><td>-2.68901</td></tr> <tr><td>C</td><td>0.79029</td><td>1.24639</td><td>-1.30078</td></tr> <tr><td>C</td><td>-0.62545</td><td>-0.68490</td><td>-1.57040</td></tr> <tr><td>H</td><td>-1.04611</td><td>-1.26280</td><td>-3.60226</td></tr> <tr><td>H</td><td>1.51693</td><td>2.13451</td><td>-3.10614</td></tr> <tr><td>C</td><td>-0.02161</td><td>0.02893</td><td>0.75043</td></tr> <tr><td>C</td><td>-0.05288</td><td>-0.26200</td><td>3.52891</td></tr> <tr><td>C</td><td>1.03458</td><td>-0.62521</td><td>1.40713</td></tr> <tr><td>C</td><td>-1.07448</td><td>0.52608</td><td>1.50883</td></tr> <tr><td>C</td><td>-1.09849</td><td>0.39182</td><td>2.89656</td></tr> <tr><td>C</td><td>1.01549</td><td>-0.76946</td><td>2.79416</td></tr> <tr><td>H</td><td>-1.91861</td><td>0.80843</td><td>3.46493</td></tr> <tr><td>H</td><td>1.82664</td><td>-1.26750</td><td>3.30337</td></tr> <tr><td>H</td><td>-0.05732</td><td>-0.37555</td><td>4.60507</td></tr> <tr><td>O</td><td>-1.35263</td><td>-1.66397</td><td>-0.94436</td></tr> <tr><td>O</td><td>2.03212</td><td>-1.07981</td><td>0.61026</td></tr> <tr><td>C</td><td>-1.88985</td><td>-2.70805</td><td>-1.74339</td></tr> <tr><td>H</td><td>-1.10062</td><td>-3.20817</td><td>-2.31175</td></tr> <tr><td>H</td><td>-2.64449</td><td>-2.32782</td><td>-2.43952</td></tr> <tr><td>H</td><td>-2.34915</td><td>-3.41141</td><td>-1.05187</td></tr> <tr><td>C</td><td>3.20143</td><td>-1.59896</td><td>1.22417</td></tr> <tr><td>H</td><td>3.65231</td><td>-0.85758</td><td>1.89034</td></tr> <tr><td>H</td><td>3.88794</td><td>-1.82925</td><td>0.41296</td></tr> <tr><td>H</td><td>2.97861</td><td>-2.50830</td><td>1.79160</td></tr> <tr><td>C</td><td>1.57293</td><td>2.24599</td><td>-0.48216</td></tr> <tr><td>N</td><td>0.87276</td><td>2.94986</td><td>0.43605</td></tr> <tr><td>H</td><td>-0.12805</td><td>2.86940</td><td>0.56376</td></tr> <tr><td>H</td><td>1.37765</td><td>3.63252</td><td>0.97615</td></tr> <tr><td>C</td><td>-2.14785</td><td>1.32426</td><td>0.82318</td></tr> <tr><td>N</td><td>-3.10739</td><td>0.60017</td><td>0.20432</td></tr> <tr><td>H</td><td>-3.76856</td><td>1.09424</td><td>-0.37379</td></tr> <tr><td>H</td><td>-2.94250</td><td>-0.37889</td><td>0.03055</td></tr> <tr><td>O</td><td>-2.13643</td><td>2.54818</td><td>0.84443</td></tr> <tr><td>O</td><td>2.76577</td><td>2.41286</td><td>-0.68544</td></tr> </tbody> </table>	H	0.30704	0.54202	-4.58149	C	0.23196	0.45627	-3.50541	C	0.03554	0.22191	-0.72567	C	-0.53612	-0.56662	-2.95372	C	0.89859	1.35244	-2.68901	C	0.79029	1.24639	-1.30078	C	-0.62545	-0.68490	-1.57040	H	-1.04611	-1.26280	-3.60226	H	1.51693	2.13451	-3.10614	C	-0.02161	0.02893	0.75043	C	-0.05288	-0.26200	3.52891	C	1.03458	-0.62521	1.40713	C	-1.07448	0.52608	1.50883	C	-1.09849	0.39182	2.89656	C	1.01549	-0.76946	2.79416	H	-1.91861	0.80843	3.46493	H	1.82664	-1.26750	3.30337	H	-0.05732	-0.37555	4.60507	O	-1.35263	-1.66397	-0.94436	O	2.03212	-1.07981	0.61026	C	-1.88985	-2.70805	-1.74339	H	-1.10062	-3.20817	-2.31175	H	-2.64449	-2.32782	-2.43952	H	-2.34915	-3.41141	-1.05187	C	3.20143	-1.59896	1.22417	H	3.65231	-0.85758	1.89034	H	3.88794	-1.82925	0.41296	H	2.97861	-2.50830	1.79160	C	1.57293	2.24599	-0.48216	N	0.87276	2.94986	0.43605	H	-0.12805	2.86940	0.56376	H	1.37765	3.63252	0.97615	C	-2.14785	1.32426	0.82318	N	-3.10739	0.60017	0.20432	H	-3.76856	1.09424	-0.37379	H	-2.94250	-0.37889	0.03055	O	-2.13643	2.54818	0.84443	O	2.76577	2.41286	-0.68544	 <p>2h -1029.588990 -1029.410860 -1030.354784</p>	<table border="1"> <tbody> <tr><td>H</td><td>0.47676</td><td>-4.59760</td><td>-0.57153</td></tr> <tr><td>C</td><td>0.26740</td><td>-3.54645</td><td>-0.42518</td></tr> <tr><td>C</td><td>-0.06626</td><td>-0.73490</td><td>-0.06262</td></tr> <tr><td>C</td><td>-0.04973</td><td>-2.73942</td><td>-1.50435</td></tr> <tr><td>C</td><td>0.19652</td><td>-3.00670</td><td>0.84900</td></tr> <tr><td>C</td><td>-0.03102</td><td>-1.64635</td><td>1.03756</td></tr> <tr><td>C</td><td>-0.29216</td><td>-1.37714</td><td>-1.31744</td></tr> <tr><td>H</td><td>-0.14572</td><td>-3.16705</td><td>-2.49029</td></tr> <tr><td>H</td><td>0.26580</td><td>-3.63333</td><td>1.72681</td></tr> <tr><td>C</td><td>0.04721</td><td>0.75412</td><td>0.06353</td></tr> <tr><td>C</td><td>-0.28678</td><td>3.56552</td><td>0.42689</td></tr> <tr><td>C</td><td>0.27363</td><td>1.39612</td><td>1.31838</td></tr> <tr><td>C</td><td>0.01133</td><td>1.66581</td><td>-1.03644</td></tr> <tr><td>C</td><td>-0.21638</td><td>3.02607</td><td>-0.84745</td></tr> <tr><td>C</td><td>0.03105</td><td>2.75831</td><td>1.50573</td></tr> <tr><td>H</td><td>-0.28617</td><td>3.65290</td><td>-1.72508</td></tr> <tr><td>H</td><td>0.12741</td><td>3.18573</td><td>2.49172</td></tr> <tr><td>H</td><td>-0.49629</td><td>4.61659</td><td>0.57358</td></tr> <tr><td>O</td><td>-0.82459</td><td>-0.62520</td><td>-2.30569</td></tr> <tr><td>O</td><td>0.80662</td><td>0.64402</td><td>2.30622</td></tr> <tr><td>C</td><td>-0.88275</td><td>-1.11959</td><td>-3.63595</td></tr> <tr><td>H</td><td>-1.59521</td><td>-1.94522</td><td>-3.71108</td></tr> <tr><td>H</td><td>0.10348</td><td>-1.45777</td><td>-3.96597</td></tr> <tr><td>H</td><td>-1.20217</td><td>-0.27517</td><td>-4.24067</td></tr> <tr><td>C</td><td>0.86532</td><td>1.13812</td><td>3.63656</td></tr> <tr><td>H</td><td>1.57766</td><td>1.96387</td><td>3.71154</td></tr> <tr><td>H</td><td>1.18515</td><td>0.29364</td><td>4.24096</td></tr> <tr><td>H</td><td>-0.12083</td><td>1.47602</td><td>3.96710</td></tr> <tr><td>C</td><td>-0.51185</td><td>-1.35288</td><td>2.44094</td></tr> <tr><td>N</td><td>-1.69398</td><td>-0.66989</td><td>2.47766</td></tr> <tr><td>H</td><td>-2.05732</td><td>-0.20973</td><td>1.66199</td></tr> <tr><td>H</td><td>-2.08737</td><td>-0.45644</td><td>3.37804</td></tr> <tr><td>C</td><td>0.49183</td><td>1.37286</td><td>-2.44004</td></tr> <tr><td>N</td><td>1.67445</td><td>0.69072</td><td>-2.47719</td></tr> <tr><td>H</td><td>2.06758</td><td>0.47746</td><td>-3.37773</td></tr> <tr><td>H</td><td>2.03810</td><td>0.23039</td><td>-1.66173</td></tr> <tr><td>O</td><td>-0.00523</td><td>1.85417</td><td>-3.44234</td></tr> <tr><td>O</td><td>-0.01536</td><td>-1.83430</td><td>3.44347</td></tr> </tbody> </table>	H	0.47676	-4.59760	-0.57153	C	0.26740	-3.54645	-0.42518	C	-0.06626	-0.73490	-0.06262	C	-0.04973	-2.73942	-1.50435	C	0.19652	-3.00670	0.84900	C	-0.03102	-1.64635	1.03756	C	-0.29216	-1.37714	-1.31744	H	-0.14572	-3.16705	-2.49029	H	0.26580	-3.63333	1.72681	C	0.04721	0.75412	0.06353	C	-0.28678	3.56552	0.42689	C	0.27363	1.39612	1.31838	C	0.01133	1.66581	-1.03644	C	-0.21638	3.02607	-0.84745	C	0.03105	2.75831	1.50573	H	-0.28617	3.65290	-1.72508	H	0.12741	3.18573	2.49172	H	-0.49629	4.61659	0.57358	O	-0.82459	-0.62520	-2.30569	O	0.80662	0.64402	2.30622	C	-0.88275	-1.11959	-3.63595	H	-1.59521	-1.94522	-3.71108	H	0.10348	-1.45777	-3.96597	H	-1.20217	-0.27517	-4.24067	C	0.86532	1.13812	3.63656	H	1.57766	1.96387	3.71154	H	1.18515	0.29364	4.24096	H	-0.12083	1.47602	3.96710	C	-0.51185	-1.35288	2.44094	N	-1.69398	-0.66989	2.47766	H	-2.05732	-0.20973	1.66199	H	-2.08737	-0.45644	3.37804	C	0.49183	1.37286	-2.44004	N	1.67445	0.69072	-2.47719	H	2.06758	0.47746	-3.37773	H	2.03810	0.23039	-1.66173	O	-0.00523	1.85417	-3.44234	O	-0.01536	-1.83430	3.44347
H	0.30704	0.54202	-4.58149																																																																																																																																																																																																																																																																																																																
C	0.23196	0.45627	-3.50541																																																																																																																																																																																																																																																																																																																
C	0.03554	0.22191	-0.72567																																																																																																																																																																																																																																																																																																																
C	-0.53612	-0.56662	-2.95372																																																																																																																																																																																																																																																																																																																
C	0.89859	1.35244	-2.68901																																																																																																																																																																																																																																																																																																																
C	0.79029	1.24639	-1.30078																																																																																																																																																																																																																																																																																																																
C	-0.62545	-0.68490	-1.57040																																																																																																																																																																																																																																																																																																																
H	-1.04611	-1.26280	-3.60226																																																																																																																																																																																																																																																																																																																
H	1.51693	2.13451	-3.10614																																																																																																																																																																																																																																																																																																																
C	-0.02161	0.02893	0.75043																																																																																																																																																																																																																																																																																																																
C	-0.05288	-0.26200	3.52891																																																																																																																																																																																																																																																																																																																
C	1.03458	-0.62521	1.40713																																																																																																																																																																																																																																																																																																																
C	-1.07448	0.52608	1.50883																																																																																																																																																																																																																																																																																																																
C	-1.09849	0.39182	2.89656																																																																																																																																																																																																																																																																																																																
C	1.01549	-0.76946	2.79416																																																																																																																																																																																																																																																																																																																
H	-1.91861	0.80843	3.46493																																																																																																																																																																																																																																																																																																																
H	1.82664	-1.26750	3.30337																																																																																																																																																																																																																																																																																																																
H	-0.05732	-0.37555	4.60507																																																																																																																																																																																																																																																																																																																
O	-1.35263	-1.66397	-0.94436																																																																																																																																																																																																																																																																																																																
O	2.03212	-1.07981	0.61026																																																																																																																																																																																																																																																																																																																
C	-1.88985	-2.70805	-1.74339																																																																																																																																																																																																																																																																																																																
H	-1.10062	-3.20817	-2.31175																																																																																																																																																																																																																																																																																																																
H	-2.64449	-2.32782	-2.43952																																																																																																																																																																																																																																																																																																																
H	-2.34915	-3.41141	-1.05187																																																																																																																																																																																																																																																																																																																
C	3.20143	-1.59896	1.22417																																																																																																																																																																																																																																																																																																																
H	3.65231	-0.85758	1.89034																																																																																																																																																																																																																																																																																																																
H	3.88794	-1.82925	0.41296																																																																																																																																																																																																																																																																																																																
H	2.97861	-2.50830	1.79160																																																																																																																																																																																																																																																																																																																
C	1.57293	2.24599	-0.48216																																																																																																																																																																																																																																																																																																																
N	0.87276	2.94986	0.43605																																																																																																																																																																																																																																																																																																																
H	-0.12805	2.86940	0.56376																																																																																																																																																																																																																																																																																																																
H	1.37765	3.63252	0.97615																																																																																																																																																																																																																																																																																																																
C	-2.14785	1.32426	0.82318																																																																																																																																																																																																																																																																																																																
N	-3.10739	0.60017	0.20432																																																																																																																																																																																																																																																																																																																
H	-3.76856	1.09424	-0.37379																																																																																																																																																																																																																																																																																																																
H	-2.94250	-0.37889	0.03055																																																																																																																																																																																																																																																																																																																
O	-2.13643	2.54818	0.84443																																																																																																																																																																																																																																																																																																																
O	2.76577	2.41286	-0.68544																																																																																																																																																																																																																																																																																																																
H	0.47676	-4.59760	-0.57153																																																																																																																																																																																																																																																																																																																
C	0.26740	-3.54645	-0.42518																																																																																																																																																																																																																																																																																																																
