## **Supporting Information**

## Calycindaphines A–J, *Daphniphyllum* alkaloids from the roots of *Daphniphyllum calycinum*

Ji Yang,<sup>a</sup> Xin Liu,<sup>a,b</sup> Jing Fu,<sup>a</sup> Hao-Yuan Lyu,<sup>a</sup> Li-Ping Bai,<sup>a</sup> Zhi-Hong Jiang,<sup>\*a</sup> and Guo-Yuan Zhu <sup>\*a</sup>

<sup>a</sup> State Key Laboratory of Quality Research in Chinese Medicine, Macau Institute for

Applied Research in Medicine and Health, Macau University of Science and

Technology, Macau, China

<sup>b</sup> Biology Institute, Qilu University of Technology (Shandong Academy of Sciences),

Jinan 250103, China

Fig. S1. HR-ESI-MS spectrum of compound 1	6
Fig. S2. <sup>1</sup> H NMR spectrum for compound <b>1</b>	6
Fig. S3. <sup>13</sup> C and DEPT135 NMR spectra for compound <b>1</b>	7
Fig. S4. HSQC NMR spectrum for compound 1	7
Fig. S5. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound <b>1</b>	8
Fig. S6. HMBC NMR spectrum for compound 1	8
Fig. S7. NOESY NMR spectrum for compound 1	9
Fig. S8. IR spectrum of compound 1 (KBr)	9
Fig. S9. UV spectrum of compound 1 in MeOH	
Fig. S10. CD spectrum of compound 1 in MeOH	10
Fig. S11. HR-ESI-MS spectrum of compound 2	11
Fig. S12. <sup>1</sup> H NMR spectrum for compound <b>2</b>	11
Fig. S13. <sup>13</sup> C and DEPT135 NMR spectra for compound 2	
Fig. S14. HSQC NMR spectrum for compound 2	12
Fig. S15. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound 2	13
Fig. S16. HMBC NMR spectrum for compound 2	13
Fig. S17. NOESY NMR spectrum for compound 2	14
Fig. S18. IR spectrum of compound 2 (KBr)	14
Fig. S19. UV spectrum of compound 2 in MeOH	15
Fig. S20. CD spectrum of compound 2 in MeOH	15
Fig. S21. HR-ESI-MS spectrum of compound 3	16
Fig. S22. <sup>1</sup> H NMR spectrum for compound <b>3</b>	16
Fig. S23. <sup>13</sup> C and DEPT135 NMR spectra for compound <b>3</b>	17
Fig. S24. HSQC NMR spectrum for compound <b>3</b>	17
Fig. S25. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound <b>3</b>	
Fig. S26. HMBC NMR spectrum for compound 3	
Fig. S27. NOESY NMR spectrum for compound 3	19
Fig. S28. IR spectrum of compound <b>3</b> (KBr)	19
Fig. S29. UV spectrum of compound <b>3</b> in MeOH	20
Fig. S30. CD spectrum of compound <b>3</b> in MeOH	20
Fig. S31. HR-ESI-MS spectrum of compound 4	21

Fig. S32. <sup>1</sup> H NMR spectrum for compound 4	21
Fig. S33. <sup>13</sup> C and DEPT135 NMR spectra for compound 4	22
Fig. S34. HSQC NMR spectrum for compound 4	22
Fig. S35. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound 4	23
Fig. S36. HMBC NMR spectrum for compound 4	23
Fig. S37. NOESY NMR spectrum for compound 4	24
Fig. S38. IR spectrum of compound 4 (KBr)	24
Fig. S39. UV spectrum of compound 4 in MeOH	25
Fig. S40. CD spectrum of compound 4 in MeOH	25
Fig. S41. HR-ESI-MS spectrum of compound 5	26
Fig. S42. <sup>1</sup> H NMR spectrum for compound <b>5</b>	26
Fig. S43. <sup>13</sup> C and DEPT135 NMR spectra for compound <b>5</b>	27
Fig. S44. HSQC NMR spectrum for compound 5	27
Fig. S45. <sup>1</sup> H <sup>-1</sup> H COSY NMR spectrum for compound <b>5</b>	
Fig. S46. HMBC NMR spectrum for compound 5	
Fig. S47. NOESY NMR spectrum for compound 5	29
Fig. S48. IR spectrum of compound 5 (KBr)	29
Fig. S49. UV spectrum of compound 5 in MeOH	
Fig. S50. CD spectrum of compound <b>5</b> in MeOH	
Fig. S51. HR-ESI-MS spectrum of compound 6	
Fig. S52. <sup>1</sup> H NMR spectrum for compound 6	
Fig. S53. <sup>13</sup> C and DEPT135 NMR spectra for compound <b>6</b>	
Fig. S54. HSQC NMR spectrum for compound 6	
Fig. S55. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound <b>6</b>	
Fig. S56. HMBC NMR spectrum for compound 6	
Fig. S57. NOESY NMR spectrum for compound 6	
Fig. S58. IR spectrum of compound 6 (KBr)	
Fig. S59. UV spectrum of compound 6 in MeOH	
Fig. S60. CD spectrum of compound 6 in MeOH	
Fig. S61. HR-ESI-MS spectrum of compound 7	
Fig. S62. <sup>1</sup> H NMR spectrum for compound 7	
Fig. S63. <sup>13</sup> C and DEPT135 NMR spectra for compound 7	

Fig. S64. HSQC NMR spectrum for compound 7	
Fig. S65. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound 7	
Fig. S66. HMBC NMR spectrum for compound 7	
Fig. S67. NOESY NMR spectrum for compound 7	
Fig. S68. IR spectrum of compound 7 (KBr)	
Fig. S69. UV spectrum of compound 7 in MeOH	40
Fig. S70. CD spectrum of compound 7 in MeOH	40
Fig. S71. HR-ESI-MS spectrum of compound 8	41
Fig. S72. <sup>1</sup> H NMR spectrum for compound 8	41
Fig. S73. <sup>13</sup> C and DEPT135 NMR spectra for compound 8	42
Fig. S74. HSQC NMR spectrum for compound 8	
Fig. S75. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound 8	43
Fig. S76. HMBC NMR spectrum for compound 8	43
Fig. S77. NOESY NMR spectrum for compound 8	
Fig. S78. IR spectrum of compound 8 (KBr)	
Fig. S79. UV spectrum of compound 8 in MeOH	45
Fig. S80. CD spectrum of compound 8 in MeOH	45
Fig. S81. HR-ESI-MS spectrum of compound 9	
Fig. S82. <sup>1</sup> H NMR spectrum for compound 9	
Fig. S83. <sup>13</sup> C and DEPT135 NMR spectra for compound 9	47
Fig. S84. HSQC NMR spectrum for compound 9	47
Fig. S85. <sup>1</sup> H <sup>-1</sup> H COSY NMR spectrum for compound 9	
Fig. S86. HMBC NMR spectrum for compound 9	
Fig. S87. NOESY NMR spectrum for compound 9	
Fig. S88. IR spectrum of compound 9 (KBr)	
Fig. S89. UV spectrum of compound 9 in MeOH	
Fig. S90. CD spectrum of compound 9 in MeOH	
Fig. S91. HR-ESI-MS spectrum of compound 10	
Fig. S92. <sup>1</sup> H NMR spectrum for compound <b>10</b>	
Fig. S93. <sup>13</sup> C and DEPT135 NMR spectra for compound <b>10</b>	
Fig. S94. HSQC NMR spectrum for compound 10	
Fig. S95. <sup>1</sup> H– <sup>1</sup> H COSY NMR spectrum for compound <b>10</b>	53

Fig. S96. HMBC NMR spectrum for compound 10	53
Fig. S97. NOESY NMR spectrum for compound 10	54
Fig. S98. IR spectrum of compound 10 (KBr)	54
Fig. S99. UV spectrum of compound <b>10</b> in MeOH	55
Fig. S100. CD spectrum of compound <b>10</b> in MeOH	55
Fig. S101. Optimized conformers of compound 1	56
Table S1. Gibbs free energiesa and equilibrium populationsb of low-energy conformers of	of <b>1</b> .
Table S2. Cartesian coordinates for the low-energy reoptimized random reseach conform of $1$ at PRE0 D3(R1)/dof2 SVR layel of theory in methanol	57 ers
of I at PBEU-D3(BJ)/det2-SVP level of theory in methanol.	57







Fig. S2. <sup>1</sup>H NMR spectrum for compound 1



Fig. S3.  $^{13}$ C and DEPT135 NMR spectra for compound 1



Fig. S4. HSQC NMR spectrum for compound 1



Fig. S5.  $^{1}H-^{1}H$  COSY NMR spectrum for compound 1



Fig. S6. HMBC NMR spectrum for compound 1



Fig. S7. NOESY NMR spectrum for compound 1



Fig. S8. IR spectrum of compound 1 (KBr)



Fig. S9. UV spectrum of compound 1 in MeOH



Fig. S10. CD spectrum of compound 1 in MeOH







Fig. S12. <sup>1</sup>H NMR spectrum for compound 2



Fig. S13. <sup>13</sup>C and DEPT135 NMR spectra for compound 2



Fig. S14. HSQC NMR spectrum for compound 2



Fig. S15. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 2



Fig. S16. HMBC NMR spectrum for compound 2



Fig. S17. NOESY NMR spectrum for compound 2



Fig. S18. IR spectrum of compound 2 (KBr)



Fig. S19. UV spectrum of compound 2 in MeOH



Fig. S20. CD spectrum of compound 2 in MeOH



Fig. S21. HR-ESI-MS spectrum of compound 3



Fig. S22. <sup>1</sup>H NMR spectrum for compound 3



Fig. S23. <sup>13</sup>C and DEPT135 NMR spectra for compound 3



Fig. S24. HSQC NMR spectrum for compound 3



Fig. S25. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 3



Fig. S26. HMBC NMR spectrum for compound 3





Fig. S28. IR spectrum of compound 3 (KBr)



Fig. S29. UV spectrum of compound 3 in MeOH



Fig. S30. CD spectrum of compound 3 in MeOH







Fig. S32. <sup>1</sup>H NMR spectrum for compound 4



Fig. S33. <sup>13</sup>C and DEPT135 NMR spectra for compound 4



Fig. S34. HSQC NMR spectrum for compound 4



Fig. S35. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 4



Fig. S36. HMBC NMR spectrum for compound 4



Fig. S37. NOESY NMR spectrum for compound 4



Fig. S38. IR spectrum of compound 4 (KBr)



Fig. S39. UV spectrum of compound 4 in MeOH



Fig. S40. CD spectrum of compound 4 in MeOH





Fig. S42. <sup>1</sup>H NMR spectrum for compound 5



Fig. S43. <sup>13</sup>C and DEPT135 NMR spectra for compound 5



Fig. S44. HSQC NMR spectrum for compound 5



Fig. S45. <sup>1</sup>H<sup>-1</sup>H COSY NMR spectrum for compound 5



Fig. S46. HMBC NMR spectrum for compound 5



Fig. S47. NOESY NMR spectrum for compound 5



Fig. S48. IR spectrum of compound 5 (KBr)



Fig. S49. UV spectrum of compound 5 in MeOH



Fig. S50. CD spectrum of compound 5 in MeOH







Fig. S52. <sup>1</sup>H NMR spectrum for compound 6



Fig. S53. <sup>13</sup>C and DEPT135 NMR spectra for compound 6



Fig. S54. HSQC NMR spectrum for compound 6



Fig. S55. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 6



Fig. S56. HMBC NMR spectrum for compound 6



Fig. S57. NOESY NMR spectrum for compound 6



Fig. S58. IR spectrum of compound 6 (KBr)



Fig. S59. UV spectrum of compound 6 in MeOH



Fig. S60. CD spectrum of compound 6 in MeOH





Fig. S62. <sup>1</sup>H NMR spectrum for compound 7


Fig. S63. <sup>13</sup>C and DEPT135 NMR spectra for compound 7



Fig. S64. HSQC NMR spectrum for compound 7



Fig. S65. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 7



Fig. S66. HMBC NMR spectrum for compound 7



Fig. S67. NOESY NMR spectrum for compound 7



Fig. S68. IR spectrum of compound 7 (KBr)



