

SUPPLEMENTARY MATERIAL S1

RUBESCIN E GEOMETRIC PARAMETER

Optimized parameters

1. opt=tight hf/6-311++g(d,p) nosymm

! Optimized Parameters !				
! (Angstroms and Degrees) !				

! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.5503	-DE/DX = 0.0	!
! R2	R(1,3)	1.5698	-DE/DX = 0.0	!
! R3	R(1,20)	1.5167	-DE/DX = 0.0	!
! R4	R(1,22)	1.5474	-DE/DX = 0.0	!
! R5	R(2,7)	1.19	-DE/DX = 0.0	!
! R6	R(2,34)	1.5041	-DE/DX = 0.0	!
! R7	R(3,4)	1.5898	-DE/DX = 0.0	!
! R8	R(3,40)	1.4814	-DE/DX = 0.0	!
! R9	R(3,59)	1.3994	-DE/DX = 0.0	!
! R10	R(4,5)	1.5515	-DE/DX = 0.0	!
! R11	R(4,12)	1.5707	-DE/DX = 0.0	!
! R12	R(4,36)	1.5501	-DE/DX = 0.0	!
! R13	R(5,6)	1.5428	-DE/DX = 0.0	!
! R14	R(5,46)	1.4556	-DE/DX = 0.0	!
! R15	R(5,61)	1.4206	-DE/DX = 0.0	!
! R16	R(6,26)	1.5259	-DE/DX = 0.0	!
! R17	R(6,42)	1.5352	-DE/DX = 0.0	!
! R18	R(6,51)	1.5703	-DE/DX = 0.0	!
! R19	R(8,16)	1.5423	-DE/DX = 0.0	!
! R20	R(8,20)	1.5256	-DE/DX = 0.0	!
! R21	R(8,29)	1.5405	-DE/DX = 0.0	!
! R22	R(8,32)	1.5036	-DE/DX = 0.0	!
! R23	R(9,10)	1.0829	-DE/DX = 0.0	!
! R24	R(9,11)	1.412	-DE/DX = 0.0	!
! R25	R(9,12)	1.5288	-DE/DX = 0.0	!
! R26	R(9,20)	1.4997	-DE/DX = 0.0	!
! R27	R(11,29)	1.4261	-DE/DX = 0.0	!
! R28	R(12,13)	1.0811	-DE/DX = 0.0	!
! R29	R(12,60)	1.4104	-DE/DX = 0.0	!
! R30	R(14,51)	1.5035	-DE/DX = 0.0	!
! R31	R(14,53)	1.4493	-DE/DX = 0.0	!
! R32	R(14,57)	1.3411	-DE/DX = 0.0	!
! R33	R(15,55)	1.3382	-DE/DX = 0.0	!
! R34	R(15,57)	1.3467	-DE/DX = 0.0	!
! R35	R(16,17)	1.0867	-DE/DX = 0.0	!
! R36	R(16,18)	1.0847	-DE/DX = 0.0	!
! R37	R(16,19)	1.0801	-DE/DX = 0.0	!
! R38	R(20,21)	1.0877	-DE/DX = 0.0	!