C	-0.06626	-0.73490	-0.06262																																																																																																																																																																																																																																																																																																																
C	-0.04973	-2.73942	-1.50435																																																																																																																																																																																																																																																																																																																
C	0.19652	-3.00670	0.84900																																																																																																																																																																																																																																																																																																																
C	-0.03102	-1.64635	1.03756																																																																																																																																																																																																																																																																																																																
C	-0.29216	-1.37714	-1.31744																																																																																																																																																																																																																																																																																																																
H	-0.14572	-3.16705	-2.49029																																																																																																																																																																																																																																																																																																																
H	0.26580	-3.63333	1.72681																																																																																																																																																																																																																																																																																																																
C	0.04721	0.75412	0.06353																																																																																																																																																																																																																																																																																																																
C	-0.28678	3.56552	0.42689																																																																																																																																																																																																																																																																																																																
C	0.27363	1.39612	1.31838																																																																																																																																																																																																																																																																																																																
C	0.01133	1.66581	-1.03644																																																																																																																																																																																																																																																																																																																
C	-0.21638	3.02607	-0.84745																																																																																																																																																																																																																																																																																																																
C	0.03105	2.75831	1.50573																																																																																																																																																																																																																																																																																																																
H	-0.28617	3.65290	-1.72508																																																																																																																																																																																																																																																																																																																
H	0.12741	3.18573	2.49172																																																																																																																																																																																																																																																																																																																
H	-0.49629	4.61659	0.57358																																																																																																																																																																																																																																																																																																																
O	-0.82459	-0.62520	-2.30569																																																																																																																																																																																																																																																																																																																
O	0.80662	0.64402	2.30622																																																																																																																																																																																																																																																																																																																
C	-0.88275	-1.11959	-3.63595																																																																																																																																																																																																																																																																																																																
H	-1.59521	-1.94522	-3.71108																																																																																																																																																																																																																																																																																																																
H	0.10348	-1.45777	-3.96597																																																																																																																																																																																																																																																																																																																
H	-1.20217	-0.27517	-4.24067																																																																																																																																																																																																																																																																																																																
C	0.86532	1.13812	3.63656																																																																																																																																																																																																																																																																																																																
H	1.57766	1.96387	3.71154																																																																																																																																																																																																																																																																																																																
H	1.18515	0.29364	4.24096																																																																																																																																																																																																																																																																																																																
H	-0.12083	1.47602	3.96710																																																																																																																																																																																																																																																																																																																
C	-0.51185	-1.35288	2.44094																																																																																																																																																																																																																																																																																																																
N	-1.69398	-0.66989	2.47766																																																																																																																																																																																																																																																																																																																
H	-2.05732	-0.20973	1.66199																																																																																																																																																																																																																																																																																																																
H	-2.08737	-0.45644	3.37804																																																																																																																																																																																																																																																																																																																
C	0.49183	1.37286	-2.44004																																																																																																																																																																																																																																																																																																																
N	1.67445	0.69072	-2.47719																																																																																																																																																																																																																																																																																																																
H	2.06758	0.47746	-3.37773																																																																																																																																																																																																																																																																																																																
H	2.03810	0.23039	-1.66173																																																																																																																																																																																																																																																																																																																
O	-0.00523	1.85417	-3.44234																																																																																																																																																																																																																																																																																																																
O	-0.01536	-1.83430	3.44347																																																																																																																																																																																																																																																																																																																
	<table border="1"> <tbody> <tr><td>C</td><td>-1.25701</td><td>-0.74450</td><td>-3.26598</td></tr> <tr><td>C</td><td>-0.48794</td><td>0.04276</td><td>-0.69320</td></tr> <tr><td>C</td><td>-1.00428</td><td>-1.70126</td><td>-2.30219</td></tr> <tr><td>C</td><td>-1.12963</td><td>0.60940</td><td>-2.96714</td></tr> <tr><td>C</td><td>-0.74455</td><td>0.99906</td><td>-1.68867</td></tr> <tr><td>C</td><td>-0.62870</td><td>-1.31144</td><td>-1.00862</td></tr> <tr><td>C</td><td>-0.08323</td><td>0.53515</td><td>0.65351</td></tr> <tr><td>C</td><td>0.53668</td><td>1.47215</td><td>3.21640</td></tr> <tr><td>C</td><td>1.24800</td><td>0.68520</td><td>1.05152</td></tr> <tr><td>C</td><td>-1.10178</td><td>0.86821</td><td>1.56071</td></tr> </tbody> </table>	C	-1.25701	-0.74450	-3.26598	C	-0.48794	0.04276	-0.69320	C	-1.00428	-1.70126	-2.30219	C	-1.12963	0.60940	-2.96714	C	-0.74455	0.99906	-1.68867	C	-0.62870	-1.31144	-1.00862	C	-0.08323	0.53515	0.65351	C	0.53668	1.47215	3.21640	C	1.24800	0.68520	1.05152	C	-1.10178	0.86821	1.56071		<table border="1"> <tbody> <tr><td>C</td><td>3.47264</td><td>0.72827</td><td>-0.55732</td></tr> <tr><td>C</td><td>0.72436</td><td>0.17542</td><td>-0.00764</td></tr> <tr><td>C</td><td>3.07721</td><td>-0.54382</td><td>-0.18676</td></tr> <tr><td>C</td><td>2.55878</td><td>1.76311</td><td>-0.44737</td></tr> <tr><td>C</td><td>1.22734</td><td>1.50642</td><td>-0.12212</td></tr> <tr><td>C</td><td>1.74994</td><td>-0.79746</td><td>0.16371</td></tr> <tr><td>C</td><td>-0.72421</td><td>-0.17593</td><td>0.00665</td></tr> <tr><td>C</td><td>-3.47290</td><td>-0.72862</td><td>0.55474</td></tr> <tr><td>C</td><td>-1.74968</td><td>0.79700</td><td>-0.16526</td></tr> <tr><td>C</td><td>-1.22727</td><td>-1.50689</td><td>0.12129</td></tr> </tbody> </table>	C	3.47264	0.72827	-0.55732	C	0.72436	0.17542	-0.00764	C	3.07721	-0.54382	-0.18676	C	2.55878	1.76311	-0.44737	C	1.22734	1.50642	-0.12212	C	1.74994	-0.79746	0.16371	C	-0.72421	-0.17593	0.00665	C	-3.47290	-0.72862	0.55474	C	-1.74968	0.79700	-0.16526	C	-1.22727	-1.50689	0.12129																																																																																																																																																																																																																																
C	-1.25701	-0.74450	-3.26598																																																																																																																																																																																																																																																																																																																
C	-0.48794	0.04276	-0.69320																																																																																																																																																																																																																																																																																																																
C	-1.00428	-1.70126	-2.30219																																																																																																																																																																																																																																																																																																																
C	-1.12963	0.60940	-2.96714																																																																																																																																																																																																																																																																																																																
C	-0.74455	0.99906	-1.68867																																																																																																																																																																																																																																																																																																																
C	-0.62870	-1.31144	-1.00862																																																																																																																																																																																																																																																																																																																
C	-0.08323	0.53515	0.65351																																																																																																																																																																																																																																																																																																																
C	0.53668	1.47215	3.21640																																																																																																																																																																																																																																																																																																																
C	1.24800	0.68520	1.05152																																																																																																																																																																																																																																																																																																																
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C	3.47264	0.72827	-0.55732																																																																																																																																																																																																																																																																																																																
C	0.72436	0.17542	-0.00764																																																																																																																																																																																																																																																																																																																
C	3.07721	-0.54382	-0.18676																																																																																																																																																																																																																																																																																																																
C	2.55878	1.76311	-0.44737																																																																																																																																																																																																																																																																																																																
C	1.22734	1.50642	-0.12212																																																																																																																																																																																																																																																																																																																
C	1.74994	-0.79746	0.16371																																																																																																																																																																																																																																																																																																																
C	-0.72421	-0.17593	0.00665																																																																																																																																																																																																																																																																																																																
C	-3.47290	-0.72862	0.55474																																																																																																																																																																																																																																																																																																																
C	-1.74968	0.79700	-0.16526																																																																																																																																																																																																																																																																																																																
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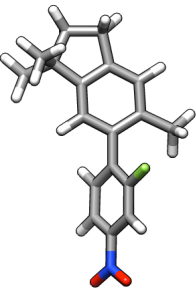
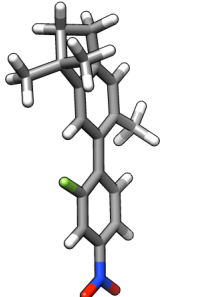