Fig. S69. UV spectrum of compound 7 in MeOH



Fig. S70. CD spectrum of compound 7 in MeOH







Fig. S72. <sup>1</sup>H NMR spectrum for compound 8



Fig. S73. <sup>13</sup>C and DEPT135 NMR spectra for compound 8



Fig. S74. HSQC NMR spectrum for compound 8



Fig. S75. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 8



Fig. S76. HMBC NMR spectrum for compound 8



Fig. S77. NOESY NMR spectrum for compound 8



Fig. S78. IR spectrum of compound 8 (KBr)



Fig. S79. UV spectrum of compound 8 in MeOH



Fig. S80. CD spectrum of compound 8 in MeOH





Fig. S82. <sup>1</sup>H NMR spectrum for compound 9



Fig. S83. <sup>13</sup>C and DEPT135 NMR spectra for compound 9



Fig. S84. HSQC NMR spectrum for compound 9



Fig. S85. <sup>1</sup>H<sup>-1</sup>H COSY NMR spectrum for compound 9



Fig. S86. HMBC NMR spectrum for compound 9



Fig. S87. NOESY NMR spectrum for compound 9



Fig. S88. IR spectrum of compound 9 (KBr)



Fig. S89. UV spectrum of compound 9 in MeOH



Fig. S90. CD spectrum of compound 9 in MeOH







Fig. S92. <sup>1</sup>H NMR spectrum for compound 10



Fig. S93. <sup>13</sup>C and DEPT135 NMR spectra for compound 10



Fig. S94. HSQC NMR spectrum for compound 10



Fig. S95. <sup>1</sup>H–<sup>1</sup>H COSY NMR spectrum for compound 10



Fig. S96. HMBC NMR spectrum for compound 10



Fig. S97. NOESY NMR spectrum for compound 10



Fig. S98. IR spectrum of compound 10 (KBr)



Fig. S99. UV spectrum of compound 10 in MeOH



Fig. S100. CD spectrum of compound 10 in MeOH



Fig. S101. Optimized conformers of compound 1

Conformers	ΔG	P(%)/100	Single point
			energy(a.u.)
1-1	8e-05	18.75	-1175.5297518288
1-2	0.00378	0.37	-1175.5260548182
1-3	1e-05	20.25	-1175.5298245595
1-4	0.00375	0.39	-1175.5260863631
1-5	0.0037	0.41	-1175.5261361246
1-6	4e-05	19.64	-1175.5297959616
1-7	0.00376	0.38	-1175.5260712545
1-8	0.00000	20.48	-1175.5298352839
1-9	5e-05	19.34	-1175.5297812377

Table S1. Gibbs free energiesa and equilibrium populationsb of low-energy conformers of **1**.

<sup>a</sup>PBE0-D3(BJ)/def2-TZVP, in kcal/mol.

<sup>b</sup>From  $\Delta$ G values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized random reseach conformers of **1** at PBE0-D3(BJ)/def2-SVP level of theory in methanol.

1-1_en		Standard Orientation (Ångstroms)			
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	0.480726	3.272757	1.477788
1	6	0	0.284551	0.458246	1.070574
2	6	0	2.518961	-0.616679	1.57233
3	6	0	4.531321	1.253707	2.294674
4	6	0	2.980948	3.671469	2.928386
5	6	0	3.403089	-3.161807	2.028121
6	6	0	6.028366	-2.916039	3.161694
7	6	0	6.108447	-0.213897	4.227905
8	6	0	-2.12111	-0.962914	0.563899
9	6	0	-1.629036	-3.517127	-0.873278
10	6	0	-0.453598	-5.66733	0.674356
11	6	0	2.140162	-5.333711	1.718142
12	6	0	-3.156348	-1.658417	3.209462
13	6	0	-4.318568	0.650957	-0.63223
14	6	0	-0.124469	-3.314655	-3.34487
15	7	0	-1.306558	-1.616392	-5.128966
16	6	0	-3.220419	2.283029	-5.341776
17	6	0	-0.767468	0.894145	-5.068249
18	6	0	-4.831209	0.455111	-6.901077
19	6	0	-3.849557	-2.132308	-6.068751

	1	1			
20	6	0	-4.087401	2.784218	-2.608284
21	8	0	1.32525	1.82022	-4.606758
22	6	0	-7.670855	0.724961	-6.710203
23	1	0	-2.989572	4.099586	-6.27727
24	1	0	-3.503718	-4.221937	-1.361479
25	1	0	5.732982	1.685772	0.667329
26	6	0	2.584012	3.868828	5.727381
27	8	0	0.78909	2.960065	6.850493
28	8	0	4.355723	5.033578	7.147402
29	6	0	6.486151	6.305061	6.015814
30	1	0	-1.137192	4.036463	2.495895
31	1	0	0.593942	4.275015	-0.318272
32	1	0	3.945974	5.348044	2.251999
33	1	0	6.430594	-4.357625	4.573612
34	1	0	7.451459	-3.106131	1.674297
35	1	0	8.026806	0.490431	4.453165
36	1	0	5.196569	-0.189641	6.077274
37	1	0	-1.731859	-6.213387	2.202779
38	1	0	-0.433884	-7.334464	-0.550108
39	1	0	3.057853	-7.06897	2.322653
40	1	0	-4.88336	-2.776597	3.046594
41	1	0	-1.786676	-2.72267	4.303889
42	1	0	-3.597628	0.042399	4.275441
43	1	0	-5.754055	-0.692058	-1.241444
44	1	0	-5.187776	1.624774	0.961596
45	1	0	1.774928	-2.630113	-2.991059
46	1	0	0.034655	-5.1859	-4.187484
47	1	0	-4.28705	0.7349	-8.87197
48	1	0	-3.772352	-3.490397	-7.615157
49	1	0	-5.035387	-2.945665	-4.600453
50	1	0	-2.882113	4.269533	-1.865278
51	1	0	-5.964615	3.632072	-2.716855
52	1	0	-8.356897	0.385189	-4.800801
53	1	0	-8.606587	-0.630833	-7.948481
54	1	0	-8.282871	2.606617	-7.281707
55	1	0	7.561545	5.054741	4.795668
56	1	0	5.866438	7.964671	4.975408
57	1	0	7.662744	6.889113	7.58861
1-1_tddft		Standard Ori	entation (Ångs	stroms)	
Center	Atomic	Atomic	X	Y	Ζ
number	number	Туре			
0	6	0	0.480726	3.272757	1.477788
1	6	0	0.284551	0.458246	1.070574

2	6	0	2.518961	-0.616679	1.57233
3	6	0	4.531321	1.253707	2.294674
4	6	0	2.980948	3.671469	2.928386
5	6	0	3.403089	-3.161807	2.028121
6	6	0	6.028366	-2.916039	3.161694
7	6	0	6.108447	-0.213897	4.227905
8	6	0	-2.12111	-0.962914	0.563899
9	6	0	-1.629036	-3.517127	-0.873278
10	6	0	-0.453598	-5.66733	0.674356
11	6	0	2.140162	-5.333711	1.718142
12	6	0	-3.156348	-1.658417	3.209462
13	6	0	-4.318568	0.650957	-0.63223
14	6	0	-0.124469	-3.314655	-3.34487
15	7	0	-1.306558	-1.616392	-5.128966
16	6	0	-3.220419	2.283029	-5.341776
17	6	0	-0.767468	0.894145	-5.068249
18	6	0	-4.831209	0.455111	-6.901077
19	6	0	-3.849557	-2.132308	-6.068751
20	6	0	-4.087401	2.784218	-2.608284
21	8	0	1.32525	1.82022	-4.606758
22	6	0	-7.670855	0.724961	-6.710203
23	1	0	-2.989572	4.099586	-6.27727
24	1	0	-3.503718	-4.221937	-1.361479
25	1	0	5.732982	1.685772	0.667329
26	6	0	2.584012	3.868828	5.727381
27	8	0	0.78909	2.960065	6.850493
28	8	0	4.355723	5.033578	7.147402
29	6	0	6.486151	6.305061	6.015814
30	1	0	-1.137192	4.036463	2.495895
31	1	0	0.593942	4.275015	-0.318272
32	1	0	3.945974	5.348044	2.251999
33	1	0	6.430594	-4.357625	4.573612
34	1	0	7.451459	-3.106131	1.674297
35	1	0	8.026806	0.490431	4.453165
36	1	0	5.196569	-0.189641	6.077274
37	1	0	-1.731859	-6.213387	2.202779
38	1	0	-0.433884	-7.334464	-0.550108
39	1	0	3.057853	-7.06897	2.322653
40	1	0	-4.88336	-2.776597	3.046594
41	1	0	-1.786676	-2.72267	4.303889
42	1	0	-3.597628	0.042399	4.275441
43	1	0	-5.754055	-0.692058	-1.241444
44	1	0	-5.187776	1.624774	0.961596

45	1	0	1.774928	-2.630113	-2.991059
46	1	0	0.034655	-5.1859	-4.187484
47	1	0	-4.28705	0.7349	-8.87197
48	1	0	-3.772352	-3.490397	-7.615157
49	1	0	-5.035387	-2.945665	-4.600453
50	1	0	-2.882113	4.269533	-1.865278
51	1	0	-5.964615	3.632072	-2.716855
52	1	0	-8.356897	0.385189	-4.800801
53	1	0	-8.606587	-0.630833	-7.948481
54	1	0	-8.282871	2.606617	-7.281707
55	1	0	7.561545	5.054741	4.795668
56	1	0	5.866438	7.964671	4.975408
57	1	0	7.662744	6.889113	7.58861
1-2_en	·	Standard Ori	entation (Ångs	troms)	·
Center	Atomic	Atomic	X	Y	Ζ
number	number	Туре			
0	6	0	1.256438	3.123307	1.24726
1	6	0	0.702509	0.330283	1.010692
2	6	0	2.791997	-0.970638	1.591975
3	6	0	4.984899	0.711299	2.240271
4	6	0	3.709002	3.234133	2.896015
5	6	0	3.419969	-3.573288	2.114095
6	6	0	6.124808	-3.583534	3.075489
7	6	0	6.580896	-0.880336	4.049489
8	6	0	-1.86868	-0.799983	0.616943
9	6	0	-1.72852	-3.497226	-0.619787
10	6	0	-0.762422	-5.656898	1.058883
11	6	0	1.907659	-5.59662	1.953681
12	6	0	-2.941024	-1.167616	3.310303
13	6	0	-3.860691	0.98955	-0.681522
14	6	0	-0.308744	-3.682297	-3.142564
15	7	0	-1.317894	-1.973307	-5.015085
16	6	0	-2.683503	2.126662	-5.490308
17	6	0	-0.440722	0.432381	-5.162041
18	6	0	-4.590152	0.430557	-6.85096
19	6	0	-3.936181	-2.204312	-5.857379
20	6	0	-3.366821	2.944631	-2.783124
21	8	0	1.770691	1.090734	-4.804042
22	6	0	-7.354488	1.114515	-6.60422
23	1	0	-2.235854	3.814678	-6.576887
24	1	0	-3.694666	-3.997245	-0.996071
25	1	0	6.109044	1.057468	0.532855
26	6	0	2.88599	3.53393	5.591208

0.992032   0.526715   0.06363   0.051656   0.58615   0.341292
5.526715 5.06363 5.051656 0.58615 5.0100 5.00100
0.06363 0.051656 0.58615 0.341292
0.051656 0.58615 0.341292
0.58615
.341292
500400
.500409
.502649
.040583
.973349
.678222
0.01845
.568195
.240746
.464791
.261021
1.225444
.845442
2.90932
3.841403
8.853633
7.310547
4.308668
2.175478
2.908923
7 314108
1.517100
4.657649
4.657649 7.701298
4.657649 7.701298 .681516
4.657649 7.701298 .681516 .314309
4.657649 7.701298 681516 314309 24699
4.657649 7.701298 681516 314309 24699
4.657649 7.701298 681516 314309 24699
4.657649 7.701298 
4.657649 7.701298 681516 314309 24699
4.657649 7.701298 681516 314309 5.24699 2 24726 010692
4.657649 7.701298 681516 314309 24699 
4.657649 7.701298 681516 314309 24699 2 24726 010692 591975 240271
4.657649 7.701298 .681516 .314309 5.24699 2. .24726 .010692 .591975 .240271 .896015
4.657649 7.701298 681516 314309 24699 24699 24726 010692 591975 240271 896015 114095
4.657649 7.701298 681516 314309 5.24699 2. .24699 2. .24726 010692 591975 240271 896015 114095 075489
4.657649 7.701298 681516 314309 24699 24699 24726 010692 591975 240271 896015 114095 075489 049489