! R39	R(22,23)	1.0823	-DE/DX = 0.0	!
! R40	R(22,24)	1.0817	-DE/DX = 0.0	!
! R41	R(22,25)	1.0804	-DE/DX = 0.0	!
! R42	R(26,27)	1.0852	-DE/DX = 0.0	!
! R43	R(26,28)	1.0849	-DE/DX = 0.0	!
! R44	R(26,40)	1.5162	-DE/DX = 0.0	!
! R45	R(29,30)	1.0847	-DE/DX = 0.0	!
! R46	R(29,31)	1.0824	-DE/DX = 0.0	!
! R47	R(32,33)	1.079	-DE/DX = 0.0	!
! R48	R(32,34)	1.327	-DE/DX = 0.0	!
! R49	R(34,35)	1.0757	-DE/DX = 0.0	!
! R50	R(36,37)	1.0831	-DE/DX = 0.0	!
! R51	R(36,38)	1.0769	-DE/DX = 0.0	!
! R52	R(36,39)	1.0814	-DE/DX = 0.0	!
! R53	R(40,41)	1.0705	-DE/DX = 0.0	!
! R54	R(40,59)	1.401	-DE/DX = 0.0	!
! R55	R(42,43)	1.0839	-DE/DX = 0.0	!
! R56	R(42,44)	1.0814	-DE/DX = 0.0	!
! R57	R(42,45)	1.0801	-DE/DX = 0.0	!
! R58	R(46,47)	1.0753	-DE/DX = 0.0	!
! R59	R(46,48)	1.5086	-DE/DX = 0.0	!
! R60	R(46,61)	1.4005	-DE/DX = 0.0	!
! R61	R(48,49)	1.0854	-DE/DX = 0.0	!
! R62	R(48,50)	1.0863	-DE/DX = 0.0	!
! R63	R(48,51)	1.5407	-DE/DX = 0.0	!
! R64	R(51,52)	1.0819	-DE/DX = 0.0	!
! R65	R(53,54)	1.0706	-DE/DX = 0.0	!
! R66	R(53,55)	1.3381	-DE/DX = 0.0	!
! R67	R(55,56)	1.0688	-DE/DX = 0.0	!
! R68	R(57,58)	1.0679	-DE/DX = 0.0	!
! R69	R(60,62)	1.3485	-DE/DX = 0.0	!
! R70	R(62,63)	1.5033	-DE/DX = 0.0	!
! R71	R(62,65)	1.181	-DE/DX = 0.0	!
! R72	R(63,64)	1.3222	-DE/DX = 0.0	!
! R73	R(63,71)	1.5153	-DE/DX = 0.0	!
! R74	R(64,66)	1.0764	-DE/DX = 0.0	!
! R75	R(64,67)	1.5001	-DE/DX = 0.0	!
! R76	R(67,68)	1.0821	-DE/DX = 0.0	!
! R77	R(67,69)	1.087	-DE/DX = 0.0	!
! R78	R(67,70)	1.0873	-DE/DX = 0.0	!
! R79	R(71,72)	1.0826	-DE/DX = 0.0	!
! R80	R(71,73)	1.0865	-DE/DX = 0.0	!
! R81	R(71,74)	1.0827	-DE/DX = 0.0	!
! A1	A(2,1,3)	115.3869	-DE/DX = 0.0	!
! A2	A(2,1,20)	104.9116	-DE/DX = 0.0	!
! A3	A(2,1,22)	104.6632	-DE/DX = 0.0	!
! A4	A(3,1,20)	105.4487	-DE/DX = 0.0	!
! A5	A(3,1,22)	110.0598	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.6507	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.6712	-DE/DX = 0.0	!
! A8	A(1,2,34)	118.8294	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.3115	-DE/DX = 0.0	!

! A10	A(1,3,4)	117.4677	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.4116	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.5239	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.7989	-DE/DX = 0.0	!
! A14	A(4,3,59)	110.9192	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.2815	-DE/DX = 0.0	!
! A16	A(3,4,12)	116.9097	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.3533	-DE/DX = 0.0	!
! A18	A(5,4,12)	110.9502	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.2096	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.7402	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.3963	-DE/DX = 0.0	!
! A22	A(4,5,46)	126.1434	-DE/DX = 0.0	!
! A23	A(4,5,61)	113.7557	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.4092	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.3436	-DE/DX = 0.0	!
! A26	A(5,6,26)	106.9225	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.7934	-DE/DX = 0.0	!
! A28	A(5,6,51)	101.8612	-DE/DX = 0.0	!
! A29	A(26,6,42)	108.8679	-DE/DX = 0.0	!
! A30	A(26,6,51)	113.8205	-DE/DX = 0.0	!
! A31	A(42,6,51)	110.5307	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.8467	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.395	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.5455	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.3773	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.3315	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.2843	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.4342	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.1563	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.4351	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.2108	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.336	-DE/DX = 0.0	!
! A43	A(12,9,20)	109.2549	-DE/DX = 0.0	!
! A44	A(9,11,29)	111.1841	-DE/DX = 0.0	!
! A45	A(4,12,9)	110.4259	-DE/DX = 0.0	!
! A46	A(4,12,13)	107.0388	-DE/DX = 0.0	!
! A47	A(4,12,60)	111.1499	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.1207	-DE/DX = 0.0	!
! A49	A(9,12,60)	109.0864	-DE/DX = 0.0	!
! A50	A(13,12,60)	108.9921	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.042	-DE/DX = 0.0	!
! A52	A(51,14,57)	129.3418	-DE/DX = 0.0	!
! A53	A(53,14,57)	104.5893	-DE/DX = 0.0	!
! A54	A(55,15,57)	107.1084	-DE/DX = 0.0	!
! A55	A(8,16,17)	108.9763	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.4211	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.6942	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.3927	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.4116	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.7317	-DE/DX = 0.0	!
! A61	A(1,20,8)	121.1479	-DE/DX = 0.0	!