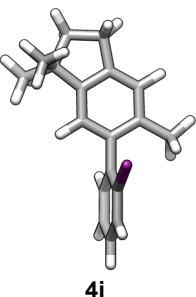
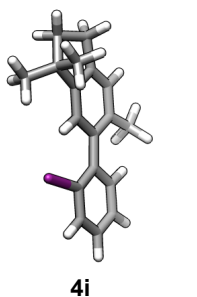
 <p>2i -1147.958720 -1147.764144 -1148.759637</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.79522</td><td>1.33671</td><td>2.83395</td></tr> <tr><td>C</td><td>1.55355</td><td>1.14528</td><td>2.34045</td></tr> <tr><td>H</td><td>-1.55472</td><td>-1.04428</td><td>-4.26210</td></tr> <tr><td>H</td><td>0.77166</td><td>1.83498</td><td>4.20830</td></tr> <tr><td>H</td><td>-1.32221</td><td>1.34665</td><td>-3.73181</td></tr> <tr><td>H</td><td>2.58575</td><td>1.24789</td><td>2.63662</td></tr> <tr><td>H</td><td>-1.10055</td><td>-2.75050</td><td>-2.53346</td></tr> <tr><td>H</td><td>-1.58035</td><td>1.58806</td><td>3.53091</td></tr> <tr><td>C</td><td>-0.39946</td><td>-2.35119</td><td>0.03547</td></tr> <tr><td>O</td><td>-0.41513</td><td>-2.16954</td><td>1.22959</td></tr> <tr><td>C</td><td>2.35351</td><td>0.37578</td><td>0.09971</td></tr> <tr><td>O</td><td>2.25428</td><td>0.31207</td><td>-1.10247</td></tr> <tr><td>O</td><td>-0.57872</td><td>2.29404</td><td>-1.31253</td></tr> <tr><td>O</td><td>-2.37017</td><td>0.68865</td><td>1.10803</td></tr> <tr><td>C</td><td>-3.44089</td><td>0.94411</td><td>1.99890</td></tr> <tr><td>H</td><td>-4.35136</td><td>0.71487</td><td>1.44928</td></tr> <tr><td>H</td><td>-3.45395</td><td>1.99353</td><td>2.31180</td></tr> <tr><td>H</td><td>-3.37391</td><td>0.30628</td><td>2.88607</td></tr> <tr><td>C</td><td>-0.76026</td><td>3.30289</td><td>-2.28958</td></tr> <tr><td>H</td><td>-1.78603</td><td>3.30260</td><td>-2.67323</td></tr> <tr><td>H</td><td>-0.06507</td><td>3.17002</td><td>-3.12467</td></tr> <tr><td>H</td><td>-0.55721</td><td>4.24721</td><td>-1.78895</td></tr> <tr><td>O</td><td>-0.17309</td><td>-3.57106</td><td>-0.50433</td></tr> <tr><td>C</td><td>0.02202</td><td>-4.63228</td><td>0.43973</td></tr> <tr><td>H</td><td>0.18764</td><td>-5.52701</td><td>-0.15561</td></tr> <tr><td>H</td><td>-0.85867</td><td>-4.74564</td><td>1.07308</td></tr> <tr><td>H</td><td>0.88488</td><td>-4.42342</td><td>1.07304</td></tr> <tr><td>O</td><td>3.53030</td><td>0.17530</td><td>0.73668</td></tr> <tr><td>C</td><td>4.65112</td><td>-0.09188</td><td>-0.11654</td></tr> <tr><td>H</td><td>4.47488</td><td>-0.99356</td><td>-0.70399</td></tr> <tr><td>H</td><td>5.50069</td><td>-0.22458</td><td>0.54905</td></tr> <tr><td>H</td><td>4.81912</td><td>0.74323</td><td>-0.79772</td></tr> </tbody> </table>	C	-0.79522	1.33671	2.83395	C	1.55355	1.14528	2.34045	H	-1.55472	-1.04428	-4.26210	H	0.77166	1.83498	4.20830	H	-1.32221	1.34665	-3.73181	H	2.58575	1.24789	2.63662	H	-1.10055	-2.75050	-2.53346	H	-1.58035	1.58806	3.53091	C	-0.39946	-2.35119	0.03547	O	-0.41513	-2.16954	1.22959	C	2.35351	0.37578	0.09971	O	2.25428	0.31207	-1.10247	O	-0.57872	2.29404	-1.31253	O	-2.37017	0.68865	1.10803	C	-3.44089	0.94411	1.99890	H	-4.35136	0.71487	1.44928	H	-3.45395	1.99353	2.31180	H	-3.37391	0.30628	2.88607	C	-0.76026	3.30289	-2.28958	H	-1.78603	3.30260	-2.67323	H	-0.06507	3.17002	-3.12467	H	-0.55721	4.24721	-1.78895	O	-0.17309	-3.57106	-0.50433	C	0.02202	-4.63228	0.43973	H	0.18764	-5.52701	-0.15561	H	-0.85867	-4.74564	1.07308	H	0.88488	-4.42342	1.07304	O	3.53030	0.17530	0.73668	C	4.65112	-0.09188	-0.11654	H	4.47488	-0.99356	-0.70399	H	5.50069	-0.22458	0.54905	H	4.81912	0.74323	-0.79772	 <p>2i -1147.915381 -1147.720077 -1148.715612</p>	<table border="1"> <tbody> <tr><td>C</td><td>-2.55893</td><td>-1.76345</td><td>0.44580</td></tr> <tr><td>C</td><td>-3.07720</td><td>0.54339</td><td>0.18424</td></tr> <tr><td>H</td><td>4.49610</td><td>0.92025</td><td>-0.84964</td></tr> <tr><td>H</td><td>-4.49659</td><td>-0.92056</td><td>0.84628</td></tr> <tr><td>H</td><td>-2.87601</td><td>-2.78840</td><td>0.56627</td></tr> <tr><td>H</td><td>2.87579</td><td>2.78810</td><td>-0.56767</td></tr> <tr><td>H</td><td>3.80300</td><td>-1.34053</td><td>-0.14737</td></tr> <tr><td>H</td><td>-3.80298</td><td>1.34007</td><td>0.14409</td></tr> <tr><td>C</td><td>-0.51008</td><td>-2.70164</td><td>-0.42474</td></tr> <tr><td>O</td><td>0.02522</td><td>-2.72033</td><td>-1.50628</td></tr> <tr><td>C</td><td>0.51024</td><td>2.70079</td><td>0.42481</td></tr> <tr><td>O</td><td>-0.02507</td><td>2.71869</td><td>1.50636</td></tr> <tr><td>O</td><td>1.40610</td><td>-1.96517</td><td>0.76089</td></tr> <tr><td>O</td><td>-1.40544</td><td>1.96483</td><td>-0.76201</td></tr> <tr><td>C</td><td>-2.35049</td><td>3.01732</td><td>-0.85789</td></tr> <tr><td>H</td><td>-2.68409</td><td>3.33019</td><td>0.13528</td></tr> <tr><td>H</td><td>-3.21267</td><td>2.71570</td><td>-1.45878</td></tr> <tr><td>H</td><td>-1.82511</td><td>3.83231</td><td>-1.34898</td></tr> <tr><td>C</td><td>2.35147</td><td>-3.01736</td><td>0.85698</td></tr> <tr><td>H</td><td>3.21404</td><td>-2.71496</td><td>1.45691</td></tr> <tr><td>H</td><td>2.68437</td><td>-3.33109</td><td>-0.13615</td></tr> <tr><td>H</td><td>1.82668</td><td>-3.83201</td><td>1.34926</td></tr> <tr><td>O</td><td>0.68587</td><td>3.81254</td><td>-0.32456</td></tr> <tr><td>O</td><td>-0.68581</td><td>-3.81282</td><td>0.32544</td></tr> <tr><td>C</td><td>-0.24967</td><td>-5.03529</td><td>-0.28506</td></tr> <tr><td>H</td><td>-0.79263</td><td>-5.21096</td><td>-1.21446</td></tr> <tr><td>H</td><td>-0.46311</td><td>-5.81741</td><td>0.43992</td></tr> <tr><td>H</td><td>0.81668</td><td>-4.99519</td><td>-0.50683</td></tr> <tr><td>C</td><td>0.24958</td><td>5.03450</td><td>0.28692</td></tr> <tr><td>H</td><td>-0.81629</td><td>4.99325</td><td>0.51076</td></tr> <tr><td>H</td><td>0.46084</td><td>5.81693</td><td>-0.43837</td></tr> <tr><td>H</td><td>0.79418</td><td>5.21063</td><td>1.21528</td></tr> </tbody> </table>	C	-2.55893	-1.76345	0.44580	C	-3.07720	0.54339	0.18424	H	4.49610	0.92025	-0.84964	H	-4.49659	-0.92056	0.84628	H	-2.87601	-2.78840	0.56627	H	2.87579	2.78810	-0.56767	H	3.80300	-1.34053	-0.14737	H	-3.80298	1.34007	0.14409	C	-0.51008	-2.70164	-0.42474	O	0.02522	-2.72033	-1.50628	C	0.51024	2.70079	0.42481	O	-0.02507	2.71869	1.50636	O	1.40610	-1.96517	0.76089	O	-1.40544	1.96483	-0.76201	C	-2.35049	3.01732	-0.85789	H	-2.68409	3.33019	0.13528	H	-3.21267	2.71570	-1.45878	H	-1.82511	3.83231	-1.34898	C	2.35147	-3.01736	0.85698	H	3.21404	-2.71496	1.45691	H	2.68437	-3.33109	-0.13615	H	1.82668	-3.83201	1.34926	O	0.68587	3.81254	-0.32456	O	-0.68581	-3.81282	0.32544	C	-0.24967	-5.03529	-0.28506	H	-0.79263	-5.21096	-1.21446	H	-0.46311	-5.81741	0.43992	H	0.81668	-4.99519	-0.50683	C	0.24958	5.03450	0.28692	H	-0.81629	4.99325	0.51076	H	0.46084	5.81693	-0.43837	H	0.79418	5.21063	1.21528																								
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H	0.77166	1.83498	4.20830																																																																																																																																																																																																																																																																																								
H	-1.32221	1.34665	-3.73181																																																																																																																																																																																																																																																																																								
H	2.58575	1.24789	2.63662																																																																																																																																																																																																																																																																																								
H	-1.10055	-2.75050	-2.53346																																																																																																																																																																																																																																																																																								
H	-1.58035	1.58806	3.53091																																																																																																																																																																																																																																																																																								
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O	-0.41513	-2.16954	1.22959																																																																																																																																																																																																																																																																																								
C	2.35351	0.37578	0.09971																																																																																																																																																																																																																																																																																								
O	2.25428	0.31207	-1.10247																																																																																																																																																																																																																																																																																								
O	-0.57872	2.29404	-1.31253																																																																																																																																																																																																																																																																																								
O	-2.37017	0.68865	1.10803																																																																																																																																																																																																																																																																																								
C	-3.44089	0.94411	1.99890																																																																																																																																																																																																																																																																																								
H	-4.35136	0.71487	1.44928																																																																																																																																																																																																																																																																																								
H	-3.45395	1.99353	2.31180																																																																																																																																																																																																																																																																																								
H	-3.37391	0.30628	2.88607																																																																																																																																																																																																																																																																																								
C	-0.76026	3.30289	-2.28958																																																																																																																																																																																																																																																																																								
H	-1.78603	3.30260	-2.67323																																																																																																																																																																																																																																																																																								
H	-0.06507	3.17002	-3.12467																																																																																																																																																																																																																																																																																								
H	-0.55721	4.24721	-1.78895																																																																																																																																																																																																																																																																																								
O	-0.17309	-3.57106	-0.50433																																																																																																																																																																																																																																																																																								
C	0.02202	-4.63228	0.43973																																																																																																																																																																																																																																																																																								
H	0.18764	-5.52701	-0.15561																																																																																																																																																																																																																																																																																								
H	-0.85867	-4.74564	1.07308																																																																																																																																																																																																																																																																																								
H	0.88488	-4.42342	1.07304																																																																																																																																																																																																																																																																																								
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C	4.65112	-0.09188	-0.11654																																																																																																																																																																																																																																																																																								
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H	-4.49659	-0.92056	0.84628																																																																																																																																																																																																																																																																																								
H	-2.87601	-2.78840	0.56627																																																																																																																																																																																																																																																																																								
H	2.87579	2.78810	-0.56767																																																																																																																																																																																																																																																																																								
H	3.80300	-1.34053	-0.14737																																																																																																																																																																																																																																																																																								
H	-3.80298	1.34007	0.14409																																																																																																																																																																																																																																																																																								
C	-0.51008	-2.70164	-0.42474																																																																																																																																																																																																																																																																																								
O	0.02522	-2.72033	-1.50628																																																																																																																																																																																																																																																																																								
C	0.51024	2.70079	0.42481																																																																																																																																																																																																																																																																																								
O	-0.02507	2.71869	1.50636																																																																																																																																																																																																																																																																																								
O	1.40610	-1.96517	0.76089																																																																																																																																																																																																																																																																																								
O	-1.40544	1.96483	-0.76201																																																																																																																																																																																																																																																																																								
C	-2.35049	3.01732	-0.85789																																																																																																																																																																																																																																																																																								
H	-2.68409	3.33019	0.13528																																																																																																																																																																																																																																																																																								
H	-3.21267	2.71570	-1.45878																																																																																																																																																																																																																																																																																								
H	-1.82511	3.83231	-1.34898																																																																																																																																																																																																																																																																																								
C	2.35147	-3.01736	0.85698																																																																																																																																																																																																																																																																																								
H	3.21404	-2.71496	1.45691																																																																																																																																																																																																																																																																																								
H	2.68437	-3.33109	-0.13615																																																																																																																																																																																																																																																																																								
H	1.82668	-3.83201	1.34926																																																																																																																																																																																																																																																																																								
O	0.68587	3.81254	-0.32456																																																																																																																																																																																																																																																																																								
