

Supplementary information

transoid conformer of n-C₄F₁₀

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	0.544864	-0.550486	-0.098555
2	6	-0.544864	0.550486	-0.098555
3	6	0.004528	1.987721	0.078956
4	6	-0.004528	-1.987721	0.078956
5	9	-0.979410	2.844762	-0.140628
6	9	0.979410	-2.844762	-0.140628
7	9	1.410662	-0.322527	0.896449
8	9	1.197655	-0.503347	-1.263230
9	9	-1.410662	0.322527	0.896449
10	9	-1.197655	0.503347	-1.263230
11	9	0.979410	2.220790	-0.785897
12	9	0.459079	2.169330	1.306372
13	9	-0.979410	-2.220790	-0.785897
14	9	-0.459079	-2.169330	1.306372

ortho conformer of n-C₄F₁₀

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.656815	-0.422389	0.527670
2	6	0.656815	0.422389	0.527670
3	6	0.656815	1.657920	-0.407006
4	6	-0.656815	-1.657920	-0.407006
5	9	1.877855	2.168779	-0.420083
6	9	-1.877855	-2.168779	-0.420083
7	9	-1.685252	0.360467	0.177203
8	9	-0.866859	-0.875882	1.765769
9	9	1.685252	-0.360467	0.177203
10	9	0.866859	0.875882	1.765769
11	9	-0.182426	2.576639	0.038325
12	9	0.321404	1.321351	-1.641657
13	9	0.182426	-2.576639	0.038325
14	9	-0.321404	-1.321351	-1.641657

gauche conformer of n-C₄F₁₀

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-0.262951	-0.730866	0.680838
2	6	0.262951	0.730866	0.680838
3	6	-0.081357	1.618332	-0.536742
4	6	0.081357	-1.618332	-0.536742
5	9	0.261137	2.865423	-0.261875
6	9	-0.261137	-2.865423	-0.261875
7	9	-1.593634	-0.709316	0.802954
8	9	0.262951	-1.313855	1.764531
9	9	1.593634	0.709316	0.802954
10	9	-0.262951	1.313855	1.764531
11	9	-1.377539	1.574744	-0.797953
12	9	0.593019	1.219127	-1.603720
13	9	1.377539	-1.574744	-0.797953
14	9	-0.593019	-1.219127	-1.603720