! A62	A(1,20,9)	118.7226	-DE/DX = 0.0	!
! A63	A(1,20,21)	103.9684	-DE/DX = 0.0	!
! A64	A(8,20,9)	103.812	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.8648	-DE/DX = 0.0	!
! A66	A(9,20,21)	103.9251	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.2273	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.4028	-DE/DX = 0.0	!
! A69	A(1,22,25)	108.9904	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.6973	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.5798	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.8015	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.4567	-DE/DX = 0.0	!
! A74	A(6,26,28)	110.7901	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.4945	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.7426	-DE/DX = 0.0	!
! A77	A(27,26,40)	108.8133	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.4113	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.4386	-DE/DX = 0.0	!
! A80	A(8,29,30)	112.144	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.6297	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.4369	-DE/DX = 0.0	!
! A83	A(11,29,31)	107.748	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.2024	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.7184	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.4664	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.714	-DE/DX = 0.0	!
! A88	A(2,34,32)	125.2907	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.2592	-DE/DX = 0.0	!
! A90	A(32,34,35)	121.3309	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.5187	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.7606	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.3595	-DE/DX = 0.0	!
! A94	A(37,36,38)	107.9887	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.4908	-DE/DX = 0.0	!
! A96	A(38,36,39)	108.5956	-DE/DX = 0.0	!
! A97	A(3,40,26)	124.7594	-DE/DX = 0.0	!
! A98	A(3,40,41)	116.9557	-DE/DX = 0.0	!
! A99	A(26,40,41)	114.7114	-DE/DX = 0.0	!
! A100	A(26,40,59)	116.1404	-DE/DX = 0.0	!
! A101	A(41,40,59)	112.6418	-DE/DX = 0.0	!
! A102	A(6,42,43)	108.6831	-DE/DX = 0.0	!
! A103	A(6,42,44)	112.6617	-DE/DX = 0.0	!
! A104	A(6,42,45)	112.2871	-DE/DX = 0.0	!
! A105	A(43,42,44)	107.7832	-DE/DX = 0.0	!
! A106	A(43,42,45)	107.9888	-DE/DX = 0.0	!
! A107	A(44,42,45)	107.2453	-DE/DX = 0.0	!
! A108	A(5,46,47)	123.8413	-DE/DX = 0.0	!
! A109	A(5,46,48)	110.0006	-DE/DX = 0.0	!
! A110	A(47,46,48)	120.8648	-DE/DX = 0.0	!
! A111	A(47,46,61)	115.3262	-DE/DX = 0.0	!
! A112	A(48,46,61)	111.574	-DE/DX = 0.0	!
! A113	A(46,48,49)	112.4899	-DE/DX = 0.0	!