O	-0.68581	-3.81282	0.32544																																																																																																																																																																																																																																																																																								
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 <p>3a -695.6309526 -695.5184002 -696.1692552</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.79854</td><td>5.18301</td><td>-1.37392</td></tr> <tr><td>C</td><td>-0.40741</td><td>3.11605</td><td>0.47322</td></tr> <tr><td>C</td><td>-1.03568</td><td>3.86148</td><td>-1.72685</td></tr> <tr><td>C</td><td>-0.37129</td><td>5.48245</td><td>-0.08465</td></tr> <tr><td>C</td><td>-0.18092</td><td>4.45180</td><td>0.82522</td></tr> <tr><td>C</td><td>-0.85014</td><td>2.81144</td><td>-0.82459</td></tr> <tr><td>H</td><td>-1.38216</td><td>3.63381</td><td>-2.72704</td></tr> <tr><td>H</td><td>0.16158</td><td>4.67241</td><td>1.82818</td></tr> <tr><td>C</td><td>-0.19372</td><td>2.07956</td><td>1.51800</td></tr> <tr><td>C</td><td>0.20056</td><td>0.18740</td><td>3.55059</td></tr> <tr><td>C</td><td>0.77846</td><td>1.07095</td><td>1.37860</td></tr> <tr><td>C</td><td>-0.93567</td><td>2.11830</td><td>2.69605</td></tr> <tr><td>C</td><td>-0.75126</td><td>1.18339</td><td>3.71175</td></tr> <tr><td>C</td><td>0.96773</td><td>0.12832</td><td>2.38919</td></tr> <tr><td>H</td><td>-1.67996</td><td>2.89678</td><td>2.80443</td></tr> <tr><td>H</td><td>-1.34818</td><td>1.23371</td><td>4.61232</td></tr> <tr><td>H</td><td>1.71339</td><td>-0.64520</td><td>2.28316</td></tr> <tr><td>H</td><td>0.35779</td><td>-0.55039</td><td>4.32669</td></tr> <tr><td>C</td><td>-1.18254</td><td>1.39958</td><td>-1.26776</td></tr> <tr><td>H</td><td>-0.96730</td><td>0.71997</td><td>-0.44540</td></tr> <tr><td>H</td><td>-0.18327</td><td>6.50714</td><td>0.20863</td></tr> <tr><td>H</td><td>-0.94971</td><td>5.97301</td><td>-2.09843</td></tr> <tr><td>C</td><td>-2.67701</td><td>1.26765</td><td>-1.59420</td></tr> <tr><td>H</td><td>-2.94961</td><td>1.92348</td><td>-2.42431</td></tr> <tr><td>H</td><td>-3.29102</td><td>1.53824</td><td>-0.73305</td></tr> <tr><td>H</td><td>-2.91307</td><td>0.23982</td><td>-1.88103</td></tr> <tr><td>C</td><td>-0.33036</td><td>0.97051</td><td>-2.46831</td></tr> <tr><td>H</td><td>-0.54775</td><td>1.59439</td><td>-3.33857</td></tr> <tr><td>H</td><td>-0.54781</td><td>-0.06669</td><td>-2.73577</td></tr> <tr><td>H</td><td>0.73076</td><td>1.06092</td><td>-2.23683</td></tr> <tr><td>O</td><td>1.50344</td><td>1.09264</td><td>0.22678</td></tr> <tr><td>C</td><td>2.44638</td><td>0.05924</td><td>0.00448</td></tr> <tr><td>H</td><td>2.87540</td><td>0.24929</td><td>-0.97711</td></tr> <tr><td>H</td><td>1.96342</td><td>-0.92329</td><td>0.01209</td></tr> <tr><td>H</td><td>3.23677</td><td>0.07503</td><td>0.76151</td></tr> </tbody> </table>	C	-0.79854	5.18301	-1.37392	C	-0.40741	3.11605	0.47322	C	-1.03568	3.86148	-1.72685	C	-0.37129	5.48245	-0.08465	C	-0.18092	4.45180	0.82522	C	-0.85014	2.81144	-0.82459	H	-1.38216	3.63381	-2.72704	H	0.16158	4.67241	1.82818	C	-0.19372	2.07956	1.51800	C	0.20056	0.18740	3.55059	C	0.77846	1.07095	1.37860	C	-0.93567	2.11830	2.69605	C	-0.75126	1.18339	3.71175	C	0.96773	0.12832	2.38919	H	-1.67996	2.89678	2.80443	H	-1.34818	1.23371	4.61232	H	1.71339	-0.64520	2.28316	H	0.35779	-0.55039	4.32669	C	-1.18254	1.39958	-1.26776	H	-0.96730	0.71997	-0.44540	H	-0.18327	6.50714	0.20863	H	-0.94971	5.97301	-2.09843	C	-2.67701	1.26765	-1.59420	H	-2.94961	1.92348	-2.42431	H	-3.29102	1.53824	-0.73305	H	-2.91307	0.23982	-1.88103	C	-0.33036	0.97051	-2.46831	H	-0.54775	1.59439	-3.33857	H	-0.54781	-0.06669	-2.73577	H	0.73076	1.06092	-2.23683	O	1.50344	1.09264	0.22678	C	2.44638	0.05924	0.00448	H	2.87540	0.24929	-0.97711	H	1.96342	-0.92329	0.01209	H	3.23677	0.07503	0.76151	 <p>3a -695.6022222 -695.4893423 -696.1419818</p>	<table border="1"> <tbody> <tr><td>C</td><td>0.05264</td><td>2.34917</td><td>-2.69108</td></tr> <tr><td>C</td><td>-0.06249</td><td>0.51954</td><td>-0.48514</td></tr> <tr><td>C</td><td>-0.00050</td><td>0.97825</td><td>-2.88278</td></tr> <tr><td>C</td><td>0.01920</td><td>2.82235</td><td>-1.39488</td></tr> <tr><td>C</td><td>-0.03755</td><td>1.92440</td><td>-0.34137</td></tr> <tr><td>C</td><td>-0.07091</td><td>0.04246</td><td>-1.84499</td></tr> <tr><td>H</td><td>0.00690</td><td>0.62195</td><td>-3.90035</td></tr> <tr><td>H</td><td>-0.06094</td><td>2.34079</td><td>0.64246</td></tr> <tr><td>C</td><td>-0.08379</td><td>-0.32346</td><td>0.77618</td></tr> <tr><td>C</td><td>-0.15013</td><td>-2.03841</td><td>3.09878</td></tr> <tr><td>C</td><td>-0.04513</td><td>0.18949</td><td>2.12032</td></tr> <tr><td>C</td><td>-0.13310</td><td>-1.72838</td><td>0.72674</td></tr> <tr><td>C</td><td>-0.16948</td><td>-2.57426</td><td>1.82680</td></tr> <tr><td>C</td><td>-0.08462</td><td>-0.66076</td><td>3.22895</td></tr> <tr><td>H</td><td>-0.13801</td><td>-2.21986</td><td>-0.21742</td></tr> <tr><td>H</td><td>-0.20826</td><td>-3.64373</td><td>1.66936</td></tr> <tr><td>H</td><td>-0.06065</td><td>-2.23788</td><td>4.22001</td></tr> <tr><td>H</td><td>-0.17834</td><td>-2.66579</td><td>3.97990</td></tr> <tr><td>C</td><td>-0.10812</td><td>-1.41627</td><td>-2.30672</td></tr> <tr><td>H</td><td>-0.82103</td><td>-1.95273</td><td>-1.68611</td></tr> <tr><td>H</td><td>0.03800</td><td>3.88398</td><td>-1.18398</td></tr> <tr><td>H</td><td>0.10715</td><td>3.01816</td><td>-3.54027</td></tr> <tr><td>O</td><td>0.03882</td><td>1.53376</td><td>2.33572</td></tr> <tr><td>C</td><td>0.10817</td><td>2.04900</td><td>3.65352</td></tr> <tr><td>H</td><td>0.98720</td><td>1.66943</td><td>4.18298</td></tr> <tr><td>H</td><td>-0.79187</td><td>1.80402</td><td>4.22541</td></tr> <tr><td>H</td><td>0.18678</td><td>3.12869</td><td>3.54139</td></tr> <tr><td>C</td><td>1.28921</td><td>-2.04978</td><td>-2.18024</td></tr> <tr><td>H</td><td>1.95644</td><td>-1.57723</td><td>-2.90486</td></tr> <tr><td>H</td><td>1.25124</td><td>-3.12061</td><td>-2.39699</td></tr> <tr><td>H</td><td>1.71908</td><td>-1.90928</td><td>-1.18895</td></tr> <tr><td>C</td><td>-0.62184</td><td>-1.65019</td><td>-3.73610</td></tr> <tr><td>H</td><td>0.09903</td><td>-1.33441</td><td>-4.49279</td></tr> <tr><td>H</td><td>-1.56410</td><td>-1.13021</td><td>-3.91586</td></tr> <tr><td>H</td><td>-0.78526</td><td>-2.72120</td><td>-3.87284</td></tr> </tbody> </table>	C	0.05264	2.34917	-2.69108	C	-0.06249	0.51954	-0.48514	C	-0.00050	0.97825	-2.88278	C	0.01920	2.82235	-1.39488	C	-0.03755	1.92440	-0.34137	C	-0.07091	0.04246	-1.84499	H	0.00690	0.62195	-3.90035	H	-0.06094	2.34079	0.64246	C	-0.08379	-0.32346	0.77618	C	-0.15013	-2.03841	3.09878	C	-0.04513	0.18949	2.12032	C	-0.13310	-1.72838	0.72674	C	-0.16948	-2.57426	1.82680	C	-0.08462	-0.66076	3.22895	H	-0.13801	-2.21986	-0.21742	H	-0.20826	-3.64373	1.66936	H	-0.06065	-2.23788	4.22001	H	-0.17834	-2.66579	3.97990	C	-0.10812	-1.41627	-2.30672	H	-0.82103	-1.95273	-1.68611	H	0.03800	3.88398	-1.18398	H	0.10715	3.01816	-3.54027	O	0.03882	1.53376	2.33572	C	0.10817	2.04900	3.65352	H	0.98720	1.66943	4.18298	H	-0.79187	1.80402	4.22541	H	0.18678	3.12869	3.54139	C	1.28921	-2.04978	-2.18024	H	1.95644	-1.57723	-2.90486	H	1.25124	-3.12061	-2.39699	H	1.71908	-1.90928	-1.18895	C	-0.62184	-1.65019	-3.73610	H	0.09903	-1.33441	-4.49279	H	-1.56410	-1.13021	-3.91586	H	-0.78526	-2.72120	-3.87284
C	-0.79854	5.18301	-1.37392																																																																																																																																																																																																																																																																																								
C	-0.40741	3.11605	0.47322																																																																																																																																																																																																																																																																																								
C	-1.03568	3.86148	-1.72685																																																																																																																																																																																																																																																																																								
C	-0.37129	5.48245	-0.08465																																																																																																																																																																																																																																																																																								
C	-0.18092	4.45180	0.82522																																																																																																																																																																																																																																																																																								
C	-0.85014	2.81144	-0.82459																																																																																																																																																																																																																																																																																								
H	-1.38216	3.63381	-2.72704																																																																																																																																																																																																																																																																																								
H	0.16158	4.67241	1.82818																																																																																																																																																																																																																																																																																								
C	-0.19372	2.07956	1.51800																																																																																																																																																																																																																																																																																								
C	0.20056	0.18740	3.55059																																																																																																																																																																																																																																																																																								
C	0.77846	1.07095	1.37860																																																																																																																																																																																																																																																																																								
C	-0.93567	2.11830	2.69605																																																																																																																																																																																																																																																																																								
C	-0.75126	1.18339	3.71175																																																																																																																																																																																																																																																																																								
C	0.96773	0.12832	2.38919																																																																																																																																																																																																																																																																																								
H	-1.67996	2.89678	2.80443																																																																																																																																																																																																																																																																																								
H	-1.34818	1.23371	4.61232																																																																																																																																																																																																																																																																																								
H	1.71339	-0.64520	2.28316																																																																																																																																																																																																																																																																																								
H	0.35779	-0.55039	4.32669																																																																																																																																																																																																																																																																																								
C	-1.18254	1.39958	-1.26776																																																																																																																																																																																																																																																																																								
H	-0.96730	0.71997	-0.44540																																																																																																																																																																																																																																																																																								
H	-0.18327	6.50714	0.20863																																																																																																																																																																																																																																																																																								
H	-0.94971	5.97301	-2.09843																																																																																																																																																																																																																																																																																								
C	-2.67701	1.26765	-1.59420																																																																																																																																																																																																																																																																																								
H	-2.94961	1.92348	-2.42431																																																																																																																																																																																																																																																																																								
H	-3.29102	1.53824	-0.73305																																																																																																																																																																																																																																																																																								
H	-2.91307	0.23982	-1.88103																																																																																																																																																																																																																																																																																								
C	-0.33036	0.97051	-2.46831																																																																																																																																																																																																																																																																																								
H	-0.54775	1.59439	-3.33857																																																																																																																																																																																																																																																																																								
H	-0.54781	-0.06669	-2.73577																																																																																																																																																																																																																																																																																								
H	0.73076	1.06092	-2.23683																																																																																																																																																																																																																																																																																								
O	1.50344	1.09264	0.22678																																																																																																																																																																																																																																																																																								
C	2.44638	0.05924	0.00448																																																																																																																																																																																																																																																																																								
H	2.87540	0.24929	-0.97711																																																																																																																																																																																																																																																																																								
H	1.96342	-0.92329	0.01209																																																																																																																																																																																																																																																																																								
H	3.23677	0.07503	0.76151																																																																																																																																																																																																																																																																																								
C	0.05264	2.34917	-2.69108																																																																																																																																																																																																																																																																																								
C	-0.06249	0.51954	-0.48514																																																																																																																																																																																																																																																																																								
C	-0.00050	0.97825	-2.88278																																																																																																																																																																																																																																																																																								
C	0.01920	2.82235	-1.39488																																																																																																																																																																																																																																																																																								
C	-0.03755	1.92440	-0.34137																																																																																																																																																																																																																																																																																								
C	-0.07091	0.04246	-1.84499																																																																																																																																																																																																																																																																																								
H	0.00690	0.62195	-3.90035																																																																																																																																																																																																																																																																																								
H	-0.06094	2.34079	0.64246																																																																																																																																																																																																																																																																																								
