

Table I:

label	x(Bohr)	y(Bohr)	z(Bohr)	q	$p_x(e \bullet Bohr)$	$p_y(e \bullet Bohr)$	$p_z(e \bullet Bohr)$
C 1	-9.565	1.113	-3.478	0.973	0.000	0.044	0.092
C 3	-7.152	0.889	-2.403	0.929	0.038	-0.017	0.029
C 5	-6.682	1.814	0.029	0.928	0.046	0.017	0.005
C 7	-8.685	2.931	1.361	0.857	-0.014	-0.025	-0.090
C 9	-11.028	3.132	0.263	1.055	0.105	-0.062	-0.039
C11	-11.494	2.232	-2.174	0.992	0.101	-0.009	0.026
N13	-4.247	1.613	1.055	0.472	-0.038	-0.096	-0.101
C15	-2.340	0.409	-0.158	0.997	-0.061	0.124	0.024
C17	-2.850	-0.583	-2.637	0.738	-0.052	0.121	0.041
C19	-5.129	-0.334	-3.709	1.046	0.019	0.001	0.116
C21	-3.738	2.886	3.487	0.859	-0.053	-0.089	-0.108
C23	-4.351	1.265	5.791	0.893	0.020	-0.005	-0.027
C25	0.000	0.000	1.050	0.421	0.000	0.000	-0.310
H27	-1.393	-1.638	-3.559	0.393	0.072	0.038	0.027
H29	-5.484	-1.128	-5.546	0.341	0.003	-0.020	-0.040
H31	-8.451	3.626	3.244	0.331	-0.016	0.024	0.046
H33	-12.532	3.997	1.319	0.347	-0.033	0.016	0.015
H35	-13.340	2.406	-2.997	0.351	-0.036	0.003	-0.016
H37	-9.869	0.384	-5.351	0.331	-0.028	-0.008	-0.037
H39	-1.778	3.440	3.479	0.319	0.024	0.010	-0.006
H41	-4.812	4.618	3.507	0.313	-0.023	0.024	-0.001
H43	-6.323	0.721	5.833	0.299	-0.033	-0.015	0.012
H45	-3.944	2.325	7.497	0.315	0.002	0.013	0.035
H47	-3.236	-0.453	5.827	0.271	0.003	-0.036	0.020