! A114 A(46,48,50)	109.6211	-DE/DX = 0.0	!
! A115 A(46,48,51)	102.6704	-DE/DX = 0.0	!
! A116 A(49,48,50)	107.9435	-DE/DX = 0.0	!
! A117 A(49,48,51)	111.84	-DE/DX = 0.0	!
! A118 A(50,48,51)	112.2754	-DE/DX = 0.0	!
! A119 A(6,51,14)	116.8638	-DE/DX = 0.0	!
! A120 A(6,51,48)	104.4966	-DE/DX = 0.0	!
! A121 A(6,51,52)	106.7226	-DE/DX = 0.0	!
! A122 A(14,51,48)	114.9685	-DE/DX = 0.0	!
! A123 A(14,51,52)	106.5843	-DE/DX = 0.0	!
! A124 A(48,51,52)	106.525	-DE/DX = 0.0	!
! A125 A(14,53,54)	127.4874	-DE/DX = 0.0	!
! A126 A(14,53,55)	106.1668	-DE/DX = 0.0	!
! A127 A(54,53,55)	126.3432	-DE/DX = 0.0	!
! A128 A(15,55,53)	110.7484	-DE/DX = 0.0	!
! A129 A(15,55,56)	116.5608	-DE/DX = 0.0	!
! A130 A(53,55,56)	132.6897	-DE/DX = 0.0	!
! A131 A(14,57,15)	111.3857	-DE/DX = 0.0	!
! A132 A(14,57,58)	132.9248	-DE/DX = 0.0	!
! A133 A(15,57,58)	115.6894	-DE/DX = 0.0	!
! A134 A(12,60,62)	123.1805	-DE/DX = 0.0	!
! A135 A(60,62,63)	118.3342	-DE/DX = 0.0	!
! A136 A(60,62,65)	118.3753	-DE/DX = 0.0	!
! A137 A(63,62,65)	123.0766	-DE/DX = 0.0	!
! A138 A(62,63,64)	116.9655	-DE/DX = 0.0	!
! A139 A(62,63,71)	117.8479	-DE/DX = 0.0	!
! A140 A(64,63,71)	125.0717	-DE/DX = 0.0	!
! A141 A(63,64,66)	117.3417	-DE/DX = 0.0	!
! A142 A(63,64,67)	127.2664	-DE/DX = 0.0	!
! A143 A(66,64,67)	115.3855	-DE/DX = 0.0	!
! A144 A(64,67,68)	113.2223	-DE/DX = 0.0	!
! A145 A(64,67,69)	109.8634	-DE/DX = 0.0	!
! A146 A(64,67,70)	109.9936	-DE/DX = 0.0	!
! A147 A(68,67,69)	108.1249	-DE/DX = 0.0	!
! A148 A(68,67,70)	108.4163	-DE/DX = 0.0	!
! A149 A(69,67,70)	107.0102	-DE/DX = 0.0	!
! A150 A(63,71,72)	110.8165	-DE/DX = 0.0	!
! A151 A(63,71,73)	112.6001	-DE/DX = 0.0	!
! A152 A(63,71,74)	110.4594	-DE/DX = 0.0	!
! A153 A(72,71,73)	107.8589	-DE/DX = 0.0	!
! A154 A(72,71,74)	107.2862	-DE/DX = 0.0	!
! A155 A(73,71,74)	107.6085	-DE/DX = 0.0	!
! D1 D(3,1,2,7)	-54.0251	-DE/DX = 0.0	!
! D2 D(3,1,2,34)	131.0437	-DE/DX = 0.0	!
! D3 D(20,1,2,7)	-169.5876	-DE/DX = 0.0	!
! D4 D(20,1,2,34)	15.4811	-DE/DX = 0.0	!
! D5 D(22,1,2,7)	67.0805	-DE/DX = 0.0	!
! D6 D(22,1,2,34)	-107.8507	-DE/DX = 0.0	!
! D7 D(2,1,3,4)	-153.6797	-DE/DX = 0.0	!
! D8 D(2,1,3,40)	8.9874	-DE/DX = 0.0	!
! D9 D(2,1,3,59)	74.6238	-DE/DX = 0.0	!
! D10 D(20,1,3,4)	-38.4239	-DE/DX = 0.0	!