C	-0.08379	-0.32346	0.77618																																																																																																																																																																																																																																																																																								
C	-0.15013	-2.03841	3.09878																																																																																																																																																																																																																																																																																								
C	-0.04513	0.18949	2.12032																																																																																																																																																																																																																																																																																								
C	-0.13310	-1.72838	0.72674																																																																																																																																																																																																																																																																																								
C	-0.16948	-2.57426	1.82680																																																																																																																																																																																																																																																																																								
C	-0.08462	-0.66076	3.22895																																																																																																																																																																																																																																																																																								
H	-0.13801	-2.21986	-0.21742																																																																																																																																																																																																																																																																																								
H	-0.20826	-3.64373	1.66936																																																																																																																																																																																																																																																																																								
H	-0.06065	-2.23788	4.22001																																																																																																																																																																																																																																																																																								
H	-0.17834	-2.66579	3.97990																																																																																																																																																																																																																																																																																								
C	-0.10812	-1.41627	-2.30672																																																																																																																																																																																																																																																																																								
H	-0.82103	-1.95273	-1.68611																																																																																																																																																																																																																																																																																								
H	0.03800	3.88398	-1.18398																																																																																																																																																																																																																																																																																								
H	0.10715	3.01816	-3.54027																																																																																																																																																																																																																																																																																								
O	0.03882	1.53376	2.33572																																																																																																																																																																																																																																																																																								
C	0.10817	2.04900	3.65352																																																																																																																																																																																																																																																																																								
H	0.98720	1.66943	4.18298																																																																																																																																																																																																																																																																																								
H	-0.79187	1.80402	4.22541																																																																																																																																																																																																																																																																																								
H	0.18678	3.12869	3.54139																																																																																																																																																																																																																																																																																								
C	1.28921	-2.04978	-2.18024																																																																																																																																																																																																																																																																																								
H	1.95644	-1.57723	-2.90486																																																																																																																																																																																																																																																																																								
H	1.25124	-3.12061	-2.39699																																																																																																																																																																																																																																																																																								
H	1.71908	-1.90928	-1.18895																																																																																																																																																																																																																																																																																								
C	-0.62184	-1.65019	-3.73610																																																																																																																																																																																																																																																																																								
H	0.09903	-1.33441	-4.49279																																																																																																																																																																																																																																																																																								
H	-1.56410	-1.13021	-3.91586																																																																																																																																																																																																																																																																																								
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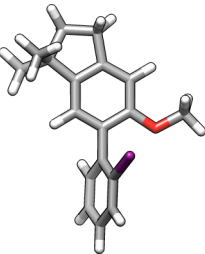
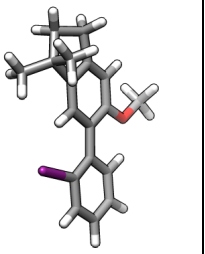
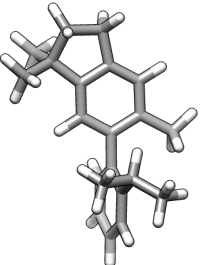
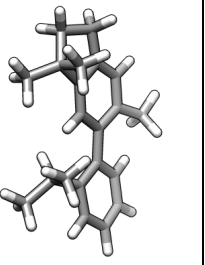
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H	1.66467	-1.83054	5.68693																																																																																																																																																																																																																																
H	2.63634	-0.80426	4.59619																																																																																																																																																																																																																																
O	-0.87906	6.19878	-2.32516																																																																																																																																																																																																																																
C	-2.08967	6.92952	-2.41506																																																																																																																																																																																																																																
H	-2.29552	7.47000	-1.48509																																																																																																																																																																																																																																
H	-1.95688	7.63919	-3.22920																																																																																																																																																																																																																																
H	-2.93464	6.26868	-2.63566																																																																																																																																																																																																																																
H	0.14544	2.19080	3.37174																																																																																																																																																																																																																																
H	-0.04629	-2.05250	3.64236																																																																																																																																																																																																																																
C	0.13740	2.51008	-1.17219																																																																																																																																																																																																																																
H	0.83643	2.61575	-0.34613																																																																																																																																																																																																																																
H	0.01812	-2.53423	-3.14646																																																																																																																																																																																																																																
O	-0.07743	-2.49964	1.07931																																																																																																																																																																																																																																
C	-0.16038	-3.65364	1.89652																																																																																																																																																																																																																																
H	-1.05512	-3.63084	2.52577																																																																																																																																																																																																																																
H	0.72447	-3.75538	2.53195																																																																																																																																																																																																																																
H	-0.21667	-4.49608	1.20968																																																																																																																																																																																																																																
C	-1.27101	2.95326	-0.73635																																																																																																																																																																																																																																
H	-1.92266	2.96380	-1.61308																																																																																																																																																																																																																																
H	-1.24770	3.96160	-0.31431																																																																																																																																																																																																																																
H	-1.70812	2.27714	-0.00228																																																																																																																																																																																																																																
C	0.65711	3.50055	-2.22464																																																																																																																																																																																																																																
H	-0.04871	3.63788	-3.04618																																																																																																																																																																																																																																
H	1.61427	3.18153	-2.64009																																																																																																																																																																																																																																
H	0.79253	4.47334	-1.74729																																																																																																																																																																																																																																
O	0.02746	-0.43866	-4.93220																																																																																																																																																																																																																																
O	0.05564	0.00926	5.47811																																																																																																																																																																																																																																
C	-0.01289	-1.70872	-5.56113																																																																																																																																																																																																																																
H	-0.91087	-2.26393	-5.27061																																																																																																																																																																																																																																
H	-0.02945	-1.51848	-6.63237																																																																																																																																																																																																																																
H	0.87029	-2.30336	-5.30533																																																																																																																																																																																																																																
C	0.11097	1.24570	5.74199																																																																																																																																																																																																																																
H	-0.75358	1.87167	5.49895																																																																																																																																																																																																																																
H	0.10073	1.00017	6.80183																																																																																																																																																																																																																																
H	1.02715	1.79266	5.49765																																																																																																																																																																																																																																
 <p>3c -5987.242631 -5989.944286 -5987.861142</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.85777</td><td>0.86927</td><td>-3.32949</td></tr> <tr><td>C</td><td>-0.39131</td><td>0.94943</td><td>-0.56587</td></tr> <tr><td>C</td><td>-0.68288</td><td>-0.31712</td><td>-2.61680</td></tr> <tr><td>C</td><td>-0.80763</td><td>2.09368</td><td>-2.66291</td></tr> <tr><td>C</td><td>-0.57890</td><td>2.12544</td><td>-1.29773</td></tr> <tr><td>C</td><td>-0.45391</td><td>-0.26793</td><td>-1.24921</td></tr> <tr><td>H</td><td>-0.72840</td><td>-1.26718</td><td>-3.12608</td></tr> <tr><td>H</td><td>-0.53210</td><td>3.07219</td><td>-0.77667</td></tr> <tr><td>C</td><td>-0.15899</td><td>1.03880</td><td>0.89767</td></tr> <tr><td>C</td><td>0.19270</td><td>1.24070</td><td>3.67193</td></tr> <tr><td>C</td><td>1.11151</td><td>0.93581</td><td>1.47035</td></tr> <tr><td>C</td><td>-1.24804</td><td>1.25632</td><td>1.74649</td></tr> <tr><td>C</td><td>-1.08225</td><td>1.35490</td><td>3.11751</td></tr> <tr><td>C</td><td>1.29482</td><td>1.03329</td><td>2.84224</td></tr> <tr><td>H</td><td>-2.23508</td><td>1.33720</td><td>1.31140</td></tr> <tr><td>H</td><td>-1.92603</td><td>1.51721</td><td>3.77281</td></tr> <tr><td>H</td><td>2.28399</td><td>0.95200</td><td>3.26529</td></tr> <tr><td>H</td><td>-0.94689</td><td>3.00412</td><td>-3.22809</td></tr> <tr><td>Br</td><td>-0.24390</td><td>-1.91831</td><td>-0.31101</td></tr> <tr><td>Br</td><td>2.65200</td><td>0.67430</td><td>0.37181</td></tr> <tr><td>C</td><td>-1.10371</td><td>0.87709</td><td>-4.79700</td></tr> <tr><td>O</td><td>-1.26431</td><td>1.87319</td><td>-5.45781</td></tr> <tr><td>O</td><td>-1.13170</td><td>-0.36477</td><td>-5.33630</td></tr> <tr><td>H</td><td>-1.29480</td><td>-0.25900</td><td>-6.28362</td></tr> <tr><td>C</td><td>0.32895</td><td>1.35019</td><td>5.14959</td></tr> <tr><td>O</td><td>-0.59018</td><td>1.53231</td><td>5.90899</td></tr> <tr><td>O</td><td>1.60842</td><td>1.22390</td><td>5.57470</td></tr> <tr><td>H</td><td>1.59689</td><td>1.30720</td><td>6.53810</td></tr> </tbody> </table>	C	-0.85777	0.86927	-3.32949	C	-0.39131	0.94943	-0.56587	C	-0.68288	-0.31712	-2.61680	C	-0.80763	2.09368	-2.66291	C	-0.57890	2.12544	-1.29773	C	-0.45391	-0.26793	-1.24921	H	-0.72840	-1.26718	-3.12608	H	-0.53210	3.07219	-0.77667	C	-0.15899	1.03880	0.89767	C	0.19270	1.24070	3.67193	C	1.11151	0.93581	1.47035	C	-1.24804	1.25632	1.74649	C	-1.08225	1.35490	3.11751	C	1.29482	1.03329	2.84224	H	-2.23508	1.33720	1.31140	H	-1.92603	1.51721	3.77281	H	2.28399	0.95200	3.26529	H	-0.94689	3.00412	-3.22809	Br	-0.24390	-1.91831	-0.31101	Br	2.65200	0.67430	0.37181	C	-1.10371	0.87709	-4.79700	O	-1.26431	1.87319	-5.45781	O	-1.13170	-0.36477	-5.33630	H	-1.29480	-0.25900	-6.28362	C	0.32895	1.35019	5.14959	O	-0.59018	1.53231	5.90899	O	1.60842	1.22390	5.57470	H	1.59689	1.30720	6.53810	 <p>3c -5987.211088 -5989.91348 -5987.832882</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.00108</td><td>0.75667</td><td>-3.55492</td></tr> <tr><td>C</td><td>-0.00134</td><td>0.10049</td><td>-0.74719</td></tr> <tr><td>C</td><td>-0.00274</td><td>-0.56213</td><td>-3.12149</td></tr> <tr><td>C</td><td>0.00070</td><td>1.75671</td><td>-2.59373</td></tr> <tr><td>C</td><td>0.00055</td><td>1.41456</td><td>-1.25611</td></tr> <tr><td>C</td><td>-0.00280</td><td>-0.89849</td><td>-1.77240</td></tr> <tr><td>H</td><td>-0.00395</td><td>-1.33832</td><td>-3.87185</td></tr> <tr><td>H</td><td>0.00200</td><td>2.22763</td><td>-0.56266</td></tr> <tr><td>C</td><td>-0.00148</td><td>-0.10044</td><td>0.74716</td></tr> <tr><td>C</td><td>-0.00114</td><td>-0.75661</td><td>3.55488</td></tr> <tr><td>C</td><td>0.00002</td><td>0.89855</td><td>1.77236</td></tr> <tr><td>C</td><td>-0.00322</td><td>-1.41451</td><td>1.25608</td></tr> <tr><td>C</td><td>-0.00311</td><td>-1.75665</td><td>2.59370</td></tr> <tr><td>C</td><td>0.00030</td><td>0.56220</td><td>3.12145</td></tr> <tr><td>H</td><td>-0.00477</td><td>-2.22758</td><td>0.56264</td></tr> <tr><td>H</td><td>-0.00453</td><td>-2.79801</td><td>2.87924</td></tr> <tr><td>H</td><td>0.00161</td><td>1.33838</td><td>3.87181</td></tr> <tr><td>H</td><td>0.00220</td><td>2.79807</td><td>-2.87926</td></tr> <tr><td>Br</td><td>-0.00475</td><td>-2.83290</td><td>-1.60973</td></tr> <tr><td>Br</td><td>0.00146</td><td>2.83295</td><td>1.60969</td></tr> <tr><td>C</td><td>-0.00120</td><td>1.01896</td><td>-5.01766</td></tr> <tr><td>O</td><td>-0.00271</td><td>0.16561</td><td>-5.86983</td></tr> <tr><td>O</td><td>0.00062</td><td>2.34130</td><td>-5.30938</td></tr> <tr><td>H</td><td>0.00043</td><td>2.41951</td><td>-6.27342</td></tr> <tr><td>C</td><td>-0.00062</td><td>-1.01889</td><td>5.01763</td></tr> <tr><td>O</td><td>0.00087</td><td>-0.16553</td><td>5.86980</td></tr> <tr><td>O</td><td>-0.00202</td><td>-2.34123</td><td>5.30936</td></tr> <tr><td>H</td><td>-0.00159</td><td>-2.41943</td><td>6.27340</td></tr> </tbody> </table>	C	-0.00108	0.75667	-3.55492	C	-0.00134	0.10049	-0.74719	C	-0.00274	-0.56213	-3.12149	C	0.00070	1.75671	-2.59373	C	0.00055	1.41456	-1.25611	C	-0.00280	-0.89849	-1.77240	H	-0.00395	-1.33832	-3.87185	H	0.00200	2.22763	-0.56266	C	-0.00148	-0.10044	0.74716	C	-0.00114	-0.75661	3.55488	C	0.00002	0.89855	1.77236	C	-0.00322	-1.41451	1.25608	C	-0.00311	-1.75665	2.59370	C	0.00030	0.56220	3.12145	H	-0.00477	-2.22758	0.56264	H	-0.00453	-2.79801	2.87924	H	0.00161	1.33838	3.87181	H	0.00220	2.79807	-2.87926	Br	-0.00475	-2.83290	-1.60973	Br	0.00146	2.83295	1.60969	C	-0.00120	1.01896	-5.01766	O	-0.00271	0.16561	-5.86983	O	0.00062	2.34130	-5.30938	H	0.00043	2.41951	-6.27342	C	-0.00062	-1.01889	5.01763	O	0.00087	-0.16553	5.86980	O	-0.00202	-2.34123	5.30936	H	-0.00159	-2.41943	6.27340