9	6	0	-1.72852	-3.497226	-0.619787
10	6	0	-0.762422	-5.656898	1.058883
11	6	0	1.907659	-5.59662	1.953681
12	6	0	-2.941024	-1.167616	3.310303
13	6	0	-3.860691	0.98955	-0.681522
14	6	0	-0.308744	-3.682297	-3.142564
15	7	0	-1.317894	-1.973307	-5.015085
16	6	0	-2.683503	2.126662	-5.490308
17	6	0	-0.440722	0.432381	-5.162041
18	6	0	-4.590152	0.430557	-6.85096
19	6	0	-3.936181	-2.204312	-5.857379
20	6	0	-3.366821	2.944631	-2.783124
21	8	0	1.770691	1.090734	-4.804042
22	6	0	-7.354488	1.114515	-6.60422
23	1	0	-2.235854	3.814678	-6.576887
24	1	0	-3.694666	-3.997245	-0.996071
25	1	0	6.109044	1.057468	0.532855
26	6	0	2.88599	3.53393	5.591208
27	8	0	2.281036	1.81037	6.992032
28	8	0	2.597571	5.899667	6.526715
29	6	0	3.204702	8.117553	5.06363
30	1	0	-0.306791	4.196745	2.051656
31	1	0	1.675792	3.969355	-0.58615
32	1	0	4.872363	4.828157	2.341292
33	1	0	6.462833	-5.029821	4.500409
34	1	0	7.40936	-3.974603	1.502649
35	1	0	8.57257	-0.363621	4.040583
36	1	0	5.882982	-0.711311	5.973349
37	1	0	-2.019804	-5.907053	2.678222
38	1	0	-1.026915	-7.402247	-0.01845
39	1	0	2.659901	-7.405717	2.568195
40	1	0	-4.799943	-2.061605	3.240746
41	1	0	-1.700456	-2.3208	4.464791
42	1	0	-3.147828	0.644182	4.261021
43	1	0	-5.448818	-0.201146	-1.225444
44	1	0	-4.61183	2.150328	0.845442
45	1	0	1.681662	-3.246678	-2.90932
46	1	0	-0.440062	-5.614812	-3.841403
47	1	0	-4.093061	0.487114	-8.853633
48	1	0	-4.08678	-3.657181	-7.310547
49	1	0	-5.168808	-2.7652	-4.308668
50	1	0	-1.916915	4.264542	-2.175478
51	1	0	-5.089725	4.073526	-2.908923

52	1	0	-7.719147	3.013242	-7.314108
53	1	0	-8.014722	1.032487	-4.657649
54	1	0	-8.518078	-0.185081	-7.701298
55	1	0	5.221059	8.214509	4.681516
56	1	0	2.131556	8.18374	3.314309
57	1	0	2.664031	9.701862	6.24699
1-3_en		Standard Ori	entation (Ångs	stroms)	
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	0.439613	3.320293	1.490025
1	6	0	0.337962	0.503411	1.064381
2	6	0	2.624267	-0.489327	1.497683
3	6	0	4.580895	1.450529	2.190751
4	6	0	2.954889	3.799585	2.889188
5	6	0	3.617672	-3.002244	1.902824
6	6	0	6.260297	-2.665561	2.970569
7	6	0	6.262449	0.025357	4.066769
8	6	0	-2.023525	-1.006057	0.605495
9	6	0	-1.472446	-3.525805	-0.868668
10	6	0	-0.17449	-5.642405	0.625936
11	6	0	2.432254	-5.218558	1.602423
12	6	0	-2.961805	-1.765275	3.27006
13	6	0	-4.313799	0.530219	-0.516832
14	6	0	-0.046815	-3.245841	-3.379318
15	7	0	-1.339929	-1.576186	-5.112166
16	6	0	-3.403672	2.249545	-5.235603
17	6	0	-0.893969	0.951912	-5.038497
18	6	0	-4.983769	0.377245	-6.77367
19	6	0	-3.882726	-2.179452	-5.999037
20	6	0	-4.219466	2.689612	-2.475517
21	8	0	1.173719	1.951649	-4.619888
22	6	0	-7.825621	0.537121	-6.505039
23	1	0	-3.267162	4.083092	-6.156562
24	1	0	-3.331675	-4.29643	-1.313417
25	1	0	5.723334	1.946804	0.538879
26	6	0	2.613903	3.952917	5.698509
27	8	0	0.879316	2.967715	6.851503
28	8	0	4.372386	5.170461	7.090181
29	6	0	6.435615	6.519273	5.923538
30	1	0	-1.182985	4.020877	2.545391
31	1	0	0.480413	4.336442	-0.30153
32	1	0	3.840115	5.519744	2.212384
33	1	0	6.756048	-4.106653	4.35287

34	1	0	7.65014	-2.782278	1.444736
35	1	0	8.156771	0.802512	4.250946
36	1	0	5.397974	-0.004703	5.938689
37	1	0	-1.388033	-6.24936	2.184137
38	1	0	-0.125048	-7.297428	-0.61399
39	1	0	3.433123	-6.922378	2.162555
40	1	0	-4.64076	-2.958416	3.140568
41	1	0	-1.520936	-2.77634	4.323065
42	1	0	-3.452576	-0.09343	4.360169
43	1	0	-5.710005	-0.863927	-1.101961
44	1	0	-5.177349	1.454068	1.109397
45	1	0	1.836009	-2.495035	-3.073974
46	1	0	0.156253	-5.102286	-4.244946
47	1	0	-4.504454	0.699782	-8.754676
48	1	0	-3.788412	-3.512853	-7.565981
49	1	0	-5.002678	-3.058853	-4.517614
50	1	0	-3.05481	4.214058	-1.747177
51	1	0	-6.131271	3.462154	-2.526824
52	1	0	-8.523494	2.396507	-7.05083
53	1	0	-8.447957	0.165574	-4.579681
54	1	0	-8.743318	-0.847935	-7.72427
55	1	0	7.515218	5.317792	4.659482
56	1	0	5.741199	8.173587	4.922402
57	1	0	7.634541	7.116973	7.474229
1-3_tddft		Standard Ori	Drientation (Ångstroms)		
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	0.439613	3.320293	1.490025
1	6	0	0.337962	0.503411	1.064381
2	6	0	2.624267	-0.489327	1.497683
3	6	0	4.580895	1.450529	2.190751
4	6	0	2.954889	3.799585	2.889188
5	6	0	3.617672	-3.002244	1.902824
6	6	0	6.260297	-2.665561	2.970569
7	6	0	6.262449	0.025357	4.066769
8	6	0	-2.023525	-1.006057	0.605495
9	6	0	-1.472446	-3.525805	-0.868668
10	6	0	-0.17449	-5.642405	0.625936
11	6	0	2.432254	-5.218558	1.602423
12	6	0	-2.961805	-1.765275	3.27006
13	6	0	-4.313799	0.530219	-0.516832
14	6	0	-0.046815	-3.245841	-3.379318
15	7	0	-1.339929	-1.576186	-5.112166

1.6			0.400.5-5	0.040747	
16	6	0	-3.403672	2.249545	-5.235603
17	6	0	-0.893969	0.951912	-5.038497
18	6	0	-4.983769	0.377245	-6.77367
19	6	0	-3.882726	-2.179452	-5.999037
20	6	0	-4.219466	2.689612	-2.475517
21	8	0	1.173719	1.951649	-4.619888
22	6	0	-7.825621	0.537121	-6.505039
23	1	0	-3.267162	4.083092	-6.156562
24	1	0	-3.331675	-4.29643	-1.313417
25	1	0	5.723334	1.946804	0.538879
26	6	0	2.613903	3.952917	5.698509
27	8	0	0.879316	2.967715	6.851503
28	8	0	4.372386	5.170461	7.090181
29	6	0	6.435615	6.519273	5.923538
30	1	0	-1.182985	4.020877	2.545391
31	1	0	0.480413	4.336442	-0.30153
32	1	0	3.840115	5.519744	2.212384
33	1	0	6.756048	-4.106653	4.35287
34	1	0	7.65014	-2.782278	1.444736
35	1	0	8.156771	0.802512	4.250946
36	1	0	5.397974	-0.004703	5.938689
37	1	0	-1.388033	-6.24936	2.184137
38	1	0	-0.125048	-7.297428	-0.61399
39	1	0	3.433123	-6.922378	2.162555
40	1	0	-4.64076	-2.958416	3.140568
41	1	0	-1.520936	-2.77634	4.323065
42	1	0	-3.452576	-0.09343	4.360169
43	1	0	-5.710005	-0.863927	-1.101961
44	1	0	-5.177349	1.454068	1.109397
45	1	0	1.836009	-2.495035	-3.073974
46	1	0	0.156253	-5.102286	-4.244946
47	1	0	-4.504454	0.699782	-8.754676
48	1	0	-3.788412	-3.512853	-7.565981
49	1	0	-5.002678	-3.058853	-4.517614
50	1	0	-3.05481	4.214058	-1.747177
51	1	0	-6.131271	3.462154	-2.526824
52	1	0	-8.523494	2.396507	-7.05083
53	1	0	-8.447957	0.165574	-4.579681
54	1	0	-8.743318	-0.847935	-7.72427
55	1	0	7.515218	5.317792	4.659482
56	1	0	5.741199	8.173587	4.922402
57	1	0	7.634541	7.116973	7.474229
1-4 en	1	Standard Ori	entation (Ångs	stroms)	
			\ <b>0</b> °	/	

Center	Atomic	Atomic	X	Y	Ζ
number	number	Туре			
0	6	0	1.286825	3.163802	1.301364
1	6	0	0.694255	0.375592	1.101933
2	6	0	2.774994	-0.948549	1.662774
3	6	0	5.003256	0.70776	2.260893
4	6	0	3.775684	3.261287	2.898547
5	6	0	3.370559	-3.555073	2.206328
6	6	0	6.084544	-3.593181	3.14508
7	6	0	6.58627	-0.88492	4.082653
8	6	0	-1.896355	-0.728484	0.751839
9	6	0	-1.803909	-3.432948	-0.474291
10	6	0	-0.850506	-5.594663	1.208536
11	6	0	1.827444	-5.558916	2.082501
12	6	0	-2.933306	-1.07024	3.463961
13	6	0	-3.884533	1.077215	-0.529487
14	6	0	-0.404089	-3.643573	-3.005839
15	7	0	-1.413141	-1.935317	-4.884117
16	6	0	-2.741661	2.178857	-5.360046
17	6	0	-0.51041	0.463403	-5.050044
18	6	0	-4.677767	0.496123	-6.698131
19	6	0	-4.043601	-2.139679	-5.695223
20	6	0	-3.395749	3.015492	-2.649058
21	8	0	1.712496	1.099494	-4.726602
22	6	0	-7.433891	1.207328	-6.425837
23	1	0	-2.291196	3.859924	-6.455194
24	1	0	-3.777342	-3.910768	-0.833586
25	1	0	6.117484	1.006348	0.539353
26	6	0	3.010151	3.612019	5.606502
27	8	0	2.397453	1.915901	7.038116
28	8	0	2.83259	5.99231	6.530585
29	6	0	3.464242	8.179333	5.031368
30	1	0	-0.245318	4.261125	2.13253
31	1	0	1.674019	3.985411	-0.549219
32	1	0	4.952679	4.824461	2.293079
33	1	0	6.413011	-5.025781	4.585908
34	1	0	7.349997	-4.021391	1.566788
35	1	0	8.585108	-0.397664	4.060527
36	1	0	5.895294	-0.682502	6.005875
37	1	0	-2.096353	-5.819859	2.840013
38	1	0	-1.141908	-7.340696	0.140002
39	1	0	2.557256	-7.371765	2.714716
40	1	0	-4.798068	-1.954063	3.426766