! D11	D(20,1,3,40)	124.2431	-DE/DX = 0.0	!
! D12	D(20,1,3,59)	-170.1205	-DE/DX = 0.0	!
! D13	D(22,1,3,4)	88.1837	-DE/DX = 0.0	!
! D14	D(22,1,3,40)	-109.1492	-DE/DX = 0.0	!
! D15	D(22,1,3,59)	-43.5128	-DE/DX = 0.0	!
! D16	D(2,1,20,8)	-50.1404	-DE/DX = 0.0	!
! D17	D(2,1,20,9)	179.3716	-DE/DX = 0.0	!
! D18	D(2,1,20,21)	64.5944	-DE/DX = 0.0	!
! D19	D(3,1,20,8)	-172.4093	-DE/DX = 0.0	!
! D20	D(3,1,20,9)	57.1027	-DE/DX = 0.0	!
! D21	D(3,1,20,21)	-57.6746	-DE/DX = 0.0	!
! D22	D(22,1,20,8)	65.1207	-DE/DX = 0.0	!
! D23	D(22,1,20,9)	-65.3673	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	179.8555	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	39.5213	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	160.3755	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-78.9254	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	164.0854	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-75.0604	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	45.6387	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-75.8783	-DE/DX = 0.0	!
! D32	D(20,1,22,24)	44.9759	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	165.675	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	7.7985	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-176.1461	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-167.3555	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	8.6999	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	160.6895	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	34.5354	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-82.693	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-2.0881	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-128.2421	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	114.5295	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-66.4436	-DE/DX = 0.0	!
! D45	D(59,3,4,12)	167.4023	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	50.1739	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-158.1678	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.6811	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	4.097	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	161.5838	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-31.1298	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	170.9607	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	103.9327	-DE/DX = 0.0	!
! D54	D(12,4,5,6)	98.4288	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-59.4806	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-126.5087	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-147.1927	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	54.8979	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-12.1302	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-39.6689	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-159.5409	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	81.5432	-DE/DX = 0.0	!

! D63	D(5,4,12,9)	-164.4888	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	75.6392	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-43.2767	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	78.9769	-DE/DX = 0.0	!
! D67	D(36,4,12,13)	-40.895	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-159.8109	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-170.9416	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-51.3036	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	69.6558	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-54.2768	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	65.3612	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-173.6794	-DE/DX = 0.0	!
! D75	D(12,4,36,37)	64.1325	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-176.2295	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-55.2702	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	59.7117	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-61.1446	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	179.3988	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-138.9557	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	100.188	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-19.2685	-DE/DX = 0.0	!
! D84	D(61,5,6,26)	-77.0396	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	162.1041	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	42.6476	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	4.0207	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	158.3559	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-156.427	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-2.0918	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-172.0749	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	68.6153	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-50.956	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-47.52	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-166.8298	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	73.5989	-DE/DX = 0.0	!
! D97	D(51,6,26,27)	76.2605	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-43.0493	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-162.6206	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-179.4956	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-60.1178	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	61.1028	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	60.7223	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.8999	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.6793	-DE/DX = 0.0	!
! D106	D(51,6,42,43)	-64.9916	-DE/DX = 0.0	!
! D107	D(51,6,42,44)	54.3862	-DE/DX = 0.0	!
! D108	D(51,6,42,45)	175.6067	-DE/DX = 0.0	!
! D109	D(5,6,51,14)	161.3596	-DE/DX = 0.0	!
! D110	D(5,6,51,48)	33.0644	-DE/DX = 0.0	!
! D111	D(5,6,51,52)	-79.5447	-DE/DX = 0.0	!
! D112	D(26,6,51,14)	-83.9417	-DE/DX = 0.0	!
! D113	D(26,6,51,48)	147.7632	-DE/DX = 0.0	!
! D114	D(26,6,51,52)	35.154	-DE/DX = 0.0	!