C	-0.85777	0.86927	-3.32949																																																																																																																																																																																																																																
C	-0.39131	0.94943	-0.56587																																																																																																																																																																																																																																
C	-0.68288	-0.31712	-2.61680																																																																																																																																																																																																																																
C	-0.80763	2.09368	-2.66291																																																																																																																																																																																																																																
C	-0.57890	2.12544	-1.29773																																																																																																																																																																																																																																
C	-0.45391	-0.26793	-1.24921																																																																																																																																																																																																																																
H	-0.72840	-1.26718	-3.12608																																																																																																																																																																																																																																
H	-0.53210	3.07219	-0.77667																																																																																																																																																																																																																																
C	-0.15899	1.03880	0.89767																																																																																																																																																																																																																																
C	0.19270	1.24070	3.67193																																																																																																																																																																																																																																
C	1.11151	0.93581	1.47035																																																																																																																																																																																																																																
C	-1.24804	1.25632	1.74649																																																																																																																																																																																																																																
C	-1.08225	1.35490	3.11751																																																																																																																																																																																																																																
C	1.29482	1.03329	2.84224																																																																																																																																																																																																																																
H	-2.23508	1.33720	1.31140																																																																																																																																																																																																																																
H	-1.92603	1.51721	3.77281																																																																																																																																																																																																																																
H	2.28399	0.95200	3.26529																																																																																																																																																																																																																																
H	-0.94689	3.00412	-3.22809																																																																																																																																																																																																																																
Br	-0.24390	-1.91831	-0.31101																																																																																																																																																																																																																																
Br	2.65200	0.67430	0.37181																																																																																																																																																																																																																																
C	-1.10371	0.87709	-4.79700																																																																																																																																																																																																																																
O	-1.26431	1.87319	-5.45781																																																																																																																																																																																																																																
O	-1.13170	-0.36477	-5.33630																																																																																																																																																																																																																																
H	-1.29480	-0.25900	-6.28362																																																																																																																																																																																																																																
C	0.32895	1.35019	5.14959																																																																																																																																																																																																																																
O	-0.59018	1.53231	5.90899																																																																																																																																																																																																																																
O	1.60842	1.22390	5.57470																																																																																																																																																																																																																																
H	1.59689	1.30720	6.53810																																																																																																																																																																																																																																
C	-0.00108	0.75667	-3.55492																																																																																																																																																																																																																																
C	-0.00134	0.10049	-0.74719																																																																																																																																																																																																																																
C	-0.00274	-0.56213	-3.12149																																																																																																																																																																																																																																
C	0.00070	1.75671	-2.59373																																																																																																																																																																																																																																
C	0.00055	1.41456	-1.25611																																																																																																																																																																																																																																
C	-0.00280	-0.89849	-1.77240																																																																																																																																																																																																																																
H	-0.00395	-1.33832	-3.87185																																																																																																																																																																																																																																
H	0.00200	2.22763	-0.56266																																																																																																																																																																																																																																
C	-0.00148	-0.10044	0.74716																																																																																																																																																																																																																																
C	-0.00114	-0.75661	3.55488																																																																																																																																																																																																																																
C	0.00002	0.89855	1.77236																																																																																																																																																																																																																																
C	-0.00322	-1.41451	1.25608																																																																																																																																																																																																																																
C	-0.00311	-1.75665	2.59370																																																																																																																																																																																																																																
C	0.00030	0.56220	3.12145																																																																																																																																																																																																																																
H	-0.00477	-2.22758	0.56264																																																																																																																																																																																																																																
H	-0.00453	-2.79801	2.87924																																																																																																																																																																																																																																
H	0.00161	1.33838	3.87181																																																																																																																																																																																																																																
H	0.00220	2.79807	-2.87926																																																																																																																																																																																																																																
Br	-0.00475	-2.83290	-1.60973																																																																																																																																																																																																																																
Br	0.00146	2.83295	1.60969																																																																																																																																																																																																																																
C	-0.00120	1.01896	-5.01766																																																																																																																																																																																																																																
O	-0.00271	0.16561	-5.86983																																																																																																																																																																																																																																
O	0.00062	2.34130	-5.30938																																																																																																																																																																																																																																
H	0.00043	2.41951	-6.27342																																																																																																																																																																																																																																
C	-0.00062	-1.01889	5.01763																																																																																																																																																																																																																																
O	0.00087	-0.16553	5.86980																																																																																																																																																																																																																																
O	-0.00202	-2.34123	5.30936																																																																																																																																																																																																																																
H	-0.00159	-2.41943	6.27340																																																																																																																																																																																																																																
 <p>4a -3271.271538 -3272.584469 -3271.851993</p>	<table border="1"> <tbody> <tr><td>C</td><td>0.13906</td><td>-0.05931</td><td>1.12041</td></tr> <tr><td>C</td><td>0.14762</td><td>-0.07230</td><td>3.89996</td></tr> <tr><td>C</td><td>0.38616</td><td>-1.24078</td><td>1.80324</td></tr> <tr><td>C</td><td>-0.11213</td><td>1.11655</td><td>1.82134</td></tr> <tr><td>C</td><td>-0.10990</td><td>1.11246</td><td>3.20653</td></tr> <tr><td>C</td><td>0.39309</td><td>-1.26533</td><td>3.19993</td></tr> <tr><td>H</td><td>0.56612</td><td>-2.16208</td><td>1.26066</td></tr> <tr><td>H</td><td>-0.30298</td><td>2.02125</td><td>3.76361</td></tr> <tr><td>C</td><td>0.12094</td><td>-0.05382</td><td>5.38653</td></tr> <tr><td>C</td><td>-0.03100</td><td>-0.01915</td><td>8.19716</td></tr> <tr><td>C</td><td>1.27210</td><td>-0.06909</td><td>6.17871</td></tr> <tr><td>C</td><td>-1.11065</td><td>-0.00938</td><td>6.04919</td></tr> <tr><td>C</td><td>-1.19432</td><td>0.00750</td><td>7.43556</td></tr> <tr><td>C</td><td>1.20770</td><td>-0.05431</td><td>7.56807</td></tr> <tr><td>H</td><td>-2.01130</td><td>0.00569</td><td>5.44931</td></tr> <tr><td>H</td><td>-2.16233</td><td>0.03917</td><td>7.91784</td></tr> <tr><td>H</td><td>2.11858</td><td>-0.06377</td><td>8.14946</td></tr> <tr><td>H</td><td>-0.08068</td><td>-0.00812</td><td>9.27797</td></tr> <tr><td>C</td><td>0.64839</td><td>-2.55576</td><td>3.93323</td></tr> <tr><td>H</td><td>-0.11597</td><td>-2.73775</td><td>4.69211</td></tr> <tr><td>H</td><td>1.61160</td><td>-2.52875</td><td>4.44896</td></tr> <tr><td>H</td><td>0.65678</td><td>-3.39746</td><td>3.23974</td></tr> <tr><td>C</td><td>-0.31245</td><td>2.28712</td><td>0.87837</td></tr> <tr><td>C</td><td>0.10170</td><td>0.19833</td><td>-0.36608</td></tr> <tr><td>H</td><td>1.11987</td><td>0.27421</td><td>-0.76213</td></tr> <tr><td>H</td><td>-0.40316</td><td>-0.59101</td><td>-0.92581</td></tr> </tbody> </table>	C	0.13906	-0.05931	1.12041	C	0.14762	-0.07230	3.89996	C	0.38616	-1.24078	1.80324	C	-0.11213	1.11655	1.82134	C	-0.10990	1.11246	3.20653	C	0.39309	-1.26533	3.19993	H	0.56612	-2.16208	1.26066	H	-0.30298	2.02125	3.76361	C	0.12094	-0.05382	5.38653	C	-0.03100	-0.01915	8.19716	C	1.27210	-0.06909	6.17871	C	-1.11065	-0.00938	6.04919	C	-1.19432	0.00750	7.43556	C	1.20770	-0.05431	7.56807	H	-2.01130	0.00569	5.44931	H	-2.16233	0.03917	7.91784	H	2.11858	-0.06377	8.14946	H	-0.08068	-0.00812	9.27797	C	0.64839	-2.55576	3.93323	H	-0.11597	-2.73775	4.69211	H	1.61160	-2.52875	4.44896	H	0.65678	-3.39746	3.23974	C	-0.31245	2.28712	0.87837	C	0.10170	0.19833	-0.36608	H	1.11987	0.27421	-0.76213	H	-0.40316	-0.59101	-0.92581	 <p>4a -3271.24226 -3272.555293 -3271.824944</p>	<table border="1"> <tbody> <tr><td>C</td><td>-0.06752</td><td>-1.36423</td><td>-2.67418</td></tr> <tr><td>C</td><td>0.00066</td><td>-1.12109</td><td>0.16938</td></tr> <tr><td>C</td><td>-0.05895</td><td>-2.48449</td><td>-1.86671</td></tr> <tr><td>C</td><td>-0.04331</td><td>-0.11980</td><td>-2.07270</td></tr> <tr><td>C</td><td>-0.00758</td><td>-0.01314</td><td>-0.69892</td></tr> <tr><td>C</td><td>-0.02925</td><td>-2.41158</td><td>-0.46549</td></tr> <tr><td>H</td><td>-0.08450</td><td>-3.46518</td><td>-2.32666</td></tr> <tr><td>H</td><td>0.00711</td><td>0.97611</td><td>-0.29432</td></tr> <tr><td>C</td><td>0.03620</td><td>-0.87085</td><td>1.65994</td></tr> <tr><td>C</td><td>0.10290</td><td>-0.65959</td><td>4.54854</td></tr> <tr><td>C</td><td>0.06703</td><td>0.37918</td><td>2.35080</td></tr> <tr><td>C</td><td>0.04454</td><td>-1.97134</td><td>2.54694</td></tr> <tr><td>C</td><td>0.07590</td><td>-1.89511</td><td>3.92830</td></tr> <tr><td>C</td><td>0.09855</td><td>0.46546</td><td>3.74392</td></tr> <tr><td>H</td><td>0.02621</td><td>-2.95629</td><td>2.14390</td></tr> <tr><td>H</td><td>0.07892</td><td>-2.81049</td><td>4.50523</td></tr> 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</table>	C	-0.06752	-1.36423	-2.67418	C	0.00066	-1.12109	0.16938	C	-0.05895	-2.48449	-1.86671	C	-0.04331	-0.11980	-2.07270	C	-0.00758	-0.01314	-0.69892	C	-0.02925	-2.41158	-0.46549	H	-0.08450	-3.46518	-2.32666	H	0.00711	0.97611	-0.29432	C	0.03620	-0.87085	1.65994	C	0.10290	-0.65959	4.54854	C	0.06703	0.37918	2.35080	C	0.04454	-1.97134	2.54694	C	0.07590	-1.89511	3.92830	C	0.09855	0.46546	3.74392	H	0.02621	-2.95629	2.14390	H	0.07892	-2.81049	4.50523	H	0.12043	1.44183	4.20469	H	0.12742	-0.55924	5.62515	C	-0.04127	-3.78079	0.19067	H	-0.91596	-3.93457	0.82702	H	0.85532	-3.96995	0.78573	H	-0.07431	-4.54958	-0.58093	C	-0.01550	0.99347	-3.10099	C	-0.08752	-1.23165	-4.17520	H	0.91200	-1.41356	-4.58417	H	-0.76689	-1.93379	-4.66186																