41					
• -	1	0	-1.681138	-2.220603	4.608758
42	1	0	-3.114463	0.749944	4.40338
43	1	0	-5.492472	-0.097077	-1.048102
44	1	0	-4.597848	2.254461	1.001764
45	1	0	1.588549	-3.215903	-2.784242
46	1	0	-0.55025	-5.578754	-3.691965
47	1	0	-4.197543	0.539894	-8.704447
48	1	0	-4.229799	-3.60139	-7.134439
49	1	0	-5.267379	-2.670525	-4.130116
50	1	0	-1.930245	4.326593	-2.059972
51	1	0	-5.112645	4.151974	-2.766102
52	1	0	-7.789259	3.103319	-7.148072
53	1	0	-8.066595	1.147942	-4.469637
54	1	0	-8.622584	-0.092571	-7.495438
55	1	0	2.328142	8.27493	3.324126
56	1	0	3.0278	9.789844	6.221635
57	1	0	5.465557	8.20275	4.570019
1-4_tddft		Standard Ori	entation (Ångs	troms)	
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	1.286825	3.163802	1.301364
1	6	0	0.694255	0.375592	1.101933
2	6	0	2.774994	-0.948549	1.662774
2					
3	6	0	5.003256	0.70776	2.260893
3	6 6	0 0	5.003256 3.775684	0.70776 3.261287	2.260893 2.898547
3 4 5	6 6 6	0 0 0	5.003256 3.775684 3.370559	0.70776 3.261287 -3.555073	2.260893 2.898547 2.206328
3 4 5 6	6 6 6 6	0 0 0 0	5.003256 3.775684 3.370559 6.084544	0.70776 3.261287 -3.555073 -3.593181	2.260893 2.898547 2.206328 3.14508
3 4 5 6 7	6 6 6 6 6	0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627	0.70776 3.261287 -3.555073 -3.593181 -0.88492	2.260893 2.898547 2.206328 3.14508 4.082653
3 4 5 6 7 8	6 6 6 6 6 6	0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839
3   4   5   6   7   8   9	6 6 6 6 6 6 6	0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291
3   4   5   6   7   8   9   10	6 6 6 6 6 6 6 6	0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536
3   4   5   6   7   8   9   10   11	6 6 6 6 6 6 6 6 6	0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501
3   4   5   6   7   8   9   10   11   12	6 6 6 6 6 6 6 6 6 6 6	0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961
3     4     5     6     7     8     9     10     11     12     13	6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487
3     4     5     6     7     8     9     10     11     12     13     14	6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839
3     4     5     6     7     8     9     10     11     12     13     14     15	6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     7	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117
3     4     5     6     7     8     9     10     11     12     13     14     15     16	6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     7     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046
3     4     5     6     7     8     9     10     11     12     13     14     15     16     17	6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     6     7     6     6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661 -0.51041	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857 0.463403	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046 -5.050044
3     4     5     6     7     8     9     10     11     12     13     14     15     16     17     18	6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661 -0.51041 -4.677767	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857 0.463403 0.496123	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046 -5.050044 -6.698131
3     4     5     6     7     8     9     10     11     12     13     14     15     16     17     18     19	6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661 -0.51041 -4.677767 -4.043601	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857 0.463403 0.496123 -2.139679	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046 -5.050044 -6.698131 -5.695223
3     4     5     6     7     8     9     10     11     12     13     14     15     16     17     18     19     20	6     6	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661 -0.51041 -4.677767 -4.043601 -3.395749	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857 0.463403 0.496123 -2.139679 3.015492	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046 -5.050044 -6.698131 -5.695223 -2.649058
3     4     5     6     7     8     9     10     11     12     13     14     15     16     17     18     19     20     21	6     8	0 0 0 0 0 0 0 0 0 0 0 0 0 0	5.003256 3.775684 3.370559 6.084544 6.58627 -1.896355 -1.803909 -0.850506 1.827444 -2.933306 -3.884533 -0.404089 -1.413141 -2.741661 -0.51041 -4.677767 -4.043601 -3.395749 1.712496	0.70776 3.261287 -3.555073 -3.593181 -0.88492 -0.728484 -3.432948 -5.594663 -5.558916 -1.07024 1.077215 -3.643573 -1.935317 2.178857 0.463403 0.496123 -2.139679 3.015492 1.099494	2.260893 2.898547 2.206328 3.14508 4.082653 0.751839 -0.474291 1.208536 2.082501 3.463961 -0.529487 -3.005839 -4.884117 -5.360046 -5.050044 -6.698131 -5.695223 -2.649058 -4.726602

23	1	0	-2.291196	3.859924	-6.455194		
24	1	0	-3.777342	-3.910768	-0.833586		
25	1	0	6.117484	1.006348	0.539353		
26	6	0	3.010151	3.612019	5.606502		
27	8	0	2.397453	1.915901	7.038116		
28	8	0	2.83259	5.99231	6.530585		
29	6	0	3.464242	8.179333	5.031368		
30	1	0	-0.245318	4.261125	2.13253		
31	1	0	1.674019	3.985411	-0.549219		
32	1	0	4.952679	4.824461	2.293079		
33	1	0	6.413011	-5.025781	4.585908		
34	1	0	7.349997	-4.021391	1.566788		
35	1	0	8.585108	-0.397664	4.060527		
36	1	0	5.895294	-0.682502	6.005875		
37	1	0	-2.096353	-5.819859	2.840013		
38	1	0	-1.141908	-7.340696	0.140002		
39	1	0	2.557256	-7.371765	2.714716		
40	1	0	-4.798068	-1.954063	3.426766		
41	1	0	-1.681138	-2.220603	4.608758		
42	1	0	-3.114463	0.749944	4.40338		
43	1	0	-5.492472	-0.097077	-1.048102		
44	1	0	-4.597848	2.254461	1.001764		
45	1	0	1.588549	-3.215903	-2.784242		
46	1	0	-0.55025	-5.578754	-3.691965		
47	1	0	-4.197543	0.539894	-8.704447		
48	1	0	-4.229799	-3.60139	-7.134439		
49	1	0	-5.267379	-2.670525	-4.130116		
50	1	0	-1.930245	4.326593	-2.059972		
51	1	0	-5.112645	4.151974	-2.766102		
52	1	0	-7.789259	3.103319	-7.148072		
53	1	0	-8.066595	1.147942	-4.469637		
54	1	0	-8.622584	-0.092571	-7.495438		
55	1	0	2.328142	8.27493	3.324126		
56	1	0	3.0278	9.789844	6.221635		
57	1	0	5.465557	8.20275	4.570019		
1-5_en		Standard Ori	andard Orientation (Ångstroms)				
Center	Atomic	Atomic	Х	Y	Ζ		
number	number	Туре					
0	6	0	1.363633	3.062116	1.414518		
1	6	0	0.743642	0.288896	1.110145		
2	6	0	2.795535	-1.077517	1.676182		
3	6	0	5.027967	0.530987	2.379984		
4	6	0	3.816409	3.07813	3.069582		

5	6	0	3.348576	-3.707383	2.149031
6	6	0	6.039575	-3.808285	3.147139
7	6	0	6.547925	-1.138754	4.186008
8	6	0	-1.850152	-0.773319	0.666155
9	6	0	-1.755898	-3.438435	-0.643164
10	6	0	-0.870709	-5.663691	0.992651
11	6	0	1.786525	-5.688082	1.928504
12	6	0	-2.954806	-1.186483	3.340338
13	6	0	-3.788382	1.093549	-0.604746
14	6	0	-0.290376	-3.583883	-3.141901
15	7	0	-1.236529	-1.811824	-4.994246
16	6	0	-2.516298	2.32854	-5.372398
17	6	0	-0.308832	0.582476	-5.063163
18	6	0	-4.433663	0.707138	-6.809068
19	6	0	-3.850131	-1.963004	-5.869577
20	6	0	-3.231152	3.088253	-2.654171
21	8	0	1.911414	1.186659	-4.667321
22	6	0	-7.188985	1.437637	-6.583526
23	1	0	-2.022314	4.038274	-6.402647
24	1	0	-3.723433	-3.880506	-1.07194
25	1	0	6.185782	0.870777	0.695132
26	6	0	2.993661	3.358159	5.768543
27	8	0	2.331141	1.628886	7.137031
28	8	0	2.817566	5.713335	6.755559
29	6	0	3.503072	7.9349	5.332462
30	1	0	-0.174378	4.150459	2.246588
31	1	0	1.80534	3.940679	-0.397266
32	1	0	5.025236	4.644365	2.538731
33	1	0	6.319428	-5.291733	4.546038
34	1	0	7.335925	-4.198111	1.584085
35	1	0	8.551852	-0.674412	4.229636
36	1	0	5.810072	-0.99206	6.096856
37	1	0	-2.156221	-5.922827	2.587775
38	1	0	-1.158412	-7.372004	-0.136184
39	1	0	2.481258	-7.528295	2.519791
40	1	0	-4.82791	-2.047107	3.232376
41	1	0	-1.743697	-2.385661	4.479271
42	1	0	-3.139534	0.606361	4.330831
43	1	0	-5.398213	-0.045138	-1.192894
44	1	0	-4.522749	2.233923	0.944456
45	1	0	1.698523	-3.178425	-2.855041
46	1	0	-0.432237	-5.496316	-3.890286
47	1	0	-3.903385	0.805952	-8.800879

48	1	0	-4.0204	-3.381215	-7.353511		
49	1	0	-5.114152	-2.521355	-4.346678		
50	1	0	-1.771024	4.370162	-1.991342		
51	1	0	-4.935971	4.242144	-2.780196		
52	1	0	-7.871148	1.324751	-4.646274		
53	1	0	-8.361961	0.183028	-7.722315		
54	1	0	-7.50785	3.358489	-7.255274		
55	1	0	2.411347	8.085122	3.600641		
56	1	0	3.049125	9.516405	6.55467		
57	1	0	5.515555	7.954453	4.9218		
1-5_tddft		Standard Orientation (Ångstroms)					
Center	Atomic	Atomic	X	Y	Ζ		
number	number	Туре					
0	6	0	1.363633	3.062116	1.414518		
1	6	0	0.743642	0.288896	1.110145		
2	6	0	2.795535	-1.077517	1.676182		
3	6	0	5.027967	0.530987	2.379984		
4	6	0	3.816409	3.07813	3.069582		
5	6	0	3.348576	-3.707383	2.149031		
6	6	0	6.039575	-3.808285	3.147139		
7	6	0	6.547925	-1.138754	4.186008		
8	6	0	-1.850152	-0.773319	0.666155		
9	6	0	-1.755898	-3.438435	-0.643164		
10	6	0	-0.870709	-5.663691	0.992651		
11	6	0	1.786525	-5.688082	1.928504		
12	6	0	-2.954806	-1.186483	3.340338		
13	6	0	-3.788382	1.093549	-0.604746		
14	6	0	-0.290376	-3.583883	-3.141901		
15	7	0	-1.236529	-1.811824	-4.994246		
16	6	0	-2.516298	2.32854	-5.372398		
17	6	0	-0.308832	0.582476	-5.063163		
18	6	0	-4.433663	0.707138	-6.809068		
19	6	0	-3.850131	-1.963004	-5.869577		
20	6	0	-3.231152	3.088253	-2.654171		
21	8	0	1.911414	1.186659	-4.667321		
22	6	0	-7.188985	1.437637	-6.583526		
23	1	0	-2.022314	4.038274	-6.402647		
24	1	0	-3.723433	-3.880506	-1.07194		
25	1	0	6.185782	0.870777	0.695132		
26	6	0	2.993661	3.358159	5.768543		
27	8	0	2.331141	1.628886	7.137031		
28	8	0	2.817566	5.713335	6.755559		
29	6	0	3.503072	7.9349	5.332462		