! D115	D(42,6,51,14)	38.9334	-DE/DX = 0.0	!
! D116	D(42,6,51,48)	-89.3618	-DE/DX = 0.0	!
! D117	D(42,6,51,52)	158.0291	-DE/DX = 0.0	!
! D118	D(20,8,16,17)	-173.7757	-DE/DX = 0.0	!
! D119	D(20,8,16,18)	-55.4515	-DE/DX = 0.0	!
! D120	D(20,8,16,19)	67.0947	-DE/DX = 0.0	!
! D121	D(29,8,16,17)	-65.8327	-DE/DX = 0.0	!
! D122	D(29,8,16,18)	52.4915	-DE/DX = 0.0	!
! D123	D(29,8,16,19)	175.0377	-DE/DX = 0.0	!
! D124	D(32,8,16,17)	64.5551	-DE/DX = 0.0	!
! D125	D(32,8,16,18)	-177.1207	-DE/DX = 0.0	!
! D126	D(32,8,16,19)	-54.5745	-DE/DX = 0.0	!
! D127	D(16,8,20,1)	-65.974	-DE/DX = 0.0	!
! D128	D(16,8,20,9)	70.6469	-DE/DX = 0.0	!
! D129	D(16,8,20,21)	178.7271	-DE/DX = 0.0	!
! D130	D(29,8,20,1)	179.3076	-DE/DX = 0.0	!
! D131	D(29,8,20,9)	-44.0715	-DE/DX = 0.0	!
! D132	D(29,8,20,21)	64.0086	-DE/DX = 0.0	!
! D133	D(32,8,20,1)	57.3296	-DE/DX = 0.0	!
! D134	D(32,8,20,9)	-166.0495	-DE/DX = 0.0	!
! D135	D(32,8,20,21)	-57.9694	-DE/DX = 0.0	!
! D136	D(16,8,29,11)	-83.1384	-DE/DX = 0.0	!
! D137	D(16,8,29,30)	158.4524	-DE/DX = 0.0	!
! D138	D(16,8,29,31)	34.0055	-DE/DX = 0.0	!
! D139	D(20,8,29,11)	39.0357	-DE/DX = 0.0	!
! D140	D(20,8,29,30)	-79.3736	-DE/DX = 0.0	!
! D141	D(20,8,29,31)	156.1796	-DE/DX = 0.0	!
! D142	D(32,8,29,11)	151.4591	-DE/DX = 0.0	!
! D143	D(32,8,29,30)	33.0498	-DE/DX = 0.0	!
! D144	D(32,8,29,31)	-91.397	-DE/DX = 0.0	!
! D145	D(16,8,32,33)	-75.4656	-DE/DX = 0.0	!
! D146	D(16,8,32,34)	100.8667	-DE/DX = 0.0	!
! D147	D(20,8,32,33)	156.1792	-DE/DX = 0.0	!
! D148	D(20,8,32,34)	-27.4885	-DE/DX = 0.0	!
! D149	D(29,8,32,33)	49.3746	-DE/DX = 0.0	!
! D150	D(29,8,32,34)	-134.293	-DE/DX = 0.0	!
! D151	D(10,9,11,29)	112.6116	-DE/DX = 0.0	!
! D152	D(12,9,11,29)	-126.1035	-DE/DX = 0.0	!
! D153	D(20,9,11,29)	-8.0425	-DE/DX = 0.0	!
! D154	D(10,9,12,4)	-72.4472	-DE/DX = 0.0	!
! D155	D(10,9,12,13)	45.5506	-DE/DX = 0.0	!
! D156	D(10,9,12,60)	165.1225	-DE/DX = 0.0	!
! D157	D(11,9,12,4)	166.6757	-DE/DX = 0.0	!
! D158	D(11,9,12,13)	-75.3266	-DE/DX = 0.0	!
! D159	D(11,9,12,60)	44.2453	-DE/DX = 0.0	!
! D160	D(20,9,12,4)	52.1161	-DE/DX = 0.0	!
! D161	D(20,9,12,13)	170.1138	-DE/DX = 0.0	!
! D162	D(20,9,12,60)	-70.3142	-DE/DX = 0.0	!
! D163	D(10,9,20,1)	54.739	-DE/DX = 0.0	!
! D164	D(10,9,20,8)	-83.1723	-DE/DX = 0.0	!
! D165	D(10,9,20,21)	169.5395	-DE/DX = 0.0	!
! D166	D(11,9,20,1)	171.9296	-DE/DX = 0.0	!