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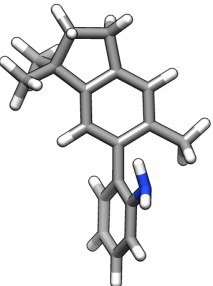
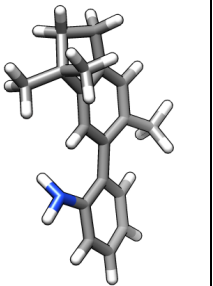
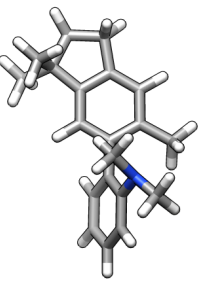
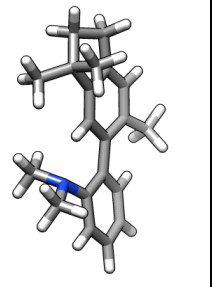
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 <p>4b -1034.903276 -1034.733099 -1035.609387</p>	<p>C -1.05725 -1.52826 -1.42782 C -0.52496 -0.81061 1.20290 C -1.62609 -2.24987 -0.38916 C -0.22151 -0.44904 -1.15671 C 0.04256 -0.08643 0.15337 C -1.36562 -1.90398 0.93870 H -2.26572 -3.10064 -0.59533 H 0.70289 0.74203 0.37559 C -0.24646 -0.39940 2.60836 C 0.17669 0.44885 5.25416 C 0.92024 -0.75888 3.30004 C -1.19044 0.38181 3.27628 C -0.98694 0.80606 4.58380 C 1.12722 -0.33329 4.61096 H -2.09423 0.65863 2.74948 H -1.73460 1.41482 5.07550 H 2.03132 -0.61823 5.12843 H 0.34624 0.77402 6.27177 C 0.26399 0.20719 -2.43447 C -1.19873 -1.71954 -2.91802 H -1.17878 -2.76844 -3.21891 H -2.14971 -1.30177 -3.26516 C -0.00467 -0.91339 -3.47432 H -0.18413 -0.51135 -4.47285 H 0.87165 -1.56417 -3.52353 C -0.60454 1.43955 -2.73865 H -0.50524 2.18225 -1.94398 H -1.65834 1.16271 -2.81521 H -0.29585 1.89738 -3.68226 C 1.73561 0.61205 -2.38103 H 2.36404 -0.24816 -2.14235 H 1.90056 1.37831 -1.61966 H 2.05324 1.02049 -3.34390 C -1.94454 -2.71991 2.06455 H -2.56602 -3.52748 1.67634 H -2.55308 -2.10617 2.73279 H -1.14849 -3.15797 2.67199 C 1.96762 -1.61364 2.62758 F 1.44946 -2.76121 2.13687 F 2.96090 -1.97088 3.46981 F 2.55621 -0.97478 1.59077</p>	 <p>4b -1034.870933 -1034.700039 -1035.579271</p>	<p>C -0.11836 -1.32552 -2.63806 C -0.03196 -1.03264 0.20231 C -0.08581 -2.43169 -1.81312 C -0.04008 -0.07267 -2.05805 C 0.01332 0.05774 -0.68776 C -0.02317 -2.33367 -0.41449 H -0.09334 -3.42078 -2.25549 H 0.10668 1.05495 -0.32940 C -0.04357 -0.77385 1.69275 C 0.23874 -0.59979 4.55815 C 0.01601 0.49178 2.37935 C -0.10838 -1.87697 2.56503 C 0.02917 -1.81711 3.94284 C 0.19632 0.53459 3.76568 H -0.28552 -2.84708 2.16362 H -0.02516 -2.73284 4.51721 H 0.27820 1.49370 4.25013 H 0.38574 -0.51562 5.62599 C 0.02600 1.02095 -3.10551 C -0.16033 -1.21660 -4.14046 H 0.82199 -1.45153 -4.56360 H -0.87968 -1.89542 -4.60208 C -0.51643 0.27327 -4.35445 H -1.60361 0.37861 -4.38235 H -0.11389 0.68084 -5.28302 C -0.80738 2.25013 -2.74908 H -0.42805 2.72691 -1.84249 H -1.84969 1.97367 -2.57813 H -0.76888 2.98366 -3.55846 C 1.49277 1.43123 -3.31828 H 2.10028 0.57001 -3.60551 H 1.90821 1.84889 -2.39872 H 1.56451 2.18568 -4.10613 C 0.11434 -3.69034 0.25550 H 0.95565 -3.72570 0.94967 H 0.29634 -4.44773 -0.50671 H -0.78706 -3.99923 0.79245 C -0.19077 1.87946 1.78446 F -1.29445 1.94790 1.00624 F 0.86513 2.32093 1.04963 F -0.37202 2.82885 2.72819</p>
 <p>4c -1157.390714 -1157.351666 -1158.023236</p>	<p>C 0.15284 -0.05721 1.12010 C 0.15973 -0.07490 3.90109 C 0.41058 -1.23709 1.80153 C -0.11064 1.11486 1.82280 C -0.10947 1.10812 3.20789 C 0.41694 -1.26442 3.19837 H 0.59718 -2.15628 1.25756 H -0.31338 2.01382 3.76618 C 0.12315 -0.05567 5.38712 C -0.04015 -0.00984 8.19689 C 1.27000 -0.12519 6.18428 C -1.10740 0.05129 6.04360 C -1.19731 0.07363 7.42965 C 1.19760 -0.10591 7.57351 H -2.00327 0.10967 5.43930 H -2.16492 0.15309 7.90712 H 2.10721 -0.15847 8.15500 H -0.09473 0.00439 9.27738 C 0.67599 -2.55739 3.92620 H -0.07392 -2.73224 4.70088 H 1.65021 -2.54079 4.42086 H 0.66101 -3.39873 3.23230 C -0.32333 2.28467 0.88147 C 0.11250 0.20209 -0.36602 H 1.12967 0.28942 -0.76233 H -0.38409 -0.59179 -0.92674 C -0.63196 1.55246 -0.45167 H -1.70684 1.36346 -0.50848 H -0.34694 2.14717 -1.32113</p>	 <p>4c -1157.363676 -1157.324577 -1157.998128</p>	<p>C -0.06632 -1.26662 -2.36665 C -0.00014 -0.74028 0.43830 C -0.05470 -2.30058 -1.45151 C -0.04639 0.03204 -1.89281 C -0.01169 0.27781 -0.53668 C -0.02570 -2.08720 -0.06486 H -0.07685 -3.32258 -1.81074 H -0.00008 1.30223 -0.23171 C 0.03419 -0.34721 1.89723 C 0.09928 0.17141 4.74644 C 0.06251 0.96882 2.45153 C 0.04401 -1.34815 2.89471 C 0.07500 -1.12380 4.26038 C 0.09292 1.20377 3.82712 H 0.02716 -2.37107 2.60013 H 0.07979 -1.97210 4.93204 H 0.11246 2.22790 4.17047 H 0.12333 0.38393 5.80663 C -0.03313 -3.38238 0.72687 H -0.90784 -3.47362 1.37507 H 0.86346 -3.50596 1.33889 H -0.06240 -4.22586 0.03748 C -0.02040 1.03594 -3.02869 C -0.08528 -1.28586 -3.87333 H 0.91512 -1.50496 -4.26140 H -0.76208 -2.03550 -4.28725 C -0.50884 0.16149 -4.21612 H -1.59942 0.21047 -4.26371 H -0.11323 0.50957 -5.17159</p>

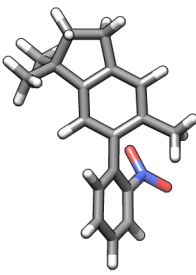
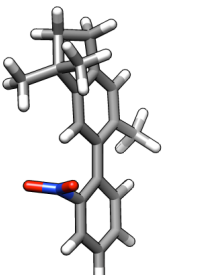
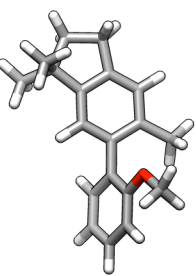
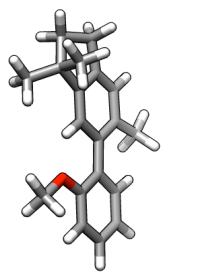
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 <p>4d -1361.898180 -1361.831504 -1362.652436</p>	<p>C -0.83389 -1.59792 -1.28645 C -0.37322 -0.16323 1.04691 C -1.03541 -2.20192 -0.05485 C -0.41280 -0.27280 -1.35866 C -0.18653 0.44616 -0.19743 C -0.80880 -1.49653 1.12959 H -1.38585 -3.22610 0.00394 H 0.13962 1.47829 -0.24030 C -0.14613 0.64579 2.27082 C 0.19973 2.21845 4.54504 C 0.94793 0.45361 3.12611 C -1.04625 1.66808 2.59234 C -0.88989 2.45843 3.72018 C 1.12863 1.22814 4.26347 H -1.89120 1.82905 1.93696 H -1.59078 3.24054 3.96730 H 1.97457 1.07666 4.91517 C -0.22284 0.16682 -2.79734 C -0.99915 -2.17084 -2.67233 H -0.13534 -2.79334 -2.92769 H -1.88782 -2.79595 -2.77446 C -1.04955 -0.90551 -3.55601 H -2.08488 -0.56412 -3.63093 H -0.67446 -1.07154 -4.56703 C -0.71940 1.58526 -3.06788 H -0.14190 2.31569 -2.49588 H -1.77149 1.68589 -2.79295 H -0.61273 1.82956 -4.12771 C 1.26594 0.05722 -3.16862 H 1.63134 -0.96022 -3.01387 H 1.86474 0.73000 -2.55099 H 1.41435 0.32428 -4.21813 C -1.05776 -2.15842 2.45964 H -0.11810 -2.38525 2.96910 H -1.60369 -3.09283 2.32628 H -1.63684 -1.51259 3.12327 Cl 2.15668 -0.74939 2.76377 N 0.38604 3.04258 5.75655 O 1.35251 2.80406 6.46394 O -0.43964 3.91472 5.97888</p>	 <p>4d -1361.872009 -1361.805480 -1362.628291</p>	<p>C -0.04117 -1.16861 -3.36700 C -0.01167 -0.79345 -0.54064 C -0.03708 -2.25124 -2.50916 C -0.03128 0.10444 -2.82623 C -0.01436 0.27726 -1.45950 C -0.02589 -2.11406 -1.11381 H -0.05146 -3.25161 -2.92447 H -0.01041 1.28390 -1.10060 C 0.00190 -0.48018 0.93205 C 0.02526 -0.12395 3.77769 C 0.01773 0.80982 1.55595 C 0.00218 -1.53725 1.87267 C 0.01318 -1.39812 3.24602 C 0.02795 0.97096 2.93783 H -0.00639 -2.54158 1.52103 H 0.01225 -2.26274 3.89136 H 0.03882 1.96080 3.36547 C 0.00308 1.16598 -3.90806 C -0.04436 -1.10912 -4.87198 H 0.96174 -1.30462 -5.25759 H -0.71227 -1.84012 -5.33077 C -0.46995 0.35241 -5.14415 H -1.56001 0.40035 -5.20156 H -0.06500 0.75013 -6.07570 C -0.90069 2.36048 -3.61130 H -0.56620 2.88615 -2.71369 H -1.93151 2.03627 -3.45484 H -0.88083 3.06873 -4.44325 C 1.45168 1.64476 -4.10222 H 2.10930 0.80788 -4.34773 H 1.82435 2.11266 -3.18855 H 1.50261 2.37591 -4.91306 C -0.03802 -3.45043 -0.39404 H 0.85178 -3.60529 0.22079 H -0.05481 -4.25456 -1.12873 H -0.92127 -3.58130 0.23555 Cl 0.02980 2.39000 0.76932 N 0.03644 0.07573 5.23361 O 0.03569 -0.92310 5.93845 O 0.04578 1.22350 5.65380</p>
 <p>4e -790.0619184 -789.9257093 -790.6823011</p>	<p>C -0.76584 -1.60713 -1.30158 C -0.35947 -0.15596 1.03894 C -0.91863 -2.22380 -0.07168 C -0.42309 -0.25832 -1.37222 C -0.22593 0.46481 -0.21124 C -0.71879 -1.51352 1.11684 H -1.21179 -3.26598 -0.01391 H 0.04321 1.51330 -0.25294 C -0.14904 0.67753 2.24790 C 0.21159 2.32558 4.50824 C 0.85779 0.40367 3.19392 C -0.94796 1.80362 2.45892 C -0.77624 2.61792 3.57146 C 1.02974 1.22350 4.31734 H -1.72256 2.02632 1.73738 H -1.41761 3.47841 3.71059 H 1.81363 0.98969 5.02454 H 0.34681 2.95461 5.37756 C -0.27381 0.19614 -2.81108 C -0.91222 -2.18281 -2.68827 H -0.01569 -2.75168 -2.95552 H -1.76328 -2.85919 -2.78426 C -1.04653 -0.91885 -3.56523 H -2.10076 -0.63741 -3.62596 H -0.67484 -1.05851 -4.58160 C -0.85305 1.58490 -3.07088 H -0.31257 2.34456 -2.50064 H -1.90642 1.62388 -2.78528 H -0.77083 1.83947 -4.13061 C 1.21444 0.17250 -3.19928 H 1.63934 -0.82239 -3.05071 H 1.78055 0.87696 -2.58620 H 1.33561 0.44965 -4.24979</p>	 <p>4e -790.0426239 -789.9064414 -790.6647340</p>	<p>C -0.06646 -1.30004 -2.26190 C -0.00017 -0.70642 0.52066 C -0.05433 -2.31314 -1.32307 C -0.04446 0.01310 -1.82277 C -0.00994 0.29161 -0.47437 C -0.02425 -2.06274 0.05700 H -0.07666 -3.34436 -1.65504 H 0.00220 1.32901 -0.06221 C 0.03067 -0.27153 1.95967 C 0.09131 0.45372 4.75561 C 0.05497 1.09037 2.40390 C 0.03993 -1.20703 3.01095 C 0.06888 -0.87291 4.35713 C 0.08421 1.42132 3.77006 H 0.02424 -2.25075 2.79345 H 0.07355 -1.66792 5.09152 H 0.10145 2.46861 4.03928 H 0.11375 0.73206 5.80010 C -0.02094 0.98801 -2.98250 C -0.08922 -1.35515 -3.76763 H 0.91101 -1.58335 -4.15075 H -0.76573 -2.11605 -4.16084 C -0.51368 0.08342 -4.14540 H -1.60433 0.13186 -4.19094 H -0.12067 0.40645 -5.11049 C -0.91405 2.20732 -2.76221 H -0.56840 2.79469 -1.90843 H -1.94501 1.90055 -2.57337 H -0.89996 2.85238 -3.64443 C 1.42721 1.44291 -3.23124 H 2.07918 0.58608 -3.41645 H 1.81049 1.98266 -2.36297 H 1.46995 2.10626 -4.09893</p>

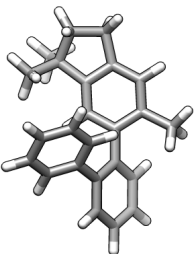
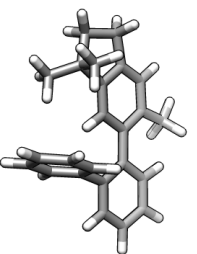
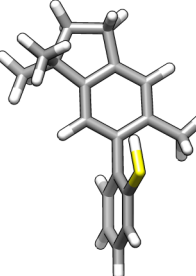
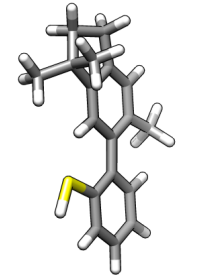
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	H	-1.67590	-3.00829	2.32038		H	-0.05144	-4.19455	0.24372
	H	-1.25797	-1.53816	3.21268		H	-0.90251	-3.38998	1.54872
	C	1.75892	-0.69143	3.01244		C	0.05489	2.27437	1.59658
	N	2.49750	-1.56792	2.89044		N	0.05850	3.30404	1.07463
	C	-0.17712	-0.91403	-1.75285		C	-0.16762	-1.31881	-2.39624
	C	-0.06136	-0.42231	0.98601		C	-0.02100	-0.87302	0.40848
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	C	-1.05061	0.89546	4.37377		C	-0.05987	-1.26354	4.21940
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	H	-0.69004	-3.77716	0.97511		H	0.42407	-4.28767	-0.03327
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	C	0.49895	-1.26336	3.19444		C	-0.02071	-1.94023	0.05161
	H	0.74427	-2.12641	1.24794		H	-0.06985	-3.21784	-1.66363
	H	-0.39287	1.97299	3.77253		H	-0.00081	1.45283	-0.18057
	C	0.10066	-0.06594	5.38693		C	0.03343	-0.17511	1.96795
	C	-0.06476	0.03596	8.20132		C	0.09840	0.57806	4.75866
	C	1.18001	-0.39087	6.20577		C	0.05602	1.16353	2.42734
	C	-1.07445	0.33211	6.03585		C	0.04701	-1.10164	3.03409
	C	-1.16421	0.38303	7.42159		C	0.07814	-0.75455	4.37726
	C	1.12143	-0.35173	7.58846		C	0.08696	1.53762	3.76035
	H	-1.92937	0.59195	5.42541		H	0.03313	-2.14780	2.82490
	H	-2.09026	0.68717	7.89082		H	0.08633	-1.54065	5.12052
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	H	-0.12523	0.06983	9.28092		H	0.12282	0.86799	5.80030
	C	0.79832	-2.56539	3.89115		C	-0.02129	-3.19992	0.89322
	H	0.20545	-2.67689	4.80046		H	-0.89485	-3.26493	1.54599
	H	1.84928	-2.62130	4.18326		H	0.87533	-3.28859	1.51102
	H	0.58492	-3.40782	3.23161		H	-0.04571	-4.07197	0.23981
	C	-0.37096	2.26950	0.89277		C	-0.02426	1.11659	-2.97860
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	H	-0.26634	-0.59102	-0.93938		H	-0.75930	-1.98450	-4.16515
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	H	-1.36076	3.61446	2.29771		H	-0.57656	2.92590	-1.91525
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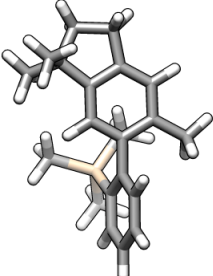
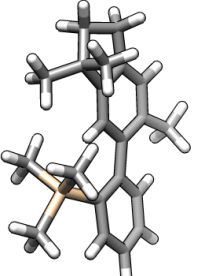
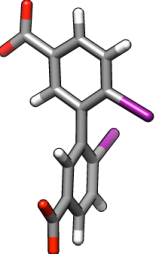
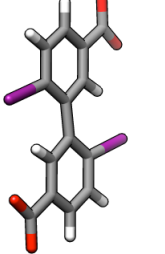
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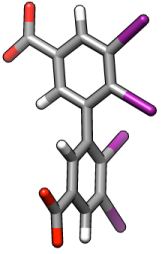
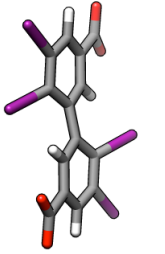
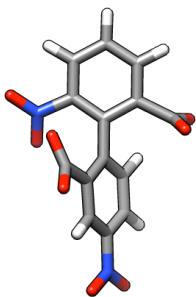
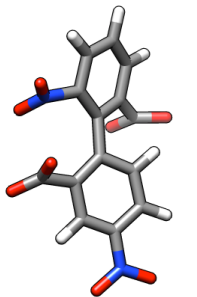
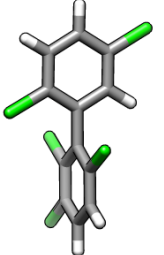
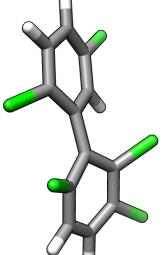
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	C	0.05882	0.41947	4.44774		C	0.03496	-1.15683	-0.28446
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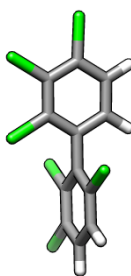
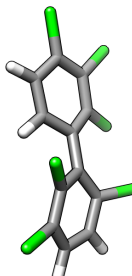
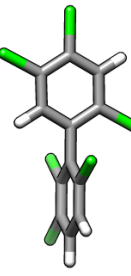
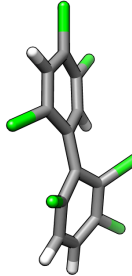
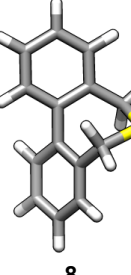
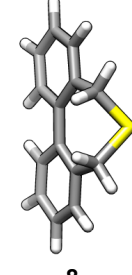
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	C	3.11560	-1.31498	2.39797		C	-0.99429	3.03948	2.63214
	H	3.77686	-2.08069	1.98434		H	-0.38240	3.42769	3.44811
	H	3.61962	-0.84596	3.24680		H	-1.89685	2.59827	3.05764
	H	2.94769	-0.55162	1.63601		H	-1.28220	3.89107	2.01171
	C	-0.69395	-0.99390	-1.82212		C	-0.15201	-1.16407	-2.22142
	C	-0.27986	-0.24252	0.83155		C	-0.04023	-0.50882	0.55610
	C	-1.20185	-1.77627	-0.79598		C	-0.08231	-2.15488	-1.26134
	C	0.01269	0.16952	-1.53100		C	-0.07448	0.15459	-1.80984
	C	0.21600	0.54597	-0.21348		C	-0.00985	0.46644	-0.46734
	C	-1.00351	-1.41537	0.54012		C	-0.00048	-1.87305	0.10977
	H	-1.76511	-2.67582	-1.01838		H	-0.06612	-3.19416	-1.56938
	H	0.77053	1.44524	0.02637		H	0.12829	1.49861	-0.21712
	C	-0.03550	0.18648	2.23439		C	-0.06112	-0.07365	1.99617
	C	0.42467	1.06168	4.85486		C	0.18112	0.55338	4.78748
	C	0.83204	-0.53635	3.07702		C	0.01972	1.28074	2.45871
	C	-0.63934	1.34423	2.72559		C	-0.18288	-1.02739	3.02851
	C	-0.42375	1.78917	4.02499		C	-0.06123	-0.75001	4.38011
	C	1.04633	-0.08590	4.38531		C	0.19167	1.54442	3.82569
	H	-1.29771	1.89592	2.06615		H	-0.40031	-2.04230	2.77715
	H	-0.91016	2.68618	4.38351		H	-0.15662	-1.55198	5.09975
	H	1.71296	-0.64671	5.03030		H	0.29812	2.57978	4.13052
	H	0.60743	1.38915	5.87036		H	0.31204	0.80419	5.83193
	C	0.42645	0.89296	-2.79836		C	-0.01414	1.09837	-2.99549
	C	-0.80291	-1.18183	-3.31567		C	-0.21430	-1.25303	-3.72523
	H	-0.66129	-2.21743	-3.63006		H	0.76135	-1.54220	-4.13014
	H	-1.79341	-0.87146	-3.66487		H	-0.94062	-1.98413	-4.08520
	C	0.29351	-0.23696	-3.85400		C	-0.57499	0.19578	-4.12774
	H	0.07432	0.15517	-4.84855		H	-1.66278	0.29761	-4.15251
	H	1.23919	-0.78229	-3.90654		H	-0.18702	0.47887	-5.10767
	C	-0.57786	2.02053	-3.09153		C	-0.83525	2.37115	-2.80084
	H	-0.56749	2.75915	-2.28713		H	-0.43511	2.96523	-1.97504
	H	-1.59223	1.62460	-3.17561		H	-1.87688	2.12816	-2.57991
	H	-0.32160	2.52289	-4.02816		H	-0.80574	2.98836	-3.70257
	C	1.84028	1.46673	-2.73427		C	1.45206	1.46609	-3.27874
	H	2.56589	0.68157	-2.51140		H	2.04886	0.56904	-3.45713
	H	1.91392	2.23314	-1.95890		H	1.88351	1.99610	-2.42683
	H	2.10842	1.92698	-3.68883		H	1.51914	2.10974	-4.16007
	C	-1.58562	-2.26037	1.64307		C	0.21456	-3.10983	0.96242
	H	-0.79886	-2.74453	2.22617		H	1.00998	-2.96907	1.69500
	H	-2.24041	-3.03026	1.23270		H	0.50530	-3.94032	0.31824
	H	-2.16170	-1.64583	2.33857		H	-0.68585	-3.42673	1.49658
	N	1.44980	-1.70413	2.63537		N	-0.05386	2.42125	1.63230
	H	1.51827	-1.80213	1.63419		H	-0.82866	2.40324	0.98580
	H	2.30145	-1.94715	3.11422		H	-0.09632	3.26998	2.17783
	C	0.59756	2.61857	-1.55725		C	-0.09981	-1.21195	-2.53554
	C	0.33884	1.53008	0.99904		C	-0.04454	-0.88434	0.29970
	C	-0.12952	1.45333	-1.37072		C	-0.09438	-2.30855	-1.69582
	C	1.18376	3.25626	-0.46771		C	-0.01000	0.04821	-1.97113
	C	1.05400	2.71799	0.80061		C	0.02225	0.20075	-0.60207
	C	-0.27241	0.89339	-0.09742		C	-0.04760	-2.19028	-0.29824
	H	-0.61567	0.97076	-2.21155		H	-0.11158	-3.30454	-2.12325
	H	1.51004	3.20295	1.65550		H	0.12875	1.18971	-0.20088
	C	0.20709	1.00337	2.38311		C	-0.04398	-0.60296	1.78268
	C	-0.25266	0.08990	4.99281		C	0.30163	-0.29746	4.61662
	C	0.68397	-0.27028	2.77371		C	0.09035	0.69421	2.39124
	C	-0.44145	1.79884	3.32815		C	-0.15019	-1.66324	2.70293
	C	-0.67879	1.35874	4.62590		C	0.01959	-1.53807	4.07432
	C	0.42719	-0.70852	4.08011		C	0.30458	0.79950	3.76994
	H	-0.79803	2.77184	3.01469		H	-0.37922	-2.64421	2.35077
	H	-1.20215	1.99207	5.32973		H	-0.06311	-2.41627	4.70117
	H	0.77863	-1.67959	4.39600		H	0.43723	1.78107	4.19946
	H	-0.43284	-0.28093	5.99385		H	0.46781	-0.16889	5.67832
	C	1.95356	4.48900	-0.90089		C	0.08221	1.12463	-3.03504
	C	0.88958	3.37696	-2.82895		C	-0.12638	-1.12305	-4.04037
	H	1.69624	2.88848	-3.38604		H	0.85599	-1.37569	-4.45357
	H	0.02960	3.44011	-3.49817		H	-0.85125	-1.79692	-4.50100
	C	1.34009	4.75679	-2.30120		C	-0.46091	0.36826	-4.27800
	H	0.46206	5.39658	-2.18329		H	-1.54664	0.48721	-4.31508
	H	2.04140	5.26457	-2.96566		H	-0.04680	0.75806	-5.20948
	C	1.78182	5.67394	0.04692		C	-0.73520	2.37135	-2.70368
	H	2.18929	5.44363	1.03437		H	-0.35500	2.85046	-1.79800
	H	0.72558	5.92622	0.16136		H	-1.78342	2.11287	-2.53950
	H	2.30907	6.55050	-0.33861		H	-0.67800	3.09636	-3.51980
	C	3.44599	4.13895	-1.02848		C	1.55584	1.51143	-3.24282
	H	3.59238	3.31495	-1.73031		H	2.15155	0.63705	-3.51396
	H	3.85094	3.83656	-0.06017		H	1.97138	1.93277	-2.32481
	H	4.01023	5.00459	-1.38590		H	1.64614	2.25470	-4.03977
	C	-1.09974	-0.35308	0.07098		C	0.06325	-3.52883	0.40767
	H	-0.45680	-1.23276	0.14325		H	0.88477	-3.54788	1.12543
	H	-1.77764	-0.48042	-0.77453		H	0.25751	-4.30838	-0.32949
	H	-1.68723	-0.31445	0.99004		H	-0.85287	-3.81369	0.93270

	N 1.37894 -1.08327 1.85469 C 2.63106 -0.55498 1.32385 H 2.90579 -1.11900 0.42976 H 3.44715 -0.65055 2.05792 H 2.52705 0.49017 1.05027 C 1.49070 -2.49344 2.16865 H 1.84318 -3.01990 1.27963 H 0.51652 -2.89336 2.45106 H 2.20169 -2.69807 2.98597		N -0.05121 1.90622 1.65892 C -1.43565 2.18576 1.28654 H -1.88892 1.30117 0.84321 H -1.45729 2.99038 0.54762 H -2.03042 2.49093 2.16076 C 0.61188 3.09325 2.16347 H 1.64057 2.85810 2.43496 H 0.11024 3.53656 3.03914 H 0.61824 3.84627 1.37210
 <p>4n -902.3318827 -902.1900026 -903.0136423</p>	C 0.18609 -0.23328 -0.46378 C -1.53764 -2.24310 0.39493 C -0.66119 -0.00602 0.60794 C 0.17035 -1.46173 -1.11963 C -0.69011 -2.45828 -0.69906 C -1.53116 -1.00334 1.05757 H -0.66798 0.95669 1.10667 H -0.70927 -3.41788 -1.20088 C -2.47340 -3.33442 0.76401 C -4.37022 -5.35717 1.33795 C -2.57768 -3.92144 2.03063 C -3.35725 -3.81318 -0.21094 C -4.28349 -4.81137 0.06057 C -3.51665 -4.90179 2.33070 H -3.31450 -3.36707 -1.19524 H -4.94654 -5.15389 -0.72297 H -3.55341 -5.30140 3.33328 H -5.09322 -6.12994 1.56009 C 1.20308 -1.50584 -2.22889 C 1.20770 0.68245 -1.09110 H 0.85830 1.71169 -1.18957 H 2.11637 0.70697 -0.48061 C 1.47501 0.00569 -2.45329 H 2.48097 0.18817 -2.83465 H 0.76045 0.38695 -3.18703 C 2.47130 -2.20744 -1.71351 H 2.25240 -3.24253 -1.44295 H 2.86178 -1.70230 -0.82771 H 3.24506 -2.20516 -2.48580 C 0.70507 -2.20270 -3.49310 H -0.20543 -1.72683 -3.86354 H 0.48888 -3.25583 -3.29677 H 1.46477 -2.15704 -4.27754 C -2.43273 -0.70754 2.22888 H -1.95196 -0.97432 3.17379 H -3.37260 -1.25791 2.17276 H -2.66129 0.35826 2.27049 N -1.64922 -3.55930 3.11936 O -2.10391 -3.52788 4.25490 O -0.48691 -3.33476 2.82898	 <p>4n -902.3082671 -902.1667832 -902.9907216</p>	C -0.01451 -1.31605 -2.44885 C 0.01179 -0.88281 0.36646 C 0.00524 -2.38042 -1.56993 C -0.02745 -0.03160 -1.93306 C -0.01279 0.17081 -0.57081 C 0.01416 -2.20887 -0.17742 H 0.00428 -3.39110 -1.96038 H -0.03056 1.19505 -0.26715 C 0.02647 -0.54786 1.83398 C 0.03450 -0.00258 4.67787 C 0.01443 0.75441 2.39208 C 0.05437 -1.54715 2.83002 C 0.05890 -1.30021 4.19491 C 0.01358 1.02652 3.75345 H 0.07586 -2.57427 2.54537 H 0.08135 -2.14047 4.87613 H -0.00082 2.05864 4.07672 H 0.03468 0.21015 5.73778 C -0.01256 1.01054 -3.03323 C -0.01739 -1.28325 -3.95528 H 0.99222 -1.46721 -4.33744 H -0.67223 -2.03382 -4.40139 C -0.46892 0.16543 -4.25428 H -1.55963 0.19278 -4.31337 H -0.06997 0.55331 -5.19265 C -0.93893 2.19286 -2.75666 H -0.61897 2.73991 -1.86671 H -1.96402 1.85198 -2.59814 H -0.92922 2.88765 -3.60019 C 1.42729 1.51313 -3.23310 H 2.10119 0.68443 -3.46231 H 1.78811 2.00490 -2.32743 H 1.46529 2.23015 -4.05724 C 0.01280 -3.51754 0.58742 H 0.90985 -3.64653 1.19774 H -0.01169 -4.34773 -0.11791 H -0.86190 -3.62282 1.23321 N 0.01349 2.02285 1.62149 O -1.06827 2.53202 1.38389 O 1.09794 2.50206 1.33753