30	1	0	-0.174378	4.150459	2.246588	
31	1	0	1.80534	3.940679	-0.397266	
32	1	0	5.025236	4.644365	2.538731	
33	1	0	6.319428	-5.291733	4.546038	
34	1	0	7.335925	-4.198111	1.584085	
35	1	0	8.551852	-0.674412	4.229636	
36	1	0	5.810072	-0.99206	6.096856	
37	1	0	-2.156221	-5.922827	2.587775	
38	1	0	-1.158412	-7.372004	-0.136184	
39	1	0	2.481258	-7.528295	2.519791	
40	1	0	-4.82791	-2.047107	3.232376	
41	1	0	-1.743697	-2.385661	4.479271	
42	1	0	-3.139534	0.606361	4.330831	
43	1	0	-5.398213	-0.045138	-1.192894	
44	1	0	-4.522749	2.233923	0.944456	
45	1	0	1.698523	-3.178425	-2.855041	
46	1	0	-0.432237	-5.496316	-3.890286	
47	1	0	-3.903385	0.805952	-8.800879	
48	1	0	-4.0204	-3.381215	-7.353511	
49	1	0	-5.114152	-2.521355	-4.346678	
50	1	0	-1.771024	4.370162	-1.991342	
51	1	0	-4.935971	4.242144	-2.780196	
52	1	0	-7.871148	1.324751	-4.646274	
53	1	0	-8.361961	0.183028	-7.722315	
54	1	0	-7.50785	3.358489	-7.255274	
55	1	0	2.411347	8.085122	3.600641	
56	1	0	3.049125	9.516405	6.55467	
57	1	0	5.515555	7.954453	4.9218	
1-6_en		Standard Orientation (Ångstroms)				
Center	Atomic	Atomic	X	Y	Ζ	
number	number	Туре				
0	6	0	0.591019	3.325337	1.378462	
1	6	0	0.36511	0.496504	1.103177	
2	6	0	2.579237	-0.577204	1.691196	
3	6	0	4.602865	1.305685	2.348694	
4	6	0	3.068329	3.761697	2.856994	
5	6	0	3.431369	-3.106164	2.276811	
6	6	0	6.047247	-2.835258	3.426199	
7	6	0	6.151353	-0.085301	4.360002	
8	6	0	-2.049266	-0.919658	0.625368	
9	6	0	-1.561612	-3.547527	-0.67639	
10	6	0	-0.43459	-5.632628	0.992754	
11	6	0	2.149053	-5.277417	2.054105	

12	6	0	-3.137428	-1.477042	3.281082
13	6	0	-4.20755	0.656289	-0.690363
14	6	0	-0.017139	-3.479408	-3.129912
15	7	0	-1.153546	-1.856106	-5.011636
16	6	0	-3.009901	2.053538	-5.444984
17	6	0	-0.58016	0.647715	-5.068205
18	6	0	-4.622849	0.170419	-6.935373
19	6	0	-3.695361	-2.382099	-5.950029
20	6	0	-3.911971	2.696804	-2.752985
21	8	0	1.519152	1.567876	-4.625951
22	6	0	-7.460678	0.491915	-6.809956
23	1	0	-2.740452	3.818041	-6.465917
24	1	0	-3.436447	-4.256123	-1.158618
25	1	0	5.819812	1.652322	0.712439
26	6	0	2.6196	4.0746	5.637815
27	8	0	0.796517	3.224466	6.761227
28	8	0	4.369761	5.287706	7.04425
29	6	0	6.535691	6.492225	5.90737
30	1	0	-1.0351	4.157727	2.326844
31	1	0	0.752721	4.238044	-0.461245
32	1	0	4.061481	5.40133	2.132341
33	1	0	6.415183	-4.209961	4.912235
34	1	0	7.483883	-3.117836	1.966515
35	1	0	8.076502	0.607572	4.561428
36	1	0	5.231794	0.038827	6.201377
37	1	0	-1.740807	-6.086942	2.526945
38	1	0	-0.418935	-7.357968	-0.148255
39	1	0	3.041342	-6.99181	2.749423
40	1	0	-4.866821	-2.594947	3.141462
41	1	0	-1.793068	-2.490306	4.452272
42	1	0	-3.591192	0.275331	4.254234
43	1	0	-5.639115	-0.700404	-1.277366
44	1	0	-5.106055	1.705319	0.838098
45	1	0	1.884004	-2.797341	-2.780332
46	1	0	0.134629	-5.390645	-3.879292
47	1	0	-4.040767	0.337814	-8.908375
48	1	0	-3.628277	-3.826305	-7.41663
49	1	0	-4.90939	-3.088123	-4.44884
50	1	0	-2.697119	4.196563	-2.056712
51	1	0	-5.773648	3.566153	-2.933244
52	1	0	-8.033718	2.343499	-7.506651
53	1	0	-8.184769	0.281138	-4.896109
54	1	0	-8.396443	-0.92373	-7.979334
	-				
-----------	--------	--------------	----------------	-----------	-----------
55	1	0	7.647851	5.171804	4.798985
56	1	0	5.953284	8.087275	4.751231
57	1	0	7.662167	7.16889	7.479821
1-6_tddft		Standard Ori	entation (Ångs	stroms)	
Center	Atomic	Atomic	Х	Y	Z
number	number	Туре			
0	6	0	0.591019	3.325337	1.378462
1	6	0	0.36511	0.496504	1.103177
2	6	0	2.579237	-0.577204	1.691196
3	6	0	4.602865	1.305685	2.348694
4	6	0	3.068329	3.761697	2.856994
5	6	0	3.431369	-3.106164	2.276811
6	6	0	6.047247	-2.835258	3.426199
7	6	0	6.151353	-0.085301	4.360002
8	6	0	-2.049266	-0.919658	0.625368
9	6	0	-1.561612	-3.547527	-0.67639
10	6	0	-0.43459	-5.632628	0.992754
11	6	0	2.149053	-5.277417	2.054105
12	6	0	-3.137428	-1.477042	3.281082
13	6	0	-4.20755	0.656289	-0.690363
14	6	0	-0.017139	-3.479408	-3.129912
15	7	0	-1.153546	-1.856106	-5.011636
16	6	0	-3.009901	2.053538	-5.444984
17	6	0	-0.58016	0.647715	-5.068205
18	6	0	-4.622849	0.170419	-6.935373
19	6	0	-3.695361	-2.382099	-5.950029
20	6	0	-3.911971	2.696804	-2.752985
21	8	0	1.519152	1.567876	-4.625951
22	6	0	-7.460678	0.491915	-6.809956
23	1	0	-2.740452	3.818041	-6.465917
24	1	0	-3.436447	-4.256123	-1.158618
25	1	0	5.819812	1.652322	0.712439
26	6	0	2.6196	4.0746	5.637815
27	8	0	0.796517	3.224466	6.761227
28	8	0	4.369761	5.287706	7.04425
29	6	0	6.535691	6.492225	5.90737
30	1	0	-1.0351	4.157727	2.326844
31	1	0	0.752721	4.238044	-0.461245
32	1	0	4.061481	5.40133	2.132341
33	1	0	6.415183	-4.209961	4.912235
34	1	0	7.483883	-3.117836	1.966515
35	1	0	8.076502	0.607572	4.561428
36	1	0	5.231794	0.038827	6.201377
N					

37	1	0	-1.740807	-6.086942	2.526945
38	1	0	-0.418935	-7.357968	-0.148255
39	1	0	3.041342	-6.99181	2.749423
40	1	0	-4.866821	-2.594947	3.141462
41	1	0	-1.793068	-2.490306	4.452272
42	1	0	-3.591192	0.275331	4.254234
43	1	0	-5.639115	-0.700404	-1.277366
44	1	0	-5.106055	1.705319	0.838098
45	1	0	1.884004	-2.797341	-2.780332
46	1	0	0.134629	-5.390645	-3.879292
47	1	0	-4.040767	0.337814	-8.908375
48	1	0	-3.628277	-3.826305	-7.41663
49	1	0	-4.90939	-3.088123	-4.44884
50	1	0	-2.697119	4.196563	-2.056712
51	1	0	-5.773648	3.566153	-2.933244
52	1	0	-8.033718	2.343499	-7.506651
53	1	0	-8.184769	0.281138	-4.896109
54	1	0	-8.396443	-0.92373	-7.979334
55	1	0	7.647851	5.171804	4.798985
56	1	0	5.953284	8.087275	4.751231
57	1	0	7.662167	7.16889	7.479821
1-7 en			^		
1-7_en		Standard Ori	entation (Ångs	troms)	
<b>1-7_en</b> Center	Atomic	Standard Ori Atomic	entation (Ångs X	troms) Y	Ζ
1-7_en Center number	Atomic number	Standard Ori Atomic Type	entation (Ångs X	troms) Y	Z
1-7_enCenternumber0	Atomic number 6	Standard Ori Atomic Type 0	entation (Ångs X 1.395201	troms) Y 3.21451	Z 1.28119
1-7_enCenternumber01	Atomic number 6 6	Standard Ori Atomic Type 0 0	entation (Ångs X 1.395201 0.768245	troms) Y 3.21451 0.429312	Z 1.28119 1.162884
1-7_enCenternumber012	Atomic number 6 6 6	Standard Ori Atomic Type 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481	troms) Y 3.21451 0.429312 -0.903972	Z 1.28119 1.162884 1.768163
1-7_en           Center           number           0           1           2           3	Atomic number 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675	troms) Y 3.21451 0.429312 -0.903972 0.740663	Z 1.28119 1.162884 1.768163 2.318615
1-7_en           Center           number           0           1           2           3           4	Atomic number 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472	Z 1.28119 1.162884 1.768163 2.318615 2.875907
1-7_en           Center           number           0           1           2           3           4           5	Atomic number 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709
1-7_en           Center           number           0           1           2           3           4           5           6	Atomic number 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528
1-7_en           Center           number           0           1           2           3           4           5           6           7	Atomic number 6 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864
1-7_en           Center           number           0           1           2           3           4           5           6           7           8	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622
1-7_en           Center           number           0           1           2           3           4           5           6           7           8           9	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori Atomic Type 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13         14	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571 -0.385935	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372 -3.712283	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504 -2.814499
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13         14         15	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571 -0.385935 -1.36213	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372 -3.712283 -2.049046	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504 -2.814499 -4.748543
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13         14         15         16	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571 -0.385935 -1.36213 -2.624228	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372 -3.712283 -2.049046 2.066951	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504 -2.814499 -4.748543 -5.364097
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13         14         15         16         17	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0           0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571 -0.385935 -1.36213 -2.624228 -0.421773	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372 -3.712283 -2.049046 2.066951 0.328247	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504 -2.814499 -4.748543 -5.364097 -4.988461
1-7_en         Center         number         0         1         2         3         4         5         6         7         8         9         10         11         12         13         14         15         16         17         18	Atomic number 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6 6	Standard Ori         Atomic         Type         0	entation (Ångs X 1.395201 0.768245 2.830481 5.079675 3.885214 3.388893 6.100637 6.640244 -1.836632 -1.782928 -0.859869 1.818028 -2.885736 -3.795571 -0.385935 -1.36213 -2.624228 -0.421773 -4.5829	troms) Y 3.21451 0.429312 -0.903972 0.740663 3.328472 -3.499418 -3.545448 -0.815306 -0.649854 -3.395034 -5.51237 -5.484419 -0.884448 1.139372 -3.712283 -2.049046 2.066951 0.328247 0.371886	Z 1.28119 1.162884 1.768163 2.318615 2.875907 2.396709 3.341528 4.190864 0.842622 -0.29206 1.461845 2.336385 3.562062 -0.504504 -2.814499 -4.748543 -5.364097 -4.988461 -6.653638