! D167 D(11,9,20,8)	34.0183	-DE/DX = 0.0	!
! D168 D(11,9,20,21)	-73.2699	-DE/DX = 0.0	!
! D169 D(12,9,20,1)	-67.2837	-DE/DX = 0.0	!
! D170 D(12,9,20,8)	154.805	-DE/DX = 0.0	!
! D171 D(12,9,20,21)	47.5168	-DE/DX = 0.0	!
! D172 D(9,11,29,8)	-20.6978	-DE/DX = 0.0	!
! D173 D(9,11,29,30)	99.5413	-DE/DX = 0.0	!
! D174 D(9,11,29,31)	-141.8283	-DE/DX = 0.0	!
! D175 D(4,12,60,62)	167.566	-DE/DX = 0.0	!
! D176 D(9,12,60,62)	-70.4399	-DE/DX = 0.0	!
! D177 D(13,12,60,62)	49.8287	-DE/DX = 0.0	!
! D178 D(53,14,51,6)	74.303	-DE/DX = 0.0	!
! D179 D(53,14,51,48)	-162.6452	-DE/DX = 0.0	!
! D180 D(53,14,51,52)	-44.867	-DE/DX = 0.0	!
! D181 D(57,14,51,6)	-107.8839	-DE/DX = 0.0	!
! D182 D(57,14,51,48)	15.1679	-DE/DX = 0.0	!
! D183 D(57,14,51,52)	132.9462	-DE/DX = 0.0	!
! D184 D(51,14,53,54)	-0.8266	-DE/DX = 0.0	!
! D185 D(51,14,53,55)	178.6105	-DE/DX = 0.0	!
! D186 D(57,14,53,54)	-179.0791	-DE/DX = 0.0	!
! D187 D(57,14,53,55)	0.3579	-DE/DX = 0.0	!
! D188 D(51,14,57,15)	-178.5301	-DE/DX = 0.0	!
! D189 D(51,14,57,58)	1.3371	-DE/DX = 0.0	!
! D190 D(53,14,57,15)	-0.3572	-DE/DX = 0.0	!
! D191 D(53,14,57,58)	179.5101	-DE/DX = 0.0	!
! D192 D(57,15,55,53)	0.0259	-DE/DX = 0.0	!
! D193 D(57,15,55,56)	179.6887	-DE/DX = 0.0	!
! D194 D(55,15,57,14)	0.2231	-DE/DX = 0.0	!
! D195 D(55,15,57,58)	-179.669	-DE/DX = 0.0	!
! D196 D(6,26,40,3)	24.7883	-DE/DX = 0.0	!
! D197 D(6,26,40,41)	-133.1439	-DE/DX = 0.0	!
! D198 D(6,26,40,59)	92.5968	-DE/DX = 0.0	!
! D199 D(27,26,40,3)	146.8604	-DE/DX = 0.0	!
! D200 D(27,26,40,41)	-11.0718	-DE/DX = 0.0	!
! D201 D(27,26,40,59)	-145.3311	-DE/DX = 0.0	!
! D202 D(28,26,40,3)	-96.7648	-DE/DX = 0.0	!
! D203 D(28,26,40,41)	105.3029	-DE/DX = 0.0	!
! D204 D(28,26,40,59)	-28.9564	-DE/DX = 0.0	!
! D205 D(8,32,34,2)	-0.863	-DE/DX = 0.0	!
! D206 D(8,32,34,35)	-176.6198	-DE/DX = 0.0	!
! D207 D(33,32,34,2)	175.4695	-DE/DX = 0.0	!
! D208 D(33,32,34,35)	-0.2873	-DE/DX = 0.0	!
! D209 D(5,46,48,49)	143.4151	-DE/DX = 0.0	!
! D210 D(5,46,48,50)	-96.4798	-DE/DX = 0.0	!
! D211 D(5,46,48,51)	23.033	-DE/DX = 0.0	!
! D212 D(47,46,48,49)	-61.3614	-DE/DX = 0.0	!
! D213 D(47,46,48,50)	58.7437	-DE/DX = 0.0	!
! D214 D(47,46,48,51)	178.2565	-DE/DX = 0.0	!
! D215 D(61,46,48,49)	79.1907	-DE/DX = 0.0	!
! D216 D(61,46,48,50)	-160.7043	-DE/DX = 0.0	!
! D217 D(61,46,48,51)	-41.1914	-DE/DX = 0.0	!
! D218 D(46,48,51,6)	-34.491	-DE/DX = 0.0	!

! D219	D(46,48,51,14)	-163.929	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	78.2593	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-155.3207	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	75.2413	-DE/DX = 0.0	!
! D223	D(49,48,51,52)	-42.5704	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	83.1563	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-46.2817	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-164.0934	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2396	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.8292	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.2058	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.3838	-DE/DX = 0.0	!
! D231	D(12,60,62,63)	-45.3512	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	139.7972	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	134.4528	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-49.2459	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-50.9538	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	125.3475	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-2.151	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	178.8186	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-178.1547	-DE/DX = 0.0	!
! D240	D(71,63,64,67)	2.8149	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-19.5718	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	101.3349	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-138.3317	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	156.3998	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-82.6935	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	37.6399	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	1.1408	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	122.1342	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-120.3209	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	-177.9059	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-56.9125	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	60.6324	-DE/DX = 0.0	!