 <p>4o -812.3439256 -812.2125694 -812.9774610</p>	C -0.35728 -0.08944 1.63442 C -0.20206 0.35149 4.38364 C -0.25094 -1.16481 2.50239 C -0.39732 1.20908 2.13367 C -0.32174 1.42913 3.49809 C -0.17212 -0.96341 3.88338 H -0.24655 -2.17961 2.11973 H -0.35147 2.43562 3.89764 C -0.16814 0.63966 5.84066 C -0.16820 1.23304 8.58337 C 0.93868 0.30776 6.64512 C -1.24546 1.28691 6.44244 C -1.25908 1.58565 7.80244 C 0.93117 0.59833 8.01007 H -2.09362 1.54633 5.82190 H -2.11403 2.08116 8.24235 H 1.77857 0.34353 8.62851 H -0.15982 1.45141 9.64341 C -0.47880 2.22685 1.01211 C -0.43937 -0.07534 0.12757 H 0.55518 -0.21917 -0.30817 H -1.08311 -0.85968 -0.27488 C -0.97043 1.34470 -0.16653 H -2.06309 1.32472 -0.15849 H -0.64652 1.73455 -1.13314 C -1.43105 3.38266 1.31130 H -1.07920 3.96396 2.16712 H -2.43198 3.00911 1.53752 H -1.49656 4.05506 0.45190 C 0.92762 2.77641 0.71871 H 1.61568 1.96629 0.46743 H 1.32333 3.29807 1.59282 H 0.89404 3.47752 -0.11966	 <p>4o -812.3228123 -812.1910039 -812.9577035</p>	C -0.06627 -1.15274 -2.45478 C -0.02436 -0.79223 0.37813 C -0.04379 -2.23912 -1.60251 C -0.06621 0.11569 -1.90409 C -0.04260 0.28677 -0.53570 C -0.02532 -2.10481 -0.20622 H -0.04796 -3.23917 -0.20200 H -0.04525 1.28871 -0.15975 C -0.00995 -0.49490 1.85804 C 0.01879 -0.07246 4.70758 C -0.00883 0.81728 2.44233 C 0.00456 -1.53068 2.80949 C 0.01860 -1.35128 4.18652 C 0.00500 0.99859 3.82732 H 0.00488 -2.54416 2.48056 H 0.02899 -2.21854 4.83307 H 0.00564 1.99816 4.23108 H 0.02948 0.10439 5.77504 C -0.04580 1.18416 -2.98075 C -0.07612 -1.08359 -3.96044 H 0.92883 -1.26610 -4.35610 H -0.74127 -1.81541 -4.42272 C -0.51704 0.37553 -4.22030 H -1.60810 0.41310 -4.27044 H -0.12195 0.78455 -5.15182 C -0.95877 2.36927 -2.67451 H -0.62592 2.88905 -1.77264 H -1.98597 2.03427 -2.51661 H -0.94771 3.08472 -3.50102 C 1.39659 1.67889 -3.17994 H 2.05949 0.84916 -3.43523 H 1.77010 2.14056 -2.26327 H 1.43811 2.41774 -3.98499

	C -0.08717 -2.15560 4.79963 H 0.94626 -2.33574 5.10409 H -0.45975 -3.05128 4.30014 H -0.66636 -1.99687 5.71113 O 1.99325 -0.27425 6.00996 C 3.12686 -0.63368 6.77978 H 2.86340 -1.35899 7.55671 H 3.57911 0.24477 7.25126 H 3.83399 -1.08069 6.08416		C -0.01312 -3.43835 0.51646 H 0.87913 -3.57234 1.13251 H -0.01754 -4.24615 -0.21537 H -0.89134 -3.57924 1.15093 O -0.02091 1.91741 1.63448 C -0.03083 3.21727 2.19654 H 0.86497 3.39789 2.79845 H -0.91904 3.37661 2.81538 H -0.04708 3.90253 1.35105
 <p>4p -928.8339249 -928.6744906 -929.5759309</p>	C -1.04626 -1.37243 -1.41614 C -0.63388 -0.84112 1.28984 C -1.80491 -2.02836 -0.46040 C -0.08250 -0.44574 -1.02584 C 0.11719 -0.17665 0.31358 C -1.60955 -1.77639 0.90239 H -2.54107 -2.76747 -0.75669 H 0.88316 0.52111 0.62604 C -0.33867 -0.56248 2.72014 C 0.16638 0.12309 5.39501 C 0.95678 -0.72093 3.25442 C -1.35344 -0.07253 3.54633 C -1.11374 0.26868 4.87049 C 1.18502 -0.36629 4.58922 H -2.34183 0.05987 3.12703 H -1.91808 0.65117 5.48540 H 2.17770 -0.50171 4.99864 H 0.36926 0.38176 6.42614 C 0.63243 0.14711 -2.22336 C -1.06865 -1.49958 -2.91962 H -1.19274 -2.52859 -3.26188 H -1.89710 -0.91793 -3.33791 C 0.29211 -0.89164 -3.32593 H 0.28428 -0.44506 -4.32173 H 1.05062 -1.67816 -3.31323 C 0.01892 1.51443 -2.56702 H 0.15443 2.21238 -1.73798 H -1.05197 1.42221 -2.76138 H 0.49887 1.93291 -3.45575 C 2.13723 0.29298 -2.00311 H 2.58068 -0.66314 -1.71810 H 2.34459 1.01261 -1.20758 H 2.62333 0.64900 -2.91528 C -2.41467 -2.55141 1.91614 H -1.80188 -2.84890 2.76892 H -2.84036 -3.44628 1.45972 H -3.24091 -1.95721 2.31559 C 2.08788 -1.25850 2.45801 C 4.24607 -2.25088 0.96248 C 1.95180 -2.41820 1.68785 C 3.32729 -0.61221 2.47279 C 4.39679 -1.10016 1.72910 C 3.01945 -2.91080 0.94982 H 0.99866 -2.92707 1.66173 H 3.44323 0.29149 3.05729 H 5.34462 -0.57753 1.74447 H 2.89351 -3.81068 0.36163 H 5.07577 -2.63098 0.38075	 <p>4p -928.8093751 -928.6499102 -929.5527741</p>	C -0.06215 -1.98240 -2.35083 C -0.01570 -1.33455 0.42847 C -0.04352 -2.97606 -1.39166 C -0.10376 -0.66446 -1.93173 C -0.08224 -0.36074 -0.58836 C -0.03729 -2.69853 -0.01533 H -0.05413 -4.01413 -1.70303 H -0.12860 0.67621 -0.33444 C 0.04553 -0.87304 1.86599 C 0.01809 -0.15807 4.65055 C 0.01036 0.49264 2.29185 C 0.14249 -1.80984 2.91420 C 0.12965 -1.48110 4.26172 C -0.02632 0.80490 3.65542 H 0.24350 -2.84837 2.69310 H 0.20577 -2.27185 4.99701 H -0.06862 1.85106 3.93010 H -0.00973 0.12562 5.69428 C -0.12147 0.29497 -3.10472 C -0.05854 -2.06179 -3.85596 H 0.95665 -2.24889 -4.22214 H -0.69367 -2.85794 -4.24887 C -0.54343 -0.65027 -4.26340 H -1.63402 -0.65615 -4.33190 H -0.14705 -0.32201 -5.22568 C -1.09038 1.46030 -2.91355 H -0.79096 2.07921 -2.06505 H -2.10266 1.09299 -2.73116 H -1.10561 2.09279 -3.80529 C 1.29855 0.83822 -3.33649 H 2.00582 0.02191 -3.50042 H 1.63049 1.40892 -2.46651 H 1.31578 1.49433 -4.21102 C -0.10392 -3.94564 0.84514 H 0.81855 -4.12442 1.40401 H -0.25950 -4.81601 0.20744 H -0.93213 -3.91424 1.55544 C 0.07318 1.72254 1.44378 C 0.23167 4.09593 -0.03662 C 1.30480 2.18696 0.97443 C -1.07175 2.47888 1.19042 C -0.99467 3.65457 0.44930 C 1.38316 3.36047 0.23420 H 2.19692 1.60839 1.17557 H -2.02721 2.12954 1.55952 H -1.89373 4.22324 0.24947 H 2.34329 3.70268 -0.13022 H 0.29162 5.00712 -0.61718
 <p>4q -1095.988885 -1095.933315 -1096.620153</p>	C -0.85104 -1.59272 -1.29591 C -0.39691 -0.14370 1.03753 C -1.06680 -2.18847 -0.06215 C -0.41459 -0.27290 -1.37070 C -0.18616 0.44953 -0.21087 C -0.84673 -1.47454 1.11901 H -1.42275 -3.21070 0.00029 H 0.15583 1.47640 -0.25545 C -0.16229 0.65810 2.26868 C 0.18374 2.21989 4.57416 C 0.97395 0.48725 3.07864 C -1.09795 1.62950 2.63343 C -0.93860 2.40700 3.77355 C 1.13420 1.27089 4.22595 H -1.96913 1.76184 2.00442 H -1.68216 3.14841 4.03407 H 2.01345 1.14038 4.84442 H 0.32563 2.81525 5.46671 C -0.20781 0.15708 -2.81019 C -1.00996 -2.17160 -2.68051 H -0.15151 -2.80540 -2.92656 H -1.90502 -2.78683 -2.78767 C -1.03884 -0.91030 -3.57094 H -2.06979 -0.55822 -3.65634 H -0.65702 -1.08535 -4.57808	 <p>4q -1095.959685 -1095.903969 -1096.593119</p>	C -0.03808 -1.28849 -2.36454 C -0.02938 -0.74440 0.44184 C -0.01437 -2.31587 -1.44166 C -0.06405 0.01258 -1.89899 C -0.05776 0.26181 -0.54282 C -0.01404 -2.09385 -0.05638 H -0.00491 -3.34039 -1.79435 H -0.08627 1.29600 -0.26560 C -0.02155 -0.33422 1.89449 C -0.01027 0.21725 4.72025 C -0.03643 1.00868 2.40293 C 0.00805 -1.32622 2.89730 C 0.01402 -1.08742 4.25985 C -0.03390 1.23624 3.78855 H 0.02986 -2.35199 2.61274 H 0.03743 -1.92398 4.94545 H -0.04958 2.25406 4.15409 H -0.00878 0.44885 5.77703 C -0.04975 1.01153 -3.03890 C -0.03103 -1.31609 -3.87139 H 0.98156 -1.50777 -4.24209 H -0.67895 -2.08712 -4.29228 C -0.49129 0.11636 -4.22935 H -1.58185 0.13270 -4.29583 H -0.08966 0.47139 -5.17975

	<p>C -0.68771 1.57920 -3.09172 H -0.10811 2.30604 -2.51747 H -1.74081 1.69140 -2.82538 H -0.56998 1.81757 -4.15188 C 1.28269 0.03129 -3.16916 H 1.63588 -0.98974 -3.00889 H 1.88310 0.69963 -2.54823 H 1.44321 0.29368 -4.21819 C -1.10844 -2.11757 2.45544 H -0.18677 -2.20591 3.03636 H -1.53217 -3.11436 2.32770 H -1.80130 -1.51721 3.04963 S 2.26775 -0.67634 2.72443 H 1.77686 -1.11381 1.55415</p>		<p>C -0.98772 2.19600 -2.81633 H -0.67572 2.77972 -1.94707 H -2.01047 1.85241 -2.64851 H -0.98033 2.85665 -3.68714 C 1.38653 1.51887 -3.25145 H 2.06781 0.68735 -3.44530 H 1.73936 2.04676 -2.36297 H 1.42389 2.20460 -4.10210 C -0.00857 -3.38280 0.74486 H 0.88484 -3.48846 1.36484 H -0.02064 -4.23190 0.06176 H -0.88634 -3.48044 1.38768 S -0.05216 2.51954 1.43069 H -0.04471 3.35621 2.47989</p>
 <p>4r -1106.456653 -1106.358940 -1107.172798</p>	<p>C -2.08483 -1.25208 -1.06270 C -1.07751 -0.01690 1.21978 C -2.92372 -0.48820 -0.26458 C -0.74545 -1.40979 -0.71978 C -0.24526 -0.80282 0.42041 C -2.43256 0.14024 0.88152 H -3.96428 -0.35010 -0.53610 H 0.79629 -0.91209 0.69389 C -0.49821 0.69181 2.39362 C 0.56442 1.94990 4.65081 C 0.34203 1.81012 2.22058 C -0.80152 0.23187 3.67650 C -0.27269 0.85023 4.80250 C 0.85839 2.41862 3.37521 H -1.45340 -0.62621 3.78470 H -0.51200 0.47570 5.78970 H 1.49939 3.28578 3.27820 H 0.98190 2.44300 5.51949 C -0.02702 -2.31062 -1.70539 C -2.39481 -2.01161 -2.32925 H -2.89560 -2.95609 -2.09160 H -3.04868 -1.46292 -3.00938 C -0.99094 -2.26419 -2.92096 H -0.71519 -1.41879 -3.55611 H -0.93439 -3.17222 -3.52362 C 1.37613 -1.82129 -2.05715 H 2.02281 -1.82590 -1.17639 H 1.34350 -0.80392 -2.45179 H 1.82909 -2.47169 -2.80978 C 0.04745 -3.73609 -1.13320 H -0.95128 -4.11639 -0.90800 H 0.63070 -3.74680 -0.20988 H 0.52211 -4.40911 -1.85223 C -3.33290 1.02786 1.70029 H -3.44150 0.65851 2.72218 H -4.32377 1.09390 1.24940 H -2.91669 2.03580 1.77682 Si 0.78450 2.55496 0.53418 C 2.20850 1.61613 -0.26665 H 2.55820 2.14691 -1.15780 H 1.90909 0.61287 -0.57151 H 3.05420 1.52480 0.42068 C -0.68907 2.58374 -0.63499 H -0.45401 3.20690 -1.50360 H -1.57401 3.00660 -0.15230 H -0.94861 1.58518 -0.98890 C 1.35179 4.32872 0.83273 H 1.56610 4.81630 -0.12270 H 2.26338 4.37230 1.43458 H 0.58483 4.91609 1.34458</p>	 <p>4r -1106.426630 -1106.328572 -1107.144459</p>	<p>C -0.15350 -1.53465 -2.69973 C -0.03413 -1.27100 0.13698 C -0.16940 -2.64820 -1.88315 C -0.02191 -0.28654 -2.11399 C 0.04048 -0.17843 -0.74212 C -0.09415 -2.56218 -0.48401 H -0.22837 -3.63330 -2.33127 H 0.16068 0.80451 -0.34605 C 0.00621 -0.98781 1.61768 C 0.36684 -0.71287 4.43767 C 0.17122 0.32088 2.20152 C -0.11066 -2.05859 2.52066 C 0.06348 -1.94385 3.89273 C 0.38397 0.38732 3.58961 H -0.35824 -3.03310 2.16268 H -0.03434 -2.82412 4.51537 H 0.54988 1.34834 4.05312 H 0.54544 -0.58986 5.49798 C 0.09539 0.80430 -3.16086 C -0.19743 -1.41580 -4.20206 H 0.77197 -1.68665 -4.63362 H -0.94645 -2.06170 -4.66377 C -0.49449 0.08784 -4.40564 H -1.57674 0.23867 -4.41736 H -0.08774 0.48415 -5.33745 C -0.66240 2.08075 -2.80399 H -0.24791 2.54015 -1.90488 H -1.71735 1.86785 -2.62172 H -0.58910 2.80552 -3.61892 C 1.58108 1.13152 -3.38960 H 2.13678 0.23606 -3.67596 H 2.03017 1.53256 -2.47887 H 1.68653 1.87573 -4.18348 C -0.03218 -3.91572 0.19684 H 0.80768 -3.98927 0.88956 H 0.09918 -4.69201 -0.55733 H -0.94673 -4.15925 0.74467 Si -0.07104 2.08891 1.50521 C -1.73385 2.23644 0.62134 H -1.90440 1.49381 -0.15539 H -1.83051 3.22808 0.16930 H -2.52828 2.13482 1.36666 C -0.20350 3.32464 2.92967 H -0.46068 4.29840 2.50135 H 0.73211 3.44687 3.48067 H -0.98698 3.05607 3.64183 C 1.39034 2.74404 0.49291 H 1.68986 2.14258 -0.36447 H 2.25779 2.82665 1.15461 H 1.15786 3.75103 0.13245</p>
 <p>5a -1433.410171 -1434.278592 -1433.765965</p>	<p>C -1.64849 0.38296 -3.36184 C -1.05945 0.49838 -0.62131 C -1.42012 -0.80392 -2.66645 C -1.58147 1.61398 -2.72123 C -1.28470 1.66075 -1.36209 C -1.13363 -0.72267 -1.30498 C -0.73713 0.52173 0.83266 C -0.20055 0.58116 3.58581 C 0.57403 0.52831 1.31387 C -1.76859 0.55269 1.78056 C -1.52601 0.58716 3.15253 C 0.85073 0.55377 2.67787 H -2.79951 0.56114 1.45151 H -1.87362 0.30977 -4.41807 H -0.02197 0.60454 4.65308 H -0.95408 -1.64735 -0.77239 I -1.14186 3.58390 -0.44751 I 2.23145 0.54299 -0.03079</p>	 <p>5a -1433.372199 -1434.240935 -1433.731574</p>	<p>C -0.12524 -0.34527 -3.61838 C -0.00635 -0.01315 -0.75885 C -0.01043 -1.45954 -2.80302 C -0.13476 0.91264 -3.04136 C -0.06157 1.09766 -1.65678 C 0.04620 -1.25327 -1.42997 C 0.00697 0.01213 0.75872 C 0.12583 0.34424 3.61826 C -0.04557 1.25225 1.42984 C 0.06219 -1.09868 1.65666 C 0.13537 -0.91366 3.04123 C 0.01103 1.45851 2.80289 H -0.18513 -0.48387 -4.68996 H 0.18570 0.48285 4.68983 H 0.14302 -2.16000 -0.86818 C 0.05597 -2.88793 -3.40888 O -0.05528 -2.94091 -4.65648 O 0.21433 -3.82027 -2.59167</p>

	<p>C -1.47096 -2.17055 -3.40633 O -1.22299 -3.17438 -2.70583 O -1.75059 -2.10592 -4.62660 C -2.68925 0.64759 4.18238 O -2.33612 0.66159 5.38519 O -3.83969 0.68100 3.69744 H -1.75284 2.53032 -3.27085 H 1.87621 0.55710 3.02337</p>		<p>I 0.03776 3.22949 -1.27159 I -0.03712 -3.23051 1.27146 H -0.14238 2.15898 0.86805 C -0.05537 2.88691 3.40877 O 0.05578 2.93987 4.65637 O -0.21363 3.81926 2.59155 H 0.18873 -1.78146 3.68361 H -0.18813 1.78043 -3.68374</p>
 <p>5b -2027.629814 -2029.525752 -2027.765952</p>	<p>C -1.63016 0.37986 -3.35506 C -1.03997 0.52516 -0.62763 C -1.44805 -0.79698 -2.63475 C -1.52474 1.61481 -2.72924 C -1.22943 1.70609 -1.36496 C -1.16027 -0.70407 -1.27763 C -0.71082 0.54269 0.82820 C -0.20691 0.59780 3.57621 C 0.61397 0.58463 1.29451 C -1.75340 0.52080 1.75582 C -1.52329 0.55305 3.12665 C 0.84790 0.61131 2.67342 H -2.77992 0.49257 1.41611 H -1.85311 0.28591 -4.40855 H -0.04953 0.62211 4.64534 H -1.01424 -1.62392 -0.72765 I -1.84094 3.31393 -3.99711 I -1.02212 3.56330 -0.35002 I 2.17958 0.63503 -0.14371 I 2.80277 0.67730 3.55021 C -1.55326 -2.17418 -3.35829 O -1.36012 -3.16869 -2.63057 O -1.81377 -2.11346 -4.58003 C -2.69545 0.55667 4.15484 O -2.34803 0.58939 5.35586 O -3.83726 0.53125 3.65329</p>	 <p>5b -2027.580164 -2029.477793 -2027.721582</p>	<p>C 0.85065 -2.04107 -2.75280 C -0.76345 -0.50773 -0.96918 C 0.19420 -2.67026 -1.70822 C 0.86398 -0.65468 -2.79016 C 0.15739 0.13347 -1.86857 C -0.58045 -1.89509 -0.85848 C -1.83293 0.17576 -0.15096 C -3.43895 1.71129 1.63773 C -2.01565 1.56303 -0.26227 C -2.75212 -0.46433 0.75099 C -3.45558 0.32483 1.67402 C -2.78474 2.33958 0.59127 H 1.37882 -2.65355 -3.46879 H -3.96270 2.32444 2.35635 H -1.05501 -2.44448 -0.06792 C 0.30759 -4.21026 -1.51684 O -0.19121 -4.64878 -0.45933 O 0.88980 -4.81965 -2.44022 I 2.06856 0.12842 -4.39916 I 0.88211 2.14202 -1.61736 I -3.47916 -2.47220 0.50132 I -4.65938 -0.45643 3.28448 H -1.54365 2.11141 -1.05512 C -2.89521 3.87994 0.40126 O -3.46550 4.49110 1.33081 O -2.40613 4.31681 -0.66153</p>
 <p>6 -1248.197974 -1247.986680 -1249.021207</p>	<p>C -0.67868 -1.00888 -3.72584 C -0.11509 -0.26140 -1.06278 C -0.89230 -1.91606 -2.69562 C -0.14111 0.23432 -3.43788 C 0.14793 0.62377 -2.12524 C -0.59094 -1.54066 -1.39526 C 0.15785 0.18170 0.33567 C 0.91923 1.02655 2.86852 C 1.48129 0.57396 0.60152 C -0.81466 0.27097 1.35384 C -0.40946 0.70911 2.61243 C 1.87919 0.97863 1.85836 H -0.91044 -1.28765 -4.74789 H 0.07443 0.93483 -4.23571 H 2.89955 1.26390 2.06177 H -1.27819 -2.90668 -2.87845 H -1.16218 0.80671 3.37859 H 2.19275 0.57627 -0.21234 C 0.77782 2.02219 -1.95985 O 2.00834 2.04289 -2.20482 O 0.00483 2.94748 -1.66412 C -2.32697 -0.06587 1.19835 O -2.62223 -0.89022 0.30647 O -3.08094 0.51170 2.00848 N -0.68897 -2.62147 -0.39058 O 0.04838 -2.57256 0.58386 O -1.42784 -3.56947 -0.62851 N 1.32043 1.43307 4.20896 O 2.50502 1.71769 4.41107 O 0.47282 1.47794 5.09858</p>	 <p>6 -1248.159299 -1247.950882 -1248.988222</p>	<p>C -0.60671 0.80017 -4.13792 C -0.08849 0.24465 -1.37127 C -0.60232 -0.50268 -3.67175 C -0.23105 1.80819 -3.26952 C 0.05732 1.55577 -1.92699 C -0.29631 -0.77275 -2.33938 C -0.15404 0.13803 0.12978 C -0.20093 0.47828 2.93058 C -0.65767 1.30634 0.75524 C 0.17772 -0.94589 0.99092 C 0.22189 -0.71630 2.37143 C -0.69673 1.49320 2.11936 H -0.84873 1.01045 -5.17382 H 0.56185 -1.52059 3.00544 H -0.15947 2.83444 -3.60614 H -0.79180 -1.33652 -4.33128 H -1.07984 2.40755 2.54366 C 0.26192 -2.46065 0.70146 O -0.81669 -2.87777 0.22091 O 1.26328 -3.07961 1.09233 H -1.03941 2.11229 0.15016 C 0.64936 2.80762 -1.21135 O 1.83319 2.67652 -0.86041 O -0.10117 3.80954 -1.16415 N 0.01939 -2.21750 -2.19194 O -0.77175 -3.03834 -2.63409 O 1.15419 -2.46706 -1.82538 N -0.17457 0.65766 4.37583 O 0.31335 -0.22606 5.07844 O -0.64629 1.69484 4.84926</p>
 <p>7a -2761.006035 -2761.298452</p>	<p>C 0.02781 2.32353 0.86278 C 1.11685 2.10649 0.01828 C 1.51688 3.13121 -0.83688 C 0.83869 4.34120 -0.84320 C -0.24621 4.55289 -0.00082 C -0.65003 3.53717 0.85444 H 2.35932 2.97669 -1.49562 H -0.76869 5.49858 -0.01239 H -1.49119 3.68499 1.51638 C 1.86251 0.82096 0.01087 C 2.97424 0.62914 0.83371 C 1.46907 -0.23274 -0.82722 C 3.68291 -0.56569 0.82997 C 2.17817 -1.43756 -0.83594 C 3.28226 -1.59422 -0.00544 H 4.53883 -0.68749 1.47743 H 3.82430 -2.52879 -0.01839</p>	 <p>7a -2760.937410 -2761.231996</p>	<p>C -0.72025 -2.66253 -2.12481 C 0.15295 -0.50047 -0.44075 C -0.37955 -2.88740 -0.80442 C -0.35631 -1.44115 -2.68943 C 0.14441 -0.41119 -1.88496 C 0.13816 -1.86215 -0.00867 C 0.10892 0.74912 0.38623 C 0.17477 3.39315 1.56398 C -0.23048 1.93733 -0.31688 C 0.21976 0.96137 1.79465 C 0.33128 2.25229 2.33163 C -0.19032 3.20447 0.23424 H -1.13819 -3.44711 -2.74360 H 0.25364 4.38259 1.99820 H -0.56287 1.86784 -1.33864 H 0.48322 2.33999 3.40136 Cl 0.97400 0.87118 -2.74023</p>

-2761.735577	Cl 3.49521 1.90036 1.90454 Cl 0.08335 -0.02061 -1.84747 Cl 1.71872 -2.75935 -1.86166 Cl -0.50381 1.06865 1.94793 Cl 1.35599 5.60949 -1.92159	-2761.672081	Cl 0.98576 -2.45712 1.39066 Cl -0.00664 -0.22732 3.05097 Cl -0.61752 4.57596 -0.75834 Cl -0.48032 -1.27257 -4.41401 H -0.45454 -3.88137 -0.37889
 7b -3220.560430 -3220.927857 -3221.362571	C 0.01176 2.30846 0.85739 C 1.10067 2.09868 0.00955 C 1.49252 3.11862 -0.85090 C 0.81906 4.32730 -0.87618 C -0.26540 4.53418 -0.03229 C -0.68320 3.52729 0.84652 H 2.33649 2.95758 -1.50714 C 1.85109 0.81571 0.01192 C 2.96263 0.63370 0.83724 C 1.46816 -0.24182 -0.82621 C 3.68103 -0.55521 0.83605 C 2.18731 -1.44074 -0.83275 C 3.29083 -1.58764 0.00044 H 4.53620 -0.66961 1.48578 H 3.84048 -2.51776 -0.01050 Cl 3.46930 1.90994 1.90884 Cl 0.08120 -0.04258 -1.84751 Cl 1.74118 -2.76669 -1.85871 Cl -0.47287 1.03439 1.92911 H 1.12571 5.11710 -1.54612 Cl -2.02969 3.78189 1.89827 Cl -1.07987 6.06508 -0.09879	 7b -3220.489400 -3220.859241 -3221.297079	C -0.51685 -3.84098 -1.03258 C 0.09705 -1.10687 -0.37999 C -0.14572 -3.50119 0.26769 C -0.29734 -2.90691 -2.02718 C 0.10028 -1.60219 -1.72129 C 0.22997 -2.18918 0.57343 C -0.07451 0.29011 0.12915 C -0.14638 2.78383 1.55707 C -0.07191 1.54800 -0.55016 C -0.42237 0.40567 1.50000 C -0.45532 1.59106 2.20447 C -0.00130 2.76815 0.16734 H -0.84114 -4.84841 -1.26293 H -0.37392 -3.18866 -3.07100 Cl 0.83877 -0.79445 -3.07678 Cl 1.09887 -1.98756 2.08088 Cl -0.09878 -4.76501 1.45897 H -0.70136 -0.48413 2.04054 Cl -0.39470 1.74104 -2.23674 H -0.70947 1.59741 3.25762 Cl 0.18183 4.26808 -0.67406 Cl -0.06304 4.25150 2.46827
 7c -3220.564736 -3220.932354 -3221.366130	C 0.08083 2.32112 0.84938 C 1.14594 2.12260 -0.02161 C 1.49441 3.15989 -0.88682 C 0.79731 4.35911 -0.88192 C -0.26670 4.54279 -0.00592 C -0.62961 3.51513 0.86903 C 1.87787 0.83007 -0.00123 C 2.95747 0.62804 0.86103 C 1.49968 -0.22232 -0.84811 C 3.64468 -0.57878 0.89290 C 2.18712 -1.43935 -0.82069 C 3.25629 -1.60779 0.05230 H 4.47683 -0.70831 1.56913 H 3.78221 -2.55152 0.06688 Cl 3.47690 1.90868 1.92100 Cl 0.16962 0.01240 -1.93518 Cl 1.74389 -2.76093 -1.85323 H 1.07760 5.15348 -1.55710 Cl -1.94581 3.68471 1.98491 Cl 2.81938 2.97030 -1.99788 H -0.20301 1.52966 1.52803 Cl -1.10880 6.05771 -0.03560	 7c -3220.497137 -3220.867022 -3221.303692	C -0.59629 -3.55062 -1.73320 C 0.12618 -1.06770 -0.47344 C -0.30333 -3.50096 -0.38342 C -0.25717 -2.44543 -2.51202 C 0.17080 -1.25807 -1.90726 C 0.14120 -2.31938 0.21501 C 0.01569 0.31270 0.09435 C -0.01116 3.13252 0.72770 C -0.32916 1.33344 -0.82978 C 0.06801 0.80007 1.43699 C 0.13694 2.16989 1.71473 C -0.34010 2.69033 -0.55850 H -0.95756 -4.45802 -2.20147 Cl 0.98086 -0.12704 -2.96987 Cl 0.94419 -2.59212 1.73515 Cl 0.10038 4.80830 1.13330 H 0.24527 2.48249 2.74574 H -0.63057 1.05728 -1.82617 Cl -0.77050 3.79887 -1.82156 Cl -0.18615 -0.12110 2.89467 Cl -0.31796 -2.61762 -4.23936 H -0.35927 -4.39655 0.22440
 8 -938.7683001 -938.7268268 -939.2696173	C -1.15891 2.48965 -0.02895 C 0.14026 2.54978 -0.56664 C 0.83002 3.76062 -0.54977 C 0.24876 4.91047 -0.02808 C -1.04439 4.85806 0.48277 C -1.73873 3.65430 0.47981 H 1.83011 3.79960 -0.96402 H 0.79900 5.84232 -0.02680 H -1.50779 5.74821 0.88780 H -2.73886 3.60289 0.89079 C -1.91001 1.21019 -0.00554 C -3.19960 1.14273 -0.53838 C -1.33932 0.05258 0.55550 C -3.91157 -0.05072 -0.54259 H -3.63460 2.03650 -0.96711 C -2.05940 -1.14048 0.53719 C -3.33640 -1.19965 -0.00868 H -4.90670 -0.08481 -0.96650 H -1.61362 -2.02799 0.96949 H -3.88128 -2.13464 -0.01090 C 0.75263 1.33088 -1.19428 H 0.01599 0.81647 -1.81190 H 1.60338 1.60189 -1.81866 C 0.01125 0.11929 1.20833 H 0.08943 1.01980 1.81800 H 0.17762 -0.74891 1.84530 S 1.41443 0.11936 0.02014	 8 -938.7393514 -938.6982208 -939.2424881	C 0.13996 -1.67397 -3.33331 C 0.07836 -0.83035 -0.57800 C 0.06874 -2.60670 -2.31335 C 0.18656 -0.34079 -2.97578 C 0.17039 0.10893 -1.64609 C 0.03668 -2.18157 -0.99761 C -0.00462 -0.57344 0.92719 C -0.25651 -0.45590 3.79600 C -0.01070 0.66792 1.62748 C -0.11465 -1.71013 1.76351 C -0.23285 -1.67487 3.14111 C -0.14708 0.68437 3.02451 H 0.15640 -1.96890 -4.37405 H -0.35858 -0.38935 4.87097 H -0.31304 -2.60543 3.68743 H 0.24218 0.40191 -3.76160 H -0.11498 -2.69805 1.34442 H -0.02925 -2.97460 -0.27765 H 0.02961 -3.66692 -2.52603 H -0.16314 1.64629 3.52113 C 0.16081 2.05349 1.05452 H -0.11343 2.78576 1.81235 H 1.20900 2.24015 0.80589 C 0.30273 1.60936 -1.55018 H 1.32182 1.88877 -1.26972 H 0.12115 2.04333 -2.53222 S -0.81034 2.46270 -0.41232

^a Except in the case of polychlorobiphenyls **7a** – **7c**, for which TPSS-D3-optimized structures were used. ^b In Hartrees; def2-TZVPP basis sets were used in all cases.