19         6         0 $-3.989978$ $-2.241852$ $-5.569623$ 20         6         0 $-3.27441$ $3.00967$ $-2.68497$ 21         8         0 $1.809656$ $0.939913$ $4.674824$ 22         6         0 $-7.328818$ $1.131145$ $-6.409703$ 23         1         0 $-3.763687$ $-3.854813$ $-0.632238$ 24         1         0 $-3.763687$ $-3.854813$ $-0.632738$ 25         1         0 $6.199441$ $0.972466$ $0.590459$ 26         6         0 $3.123021$ $3.772939$ $5.70538$ 27         8         0 $2.976309$ $6.182681$ $6.421109$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-1.790074$ $3.979977$ $-0.591621$ 32         1         0 $5.952483$			1	1		
20         6         0 $-3.27441$ $3.000967$ $-2.68497$ 21         8         0 $1.809656$ $0.939913$ $-4.674824$ 22         6         0 $-7.328818$ $1.131145$ $-6.409703$ 23         1         0 $-3.763687$ $-3.854813$ $-0.6512032$ 24         1         0 $-3.763687$ $-3.854813$ $-0.652388$ 25         1         0 $6.199441$ $0.972466$ $0.590459$ 26         6         0 $3.123021$ $3.772939$ $5.70538$ 27         8         0 $2.976309$ $6.182681$ $6.421109$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-0.123884$ $4.352431$ $2.081509$ 31         1         0 $5.058058$ $4.850175$ $2.222837$ 33         1         0 $5.058055$	19	6	0	-3.989978	-2.241852	-5.569623
21         8         0         1.809656         0.939913         4.674824           22         6         0         -7.328818         1.131145         -6.409703           23         1         0         -2.143731         3.703928         -6.512032           24         1         0         -3.763687         -3.854813         -0.635238           25         1         0         6.199441         0.972466         0.590459           26         6         0         3.123021         3.772939         5.570538           27         8         0         2.976309         6.182681         6.421109           29         6         0         3.640353         8.314419         4.858053           30         1         0         -0.123884         4.352431         2.081509           31         1         0         5.083088         4.856175         2.222837           33         1         0         5.083088         4.856175         2.222837           34         1         0         7.363047         -4.045172         1.781905           35         1         0         2.107953         -5.668055         3.100414           <	20	6	0	-3.27441	3.000967	-2.68497
22         6         0         -7.328818         1.131145         -6.409703           23         1         0         -2.143731         3.703928         -6.512032           24         1         0         -3.763687         -3.854813         -0.635238           25         1         0         6.199441         0.972466         0.590459           26         6         0         3.123021         3.772939         5.570538           27         8         0         2.976309         6.182681         6.421109           29         6         0         3.640353         8.314419         4.858053           30         1         0         -0.123884         4.352431         2.081509           31         1         0         5.083088         4.856175         2.22837           33         1         0         6.404943         -4.933729         4.830347           34         1         0         7.363047         -4.045172         1.781905           35         1         0         8.645766         -0.357519         4.153789           36         1         0         2.522016         -7.28542         3.028468           <	21	8	0	1.809656	0.939913	-4.674824
23         1         0 $-2.143731$ $3.703928$ $-6.512032$ 24         1         0 $-3.753887$ $-3.854813$ $-0.635238$ 25         1         0 $6.199441$ $0.972466$ $0.590459$ 26         6         0 $3.123021$ $3.772939$ $5.570538$ 27         8         0 $2.484672$ $2.13035$ $7.052404$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-0.123884$ $4.352431$ $2.081599$ 31         1         0 $5.083088$ $4.856175$ $2.222837$ 33         1         0 $6.404943$ $4.933729$ $4.830347$ 34         1         0 $7.363047$ $4.045172$ $1.781905$ 35         1         0 $8.645766$ $-0.357519$ $4.153789$ 36         1         0 $2.107953$ <t< td=""><td>22</td><td>6</td><td>0</td><td>-7.328818</td><td>1.131145</td><td>-6.409703</td></t<>	22	6	0	-7.328818	1.131145	-6.409703
24         1         0 $-3.763687$ $-3.854813$ $-0.635238$ 25         1         0 $6.199441$ $0.972466$ $0.590459$ 26         6         0 $3.123021$ $3.772939$ $5.570538$ 27         8         0 $2.484672$ $2.13035$ $7.052404$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-0.123884$ $4.352431$ $2.081509$ 31         1         0 $1.790074$ $3.979977$ $-0.591621$ 32         1         0 $5.083088$ $4.850175$ $2.22837$ 33         1         0 $5.083087$ $-4.045172$ $1.781905$ 35         1         0 $8.45766$ $-0.357519$ $4.153789$ 36         1         0 $2.107953$ $-5.668055$ $3.100414$ 38         1         0 $-1.174328$ <t< td=""><td>23</td><td>1</td><td>0</td><td>-2.143731</td><td>3.703928</td><td>-6.512032</td></t<>	23	1	0	-2.143731	3.703928	-6.512032
25         1         0 $6.199441$ $0.972466$ $0.590459$ 26         6         0 $3.123021$ $3.772939$ $5.570538$ 27         8         0 $2.484672$ $2.13035$ $7.052404$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-0.123884$ $4.352431$ $2.081509$ 31         1         0 $5.083088$ $4.856175$ $2.222837$ 33         1         0 $6.404943$ $-4.933729$ $4.830347$ 34         1         0 $7.363047$ $4.045172$ $1.781905$ 35         1         0 $8.645766$ $-0.357519$ $4.153789$ 36         1         0 $-2.107953$ $-5.668055$ $3.100414$ 38         1         0 $-1.174328$ $-7.285742$ $3.028468$ 40         1         0 $-2.016027$ <	24	1	0	-3.763687	-3.854813	-0.635238
26         6         0 $3.123021$ $3.772939$ $5.570538$ 27         8         0 $2.484672$ $2.13035$ $7.052404$ 28         8         0 $2.976309$ $6.182681$ $6.421109$ 29         6         0 $3.640353$ $8.314419$ $4.85053$ 30         1         0 $-0.123884$ $4.352431$ $2.081509$ 31         1         0 $5.083088$ $4.856175$ $2.222837$ 32         1         0 $6.404943$ $-4.933729$ $4.830347$ 34         1         0 $7.363047$ $-4.045172$ $1.781905$ 35         1         0 $8.645766$ $-0.357519$ $4.153789$ 36         1         0 $-2.107953$ $-5.668055$ $3.100414$ 38         1         0 $-1.174328$ $-7.285742$ $3.028468$ 40         1         0 $-4.64436$ $-1.738533$ $3.548071$ 41         1         0 $-4.649738$	25	1	0	6.199441	0.972466	0.590459
27         8         0         2.484672         2.13035         7.052404           28         8         0         2.976309         6.182681         6.421109           29         6         0         3.640353         8.314419         4.858053           30         1         0         -0.123884         4.352431         2.081509           31         1         0         1.790074         3.979977         -0.591621           32         1         0         5.083088         4.856175         2.222837           33         1         0         6.404943         -4.933729         4.830347           34         1         0         7.363047         -4.045172         1.781905           35         1         0         8.645766         -0.357519         4.153789           36         1         0         -2.107953         -5.668055         3.100414           38         1         0         -1.174328         -7.288766         0.451625           39         1         0         -2.52016         -7.285542         3.028468           40         1         0         -4.764436         -1.738533         3.548071	26	6	0	3.123021	3.772939	5.570538
28         8         0         2.976309         6.182681         6.421109           29         6         0         3.640353         8.314419         4.858053           30         1         0         -0.123884         4.352431         2.081509           31         1         0         1.790074         3.979977         -0.591621           32         1         0         6.404943         -4.933729         4.830347           34         1         0         7.363047         -4.045172         1.781905           35         1         0         8.645766         -0.357519         4.153789           36         1         0         -2.107953         -5.668055         3.100414           38         1         0         -1.174328         -7.288766         0.451625           39         1         0         2.522016         -7.285542         3.028468           40         1         0         -4.764436         -1.738533         3.548071           41         1         0         -5.418217         -0.029656         -0.988378           42         1         0         -5.418217         -0.029656         -0.988378	27	8	0	2.484672	2.13035	7.052404
29         6         0 $3.640353$ $8.314419$ $4.858053$ 30         1         0 $-0.123884$ $4.352431$ $2.081509$ 31         1         0 $1.790074$ $3.979977$ $-0.591621$ 32         1         0 $5.083088$ $4.856175$ $2.222837$ 33         1         0 $6.404943$ $-4.933729$ $4.830347$ 34         1         0 $7.363047$ $-4.045172$ $1.781905$ 35         1         0 $5.952483$ $-0.541964$ $6.106437$ 37         1         0 $-2.107953$ $-5.668055$ $3.100414$ 38         1         0 $-1.174328$ $-7.288766$ $0.451625$ 39         1         0 $2.522016$ $-7.285542$ $3.028468$ 40         1         0 $-4.676436$ $-1.738533$ $3.548071$ 41         1         0 $-5.418217$ $-0.029556$ $-0.983672$ 44         1         0 $-5.418217$	28	8	0	2.976309	6.182681	6.421109
3010 $-0.123884$ $4.352431$ $2.081509$ $31$ 10 $1.790074$ $3.979977$ $0.591621$ $32$ 10 $5.083088$ $4.856175$ $2.222837$ $33$ 10 $6.404943$ $-4.933729$ $4.830347$ $34$ 10 $7.363047$ $-4.045172$ $1.781905$ $35$ 10 $8.645766$ $-0.357519$ $4.153789$ $36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285742$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-4.187032$ $-3.314944$ $-2.603776$ $46$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 1 </td <td>29</td> <td>6</td> <td>0</td> <td>3.640353</td> <td>8.314419</td> <td>4.858053</td>	29	6	0	3.640353	8.314419	4.858053
31         1         0 $1.790074$ $3.979977$ $-0.591621$ $32$ 1         0 $5.083088$ $4.856175$ $2.222837$ $33$ 1         0 $6.404943$ $4.933729$ $4.830347$ $34$ 1         0 $7.363047$ $-4.045172$ $1.781905$ $35$ 1         0 $8.645766$ $-0.357519$ $4.153789$ $36$ 1         0 $5.952483$ $-0.541964$ $6.106437$ $37$ 1         0 $-2.107953$ $-5.668055$ $3.100414$ $38$ 1         0 $-1.174328$ $-7.288766$ $0.451625$ $39$ 1         0 $2.522016$ $-7.285542$ $3.028468$ $40$ 1         0 $-1.656001$ $-2.016027$ $4.749198$ $42$ 1         0 $-3.039715$ $0.969043$ $4.439358$ $43$ 1         0 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 1         0	30	1	0	-0.123884	4.352431	2.081509
$32$ 10 $5.083088$ $4.856175$ $2.222837$ $33$ 10 $6.404943$ $-4.933729$ $4.830347$ $34$ 10 $7.363047$ $-4.045172$ $1.781905$ $35$ 10 $8.645766$ $-0.357519$ $4.153789$ $36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.28542$ $3.028468$ $40$ 10 $-4.764366$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-7.967043$ $1.138026$ $-4.454309$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7_{tddft}$ <td< td=""><td>31</td><td>1</td><td>0</td><td>1.790074</td><td>3.979977</td><td>-0.591621</td></td<>	31	1	0	1.790074	3.979977	-0.591621
$33$ 10 $6.404943$ $-4.933729$ $4.830347$ $34$ 10 $7.363047$ $-4.045172$ $1.781905$ $35$ 10 $8.645766$ $-0.357519$ $4.153789$ $36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-1.613961$ $-3.314944$ $-2.603776$ $45$ 10 $-4.998994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.957043$ $1.138026$ $-7.443776$ $55$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7_{ctddt}$ <td< td=""><td>32</td><td>1</td><td>0</td><td>5.083088</td><td>4.856175</td><td>2.222837</td></td<>	32	1	0	5.083088	4.856175	2.222837
$34$ 10 $7.363047$ $4.045172$ $1.781905$ $35$ 10 $8.645766$ $-0.357519$ $4.153789$ $36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-7.967043$ $1.138026$ $-7.443776$ $51$ 10 $-7.967043$ $1.138026$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $16^{-1}$ <t< td=""><td>33</td><td>1</td><td>0</td><td>6.404943</td><td>-4.933729</td><td>4.830347</td></t<>	33	1	0	6.404943	-4.933729	4.830347
$35$ 10 $8.645766$ $-0.357519$ $4.153789$ $36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-1.658117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.089944$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-4.79526$ $4.15444$ $-2.844307$ $52$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Origition (Ångstorns) $-7.43776$ $6$ 0 $0$ $1.395201$ $3.21451$ $1.28119$	34	1	0	7.363047	-4.045172	1.781905
$36$ 10 $5.952483$ $-0.541964$ $6.106437$ $37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $-1.658117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-7.967043$ $1.138026$ $-7.443776$ $55$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Or- $Taget order of Aborder o$	35	1	0	8.645766	-0.357519	4.153789
$37$ 10 $-2.107953$ $-5.668055$ $3.100414$ $38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7_tddft$ Standard Ori-tration (Ångstroms) $Center$ Atomic $X$ $Y$ $Z$ $0$ $6$ 0 $1.395201$ $3.21451$ $1.28119$	36	1	0	5.952483	-0.541964	6.106437
$38$ 10 $-1.174328$ $-7.288766$ $0.451625$ $39$ 10 $2.522016$ $-7.285542$ $3.028468$ $40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.65517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7_{tddft}$ Standard Orientation (Ångstroms) $Center$ Atomic $X$ $Y$ $Z$ $0$ $6$ 0 $1.395201$ $3.21451$ $1.28119$	37	1	0	-2.107953	-5.668055	3.100414
39         1         0         2.522016         -7.285542         3.028468           40         1         0         -4.764436         -1.738533         3.548071           41         1         0         -1.656001         -2.016027         4.749198           42         1         0         -3.039715         0.969043         4.439358           43         1         0         -5.418217         -0.029656         -0.988378           44         1         0         -4.497388         2.377067         0.983672           45         1         0         1.613961         -3.314944         -2.603776           46         1         0         -0.568117         -5.665517         -3.437875           47         1         0         -4.098994         0.347522         -8.659318           48         1         0         -4.187032         -3.742316         -6.967036           49         1         0         -1.793984         4.310929         -2.132293           51         1         0         -7.65552         3.009895         -7.188204           52         1         0         -8.533524         -0.182686         -7.443776	38	1	0	-1.174328	-7.288766	0.451625
$40$ 10 $-4.764436$ $-1.738533$ $3.548071$ $41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-7.65552$ $3.009895$ $-7.188204$ $52$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1.7_{tddft}$ Standard Orientation (Ångstroms) $Center$ AtomicXYZnumbernumberType $-1.395201$ $3.21451$ $1.28119$	39	1	0	2.522016	-7.285542	3.028468
$41$ 10 $-1.656001$ $-2.016027$ $4.749198$ $42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-7.65552$ $3.009895$ $-7.188204$ $52$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Center$ AtomicXYZ $number$ $number$ Type $-1.395201$ $3.21451$ $1.28119$	40	1	0	-4.764436	-1.738533	3.548071
$42$ 10 $-3.039715$ $0.969043$ $4.439358$ $43$ 10 $-5.418217$ $-0.029656$ $-0.988378$ $44$ 10 $-4.497388$ $2.377067$ $0.983672$ $45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-7.65552$ $3.009895$ $-7.188204$ $52$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Center$ AtomicXYZnumbernumberType $-1.395201$ $3.21451$ $1.28119$	41	1	0	-1.656001	-2.016027	4.749198
4310 $-5.418217$ $-0.029656$ $-0.988378$ 4410 $-4.497388$ $2.377067$ $0.983672$ 4510 $1.613961$ $-3.314944$ $-2.603776$ 4610 $-0.568117$ $-5.665517$ $-3.437875$ 4710 $-4.098994$ $0.347522$ $-8.659318$ 4810 $-4.187032$ $-3.742316$ $-6.967036$ 4910 $-5.230984$ $-2.710874$ $-3.998856$ 5010 $-1.793984$ $4.310929$ $-2.132293$ 5110 $-4.976526$ $4.15444$ $-2.844307$ 5210 $-7.65552$ $3.009895$ $-7.188204$ 5310 $-7.967043$ $1.138026$ $-4.454309$ 5410 $3.227226$ $9.966023$ $5.999363$ 5710 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Z$ CenterAtomicXYZnumbernumberType $-1.395201$ $3.21451$ $1.28119$	42	1	0	-3.039715	0.969043	4.439358
4410 $-4.497388$ $2.377067$ $0.983672$ 4510 $1.613961$ $-3.314944$ $-2.603776$ 4610 $-0.568117$ $-5.665517$ $-3.437875$ 4710 $-4.098994$ $0.347522$ $-8.659318$ 4810 $-4.187032$ $-3.742316$ $-6.967036$ 4910 $-5.230984$ $-2.710874$ $-3.998856$ 5010 $-1.793984$ $4.310929$ $-2.132293$ 5110 $-4.976526$ $4.15444$ $-2.844307$ 5210 $-7.65552$ $3.009895$ $-7.188204$ 5310 $-7.967043$ $1.138026$ $-4.454309$ 5410 $8.533524$ $-0.182686$ $-7.443776$ 5510 $3.227226$ $9.966023$ $5.999363$ 5710 $5.64185$ $8.295592$ $4.397522$ $\mathbf{1-7\_tddft}$ Standard Orientation (Ångstroms) $\mathbf{Z}$ CenterAtomic $\mathbf{X}$ $\mathbf{Y}$ $\mathbf{Z}$ numbernumberType $ -$ 0 $6$ 0 $1.395201$ $3.21451$ $1.28119$	43	1	0	-5.418217	-0.029656	-0.988378
$45$ 10 $1.613961$ $-3.314944$ $-2.603776$ $46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Z$ CenterAtomicXYZnumbernumberType $U$ 0 $6$ 0 $1.395201$ $3.21451$ $1.28119$	44	1	0	-4.497388	2.377067	0.983672
$46$ 10 $-0.568117$ $-5.665517$ $-3.437875$ $47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Center$ AtomicXYZ $0$ $6$ 0 $1.395201$ $3.21451$ $1.28119$	45	1	0	1.613961	-3.314944	-2.603776
$47$ 10 $-4.098994$ $0.347522$ $-8.659318$ $48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms) $Center$ AtomicXYZnumbernumberType $-1.395201$ $3.21451$ $1.28119$	46	1	0	-0.568117	-5.665517	-3.437875
$48$ 10 $-4.187032$ $-3.742316$ $-6.967036$ $49$ 10 $-5.230984$ $-2.710874$ $-3.998856$ $50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType1.28119	47	1	0	-4.098994	0.347522	-8.659318
4910 $-5.230984$ $-2.710874$ $-3.998856$ 5010 $-1.793984$ $4.310929$ $-2.132293$ 5110 $-4.976526$ $4.15444$ $-2.844307$ 5210 $-7.65552$ $3.009895$ $-7.188204$ 5310 $-7.967043$ $1.138026$ $-4.454309$ 5410 $-8.533524$ $-0.182686$ $-7.443776$ 5510 $2.506556$ $8.376124$ $3.147517$ 5610 $3.227226$ $9.966023$ $5.999363$ 5710 $5.64185$ $8.295592$ $4.397522$ <b>1-7_tddft</b> Standard Orientation (Ångstroms)CenterAtomicXYZ060 $1.395201$ $3.21451$ $1.28119$	48	1	0	-4.187032	-3.742316	-6.967036
$50$ 10 $-1.793984$ $4.310929$ $-2.132293$ $51$ 10 $-4.976526$ $4.15444$ $-2.844307$ $52$ 10 $-7.65552$ $3.009895$ $-7.188204$ $53$ 10 $-7.967043$ $1.138026$ $-4.454309$ $54$ 10 $-8.533524$ $-0.182686$ $-7.443776$ $55$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType1.28119	49	1	0	-5.230984	-2.710874	-3.998856
$51$ 10-4.9765264.15444-2.844307 $52$ 10-7.65552 $3.009895$ -7.188204 $53$ 10-7.967043 $1.138026$ -4.454309 $54$ 10-8.533524-0.182686-7.443776 $55$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType1.28119	50	1	0	-1.793984	4.310929	-2.132293
$52$ 10-7.65552 $3.009895$ -7.188204 $53$ 10-7.967043 $1.138026$ - $4.454309$ $54$ 10- $8.533524$ - $0.182686$ - $7.443776$ $55$ 10 $2.506556$ $8.376124$ $3.147517$ $56$ 10 $3.227226$ $9.966023$ $5.999363$ $57$ 10 $5.64185$ $8.295592$ $4.397522$ $1-7\_tddft$ Standard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType060 $1.395201$ $3.21451$ $1.28119$	51	1	0	-4.976526	4.15444	-2.844307
5310 $-7.967043$ $1.138026$ $-4.454309$ 5410 $-8.533524$ $-0.182686$ $-7.443776$ 5510 $2.506556$ $8.376124$ $3.147517$ 5610 $3.227226$ $9.966023$ $5.999363$ 5710 $5.64185$ $8.295592$ $4.397522$ I-7_tddftStandard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType060 $1.395201$ $3.21451$ $1.28119$	52	1	0	-7.65552	3.009895	-7.188204
	53	1	0	-7.967043	1.138026	-4.454309
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	54	1	0	-8.533524	-0.182686	-7.443776
56         1         0         3.227226         9.966023         5.999363           57         1         0         5.64185         8.295592         4.397522           1-7_tddft         Standard Orientation (Ångstroms)           Center         Atomic         X         Y         Z           number         number         Type         1.395201         3.21451         1.28119	55	1	0	2.506556	8.376124	3.147517
	56	1	0	3.227226	9.966023	5.999363
1-7_tddftStandard Orientation (Ångstroms)CenterAtomicXYZnumbernumberType0601.3952013.214511.28119	57	1	0	5.64185	8.295592	4.397522
Center numberAtomic numberXYZ0601.3952013.214511.28119	1-7_tddft Standard Orientation (Ångstroms)					
number         number         Type	Center	Atomic	Atomic	X	Y	Ζ
0 6 0 1.395201 3.21451 1.28119	number	number	Туре			
	0	6	0	1.395201	3.21451	1.28119

1	6	0	0.768245	0.429312	1.162884
2	6	0	2.830481	-0.903972	1.768163
3	6	0	5.079675	0.740663	2.318615
4	6	0	3.885214	3.328472	2.875907
5	6	0	3.388893	-3.499418	2.396709
6	6	0	6.100637	-3.545448	3.341528
7	6	0	6.640244	-0.815306	4.190864
8	6	0	-1.836632	-0.649854	0.842622
9	6	0	-1.782928	-3.395034	-0.29206
10	6	0	-0.859869	-5.51237	1.461845
11	6	0	1.818028	-5.484419	2.336385
12	6	0	-2.885736	-0.884448	3.562062
13	6	0	-3.795571	1.139372	-0.504504
14	6	0	-0.385935	-3.712283	-2.814499
15	7	0	-1.36213	-2.049046	-4.748543
16	6	0	-2.624228	2.066951	-5.364097
17	6	0	-0.421773	0.328247	-4.988461
18	6	0	-4.5829	0.371886	-6.653638
19	6	0	-3.989978	-2.241852	-5.569623
20	6	0	-3.27441	3.000967	-2.68497
21	8	0	1.809656	0.939913	-4.674824
22	6	0	-7.328818	1.131145	-6.409703
23	1	0	-2.143731	3.703928	-6.512032
24	1	0	-3.763687	-3.854813	-0.635238
25	1	0	6.199441	0.972466	0.590459
26	6	0	3.123021	3.772939	5.570538
27	8	0	2.484672	2.13035	7.052404
28	8	0	2.976309	6.182681	6.421109
29	6	0	3.640353	8.314419	4.858053
30	1	0	-0.123884	4.352431	2.081509
31	1	0	1.790074	3.979977	-0.591621
32	1	0	5.083088	4.856175	2.222837
33	1	0	6.404943	-4.933729	4.830347
34	1	0	7.363047	-4.045172	1.781905
35	1	0	8.645766	-0.357519	4.153789
36	1	0	5.952483	-0.541964	6.106437
37	1	0	-2.107953	-5.668055	3.100414
38	1	0	-1.174328	-7.288766	0.451625
39	1	0	2.522016	-7.285542	3.028468
40	1	0	-4.764436	-1.738533	3.548071
41	1	0	-1.656001	-2.016027	4.749198
42	1	0	-3.039715	0.969043	4.439358
43	1	0	-5.418217	-0.029656	-0.988378

44	1	0	-4.497388	2.377067	0.983672
45	1	0	1.613961	-3.314944	-2.603776
46	1	0	-0.568117	-5.665517	-3.437875
47	1	0	-4.098994	0.347522	-8.659318
48	1	0	-4.187032	-3.742316	-6.967036
49	1	0	-5.230984	-2.710874	-3.998856
50	1	0	-1.793984	4.310929	-2.132293
51	1	0	-4.976526	4.15444	-2.844307
52	1	0	-7.65552	3.009895	-7.188204
53	1	0	-7.967043	1.138026	-4.454309
54	1	0	-8.533524	-0.182686	-7.443776
55	1	0	2.506556	8.376124	3.147517
56	1	0	3.227226	9.966023	5.999363
57	1	0	5.64185	8.295592	4.397522
1-8_en	·	Standard Ori	entation (Ångs	troms)	·
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	0.7328	3.334989	1.149382
1	6	0	0.368644	0.510719	1.007963
2	6	0	2.511533	-0.637842	1.707825
3	6	0	4.60669	1.178871	2.329741
4	6	0	3.174249	3.719042	2.699637
5	6	0	3.230371	-3.173795	2.42381
6	6	0	5.833	-2.973965	3.617082
7	6	0	6.054068	-0.192113	4.427858
8	6	0	-2.098948	-0.80966	0.529729
9	6	0	-1.709173	-3.518169	-0.631966
10	6	0	-0.722563	-5.571535	1.160943
11	6	0	1.853397	-5.291854	2.262678
12	6	0	-3.281767	-1.18663	3.175363
13	6	0	-4.142265	0.798375	-0.922735
14	6	0	-0.110945	-3.64886	-3.049463
15	7	0	-1.114111	-2.05835	-5.032042
16	6	0	-2.752366	1.917323	-5.691651
17	6	0	-0.409691	0.407832	-5.185997
18	6	0	-4.426483	0.05114	-7.135301
19	6	0	-3.654267	-2.498037	-6.01738
20	6	0	-3.687769	2.730889	-3.057667
21	8	0	1.723544	1.238062	-4.728754
22	6	0	-7.245976	0.521578	-7.099397
23	1	0	-2.367773	3.615872	-6.785081
24	1	0	-3.606216	-4.158362	-1.124184
25	1	0	5.866224	1.400883	0.703679

26	6	0	2.640038	4.155617	5.448896
27	8	0	0.737688	3.43574	6.530791
28	8	0	4.391152	5.341804	6.877128
29	6	0	6.653762	6.399655	5.784428
30	1	0	-0.879188	4.306075	1.982033
31	1	0	1.019737	4.134277	-0.72756
32	1	0	4.263545	5.286897	1.953487
33	1	0	6.105867	-4.294764	5.171174
34	1	0	7.282492	-3.391587	2.203352
35	1	0	8.007483	0.416257	4.630961
36	1	0	5.115612	0.062941	6.246213
37	1	0	-2.079932	-5.885061	2.686086
38	1	0	-0.772249	-7.349127	0.104553
39	1	0	2.650384	-7.013914	3.048751
40	1	0	-5.057566	-2.230031	3.039015
41	1	0	-2.016908	-2.201735	4.430596
42	1	0	-3.677734	0.629885	4.051181
43	1	0	-5.609945	-0.519825	-1.507915
44	1	0	-5.047085	1.947304	0.527891
45	1	0	1.819009	-3.058757	-2.689322
46	1	0	-0.050421	-5.598907	-3.706515
47	1	0	-3.792588	0.099294	-9.098741
48	1	0	-3.622244	-4.005618	-7.420202
49	1	0	-4.939061	-3.080547	-4.521976
50	1	0	-2.414346	4.195569	-2.392754
51	1	0	-5.495364	3.686185	-3.328722
52	1	0	-8.033542	0.433123	-5.200494
53	1	0	-8.223873	-0.893975	-8.233956
54	1	0	-7.704393	2.367646	-7.889718
55	1	0	6.192738	7.971178	4.54428
56	1	0	7.74745	7.089112	7.374438
57	1	0	7.746066	4.985822	4.77637
1-8_tddft		Standard Or	ientation (Ångs	stroms)	
Center	Atomic	Atomic	X	Y	Ζ
number	number	Туре			
0	6	0	0.7328	3.334989	1.149382
1	6	0	0.368644	0.510719	1.007963
2	6	0	2.511533	-0.637842	1.707825
3	6	0	4.60669	1.178871	2.329741
4	6	0	3.174249	3.719042	2.699637
5	6	0	3.230371	-3.173795	2.42381
6	6	0	5.833	-2.973965	3.617082
7	6	0	6.054068	-0.192113	4.427858

8	6	0	-2.098948	-0.80966	0.529729
9	6	0	-1.709173	-3.518169	-0.631966
10	6	0	-0.722563	-5.571535	1.160943
11	6	0	1.853397	-5.291854	2.262678
12	6	0	-3.281767	-1.18663	3.175363
13	6	0	-4.142265	0.798375	-0.922735
14	6	0	-0.110945	-3.64886	-3.049463
15	7	0	-1.114111	-2.05835	-5.032042
16	6	0	-2.752366	1.917323	-5.691651
17	6	0	-0.409691	0.407832	-5.185997
18	6	0	-4.426483	0.05114	-7.135301
19	6	0	-3.654267	-2.498037	-6.01738
20	6	0	-3.687769	2.730889	-3.057667
21	8	0	1.723544	1.238062	-4.728754
22	6	0	-7.245976	0.521578	-7.099397
23	1	0	-2.367773	3.615872	-6.785081
24	1	0	-3.606216	-4.158362	-1.124184
25	1	0	5.866224	1.400883	0.703679
26	6	0	2.640038	4.155617	5.448896
27	8	0	0.737688	3.43574	6.530791
28	8	0	4.391152	5.341804	6.877128
29	6	0	6.653762	6.399655	5.784428
30	1	0	-0.879188	4.306075	1.982033
31	1	0	1.019737	4.134277	-0.72756
32	1	0	4.263545	5.286897	1.953487
33	1	0	6.105867	-4.294764	5.171174
34	1	0	7.282492	-3.391587	2.203352
35	1	0	8.007483	0.416257	4.630961
36	1	0	5.115612	0.062941	6.246213
37	1	0	-2.079932	-5.885061	2.686086
38	1	0	-0.772249	-7.349127	0.104553
39	1	0	2.650384	-7.013914	3.048751
40	1	0	-5.057566	-2.230031	3.039015
41	1	0	-2.016908	-2.201735	4.430596
42	1	0	-3.677734	0.629885	4.051181
43	1	0	-5.609945	-0.519825	-1.507915
44	1	0	-5.047085	1.947304	0.527891
45	1	0	1.819009	-3.058757	-2.689322
46	1	0	-0.050421	-5.598907	-3.706515
47	1	0	-3.792588	0.099294	-9.098741
48	1	0	-3.622244	-4.005618	-7.420202
49	1	0	-4.939061	-3.080547	-4.521976
50	1	0	-2.414346	4.195569	-2.392754

51	1	0	-5.495364	3.686185	-3.328722
52	1	0	-8.033542	0.433123	-5.200494
53	1	0	-8.223873	-0.893975	-8.233956
54	1	0	-7.704393	2.367646	-7.889718
55	1	0	6.192738	7.971178	4.54428
56	1	0	7.74745	7.089112	7.374438
57	1	0	7.746066	4.985822	4.77637
1-9_en		Standard Ori	entation (Ångs	troms)	
Center	Atomic	Atomic	Х	Υ	Ζ
number	number	Туре			
0	6	0	0.716635	3.048718	1.720304
1	6	0	0.455151	0.247321	1.263386
2	6	0	2.676597	-0.881757	1.698324
3	6	0	4.741069	0.933938	2.414012
4	6	0	3.253989	3.369612	3.125567
5	6	0	3.518071	-3.452317	2.086375
6	6	0	6.170536	-3.281017	3.16905
7	6	0	6.328034	-0.602207	4.284914
8	6	0	-1.988441	-1.114912	0.778263
9	6	0	-1.57647	-3.648375	-0.718337
10	6	0	-0.415107	-5.852321	0.762761
11	6	0	2.20533	-5.59205	1.759957
12	6	0	-2.984037	-1.841045	3.430499
13	6	0	-4.175855	0.564775	-0.341409
14	6	0	-0.117245	-3.427535	-3.215816
15	7	0	-1.296091	-1.668204	-4.941345
16	6	0	-3.13478	2.271723	-5.037474
17	6	0	-0.706026	0.829284	-4.838379
18	6	0	-4.81045	0.509237	-6.603776
19	6	0	-3.865104	-2.114485	-5.845594
20	6	0	-3.940426	2.733144	-2.278106
21	8	0	1.412795	1.70404	-4.396162
22	6	0	-7.640268	0.83176	-6.354881
23	1	0	-2.884582	4.102714	-5.93919
24	1	0	-3.474107	-4.305686	-1.183522
25	1	0	5.917504	1.373212	0.770027
26	6	0	2.918141	3.522831	5.935169
27	8	0	1.128606	2.629154	7.078721
28	8	0	4.740881	4.627635	7.338442
29	6	0	6.871384	5.878936	6.184512
30	1	0	-0.864353	3.825206	2.785566
31	1	0	0.814733	4.082692	-0.058606
32	1	0	4.238574	5.03927	2.460864
h					

33	1	0	6.573336	-4.757837	4.543913
34	1	0	7.557769	-3.469918	1.648038
35	1	0	8.264836	0.058699	4.482173
36	1	0	5.455905	-0.594924	6.153574
37	1	0	-1.673621	-6.402726	2.305926
38	1	0	-0.454403	-7.49483	-0.494165
39	1	0	3.099548	-7.357101	2.311076
40	1	0	-4.742012	-2.912317	3.283266
41	1	0	-1.618447	-2.962625	4.471843
42	1	0	-3.358525	-0.152147	4.540043
43	1	0	-5.648744	-0.737589	-0.949842
44	1	0	-4.995041	1.522114	1.288497
45	1	0	1.804823	-2.794196	-2.889789
46	1	0	-0.018435	-5.284145	-4.099234
47	1	0	-4.297358	0.820615	-8.578185
48	1	0	-3.841027	-3.43932	-7.42246
49	1	0	-5.040185	-2.93856	-4.374701
50	1	0	-2.691334	4.178927	-1.528845
51	1	0	-5.801756	3.620381	-2.332678
52	1	0	-8.300317	0.463758	-4.441476
53	1	0	-8.625586	-0.476562	-7.605664
54	1	0	-8.223258	2.737837	-6.873334
55	1	0	6.263214	7.576667	5.200125
56	1	0	8.099535	6.398136	7.740515
57	1	0	7.887546	4.636074	4.907432
1-9_tddft	•	Standard Or	ientation (Ångs	stroms)	•
Center	Atomic	Atomic	Х	Y	Ζ
number	number	Туре			
0	6	0	0.716635	3.048718	1.720304
1	6	0	0.455151	0.247321	1.263386
2	6	0	2.676597	-0.881757	1.698324
3	6	0	4.741069	0.933938	2.414012
4	6	0	3.253989	3.369612	3.125567
5	6	0	3.518071	-3.452317	2.086375
6	6	0	6.170536	-3.281017	3.16905
7	6	0	6.328034	-0.602207	4.284914
8	6	0	-1.988441	-1.114912	0.778263
9	6	0	-1.57647	-3.648375	-0.718337
10	6	0	-0.415107	-5.852321	0.762761
11	6	0	2.20533	-5.59205	1.759957
12	6	0	-2.984037	-1.841045	3.430499
13	6	0	-4.175855	0.564775	-0.341409
1/	6	0	-0.117245	-3.427535	-3.215816

-	1	1	1	1	l.
15	7	0	-1.296091	-1.668204	-4.941345
16	6	0	-3.13478	2.271723	-5.037474
17	6	0	-0.706026	0.829284	-4.838379
18	6	0	-4.81045	0.509237	-6.603776
19	6	0	-3.865104	-2.114485	-5.845594
20	6	0	-3.940426	2.733144	-2.278106
21	8	0	1.412795	1.70404	-4.396162
22	6	0	-7.640268	0.83176	-6.354881
23	1	0	-2.884582	4.102714	-5.93919
24	1	0	-3.474107	-4.305686	-1.183522
25	1	0	5.917504	1.373212	0.770027
26	6	0	2.918141	3.522831	5.935169
27	8	0	1.128606	2.629154	7.078721
28	8	0	4.740881	4.627635	7.338442
29	6	0	6.871384	5.878936	6.184512
30	1	0	-0.864353	3.825206	2.785566
31	1	0	0.814733	4.082692	-0.058606
32	1	0	4.238574	5.03927	2.460864
33	1	0	6.573336	-4.757837	4.543913
34	1	0	7.557769	-3.469918	1.648038
35	1	0	8.264836	0.058699	4.482173
36	1	0	5.455905	-0.594924	6.153574
37	1	0	-1.673621	-6.402726	2.305926
38	1	0	-0.454403	-7.49483	-0.494165
39	1	0	3.099548	-7.357101	2.311076
40	1	0	-4.742012	-2.912317	3.283266
41	1	0	-1.618447	-2.962625	4.471843
42	1	0	-3.358525	-0.152147	4.540043
43	1	0	-5.648744	-0.737589	-0.949842
44	1	0	-4.995041	1.522114	1.288497
45	1	0	1.804823	-2.794196	-2.889789
46	1	0	-0.018435	-5.284145	-4.099234
47	1	0	-4.297358	0.820615	-8.578185
48	1	0	-3.841027	-3.43932	-7.42246
49	1	0	-5.040185	-2.93856	-4.374701
50	1	0	-2.691334	4.178927	-1.528845
51	1	0	-5.801756	3.620381	-2.332678
52	1	0	-8.300317	0.463758	-4.441476
53	1	0	-8.625586	-0.476562	-7.605664
54	1	0	-8.223258	2.737837	-6.873334
55	1	0	6.263214	7.576667	5.200125
56	1	0	8.099535	6.398136	7.740515
57	1	0	7.887546	4.636074	4.907432
L					