2. opt=tight hf/6-311++g(d,p) scrf=(cpcm,solvent=chloroform,read) nosymm

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! Optimized Parameters !
! (Angstroms and Degrees) !
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! Name Definition      Value      Derivative Info.      !
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! R1  R(1,2)           1.549      -DE/DX = 0.0          !
! R2  R(1,3)           1.5672     -DE/DX = 0.0          !
! R3  R(1,20)          1.5157     -DE/DX = 0.0          !
! R4  R(1,22)          1.5481     -DE/DX = 0.0          !
! R5  R(2,7)           1.1948     -DE/DX = 0.0          !
! R6  R(2,34)          1.4992     -DE/DX = 0.0          !
! R7  R(3,4)           1.5887     -DE/DX = 0.0          !

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! R8	R(3,40)	1.48	-DE/DX = 0.0	!
! R9	R(3,59)	1.4024	-DE/DX = 0.0	!
! R10	R(4,5)	1.5518	-DE/DX = 0.0	!
! R11	R(4,12)	1.5733	-DE/DX = 0.0	!
! R12	R(4,36)	1.5503	-DE/DX = 0.0	!
! R13	R(5,6)	1.5442	-DE/DX = 0.0	!
! R14	R(5,46)	1.4553	-DE/DX = 0.0	!
! R15	R(5,61)	1.4235	-DE/DX = 0.0	!
! R16	R(6,26)	1.526	-DE/DX = 0.0	!
! R17	R(6,42)	1.535	-DE/DX = 0.0	!
! R18	R(6,51)	1.5708	-DE/DX = 0.0	!
! R19	R(8,16)	1.5424	-DE/DX = 0.0	!
! R20	R(8,20)	1.5244	-DE/DX = 0.0	!
! R21	R(8,29)	1.5402	-DE/DX = 0.0	!
! R22	R(8,32)	1.5036	-DE/DX = 0.0	!
! R23	R(9,10)	1.0821	-DE/DX = 0.0	!
! R24	R(9,11)	1.4133	-DE/DX = 0.0	!
! R25	R(9,12)	1.5302	-DE/DX = 0.0	!
! R26	R(9,20)	1.4993	-DE/DX = 0.0	!
! R27	R(11,29)	1.4287	-DE/DX = 0.0	!
! R28	R(12,13)	1.0795	-DE/DX = 0.0	!
! R29	R(12,60)	1.4131	-DE/DX = 0.0	!
! R30	R(14,51)	1.5041	-DE/DX = 0.0	!
! R31	R(14,53)	1.4505	-DE/DX = 0.0	!
! R32	R(14,57)	1.341	-DE/DX = 0.0	!
! R33	R(15,55)	1.3412	-DE/DX = 0.0	!
! R34	R(15,57)	1.3496	-DE/DX = 0.0	!
! R35	R(16,17)	1.0861	-DE/DX = 0.0	!
! R36	R(16,18)	1.0846	-DE/DX = 0.0	!
! R37	R(16,19)	1.0803	-DE/DX = 0.0	!
! R38	R(20,21)	1.0878	-DE/DX = 0.0	!
! R39	R(22,23)	1.0819	-DE/DX = 0.0	!
! R40	R(22,24)	1.0806	-DE/DX = 0.0	!
! R41	R(22,25)	1.0807	-DE/DX = 0.0	!
! R42	R(26,27)	1.0845	-DE/DX = 0.0	!
! R43	R(26,28)	1.0849	-DE/DX = 0.0	!
! R44	R(26,40)	1.5158	-DE/DX = 0.0	!
! R45	R(29,30)	1.0847	-DE/DX = 0.0	!
! R46	R(29,31)	1.0814	-DE/DX = 0.0	!
! R47	R(32,33)	1.0783	-DE/DX = 0.0	!
! R48	R(32,34)	1.3285	-DE/DX = 0.0	!
! R49	R(34,35)	1.0758	-DE/DX = 0.0	!
! R50	R(36,37)	1.0824	-DE/DX = 0.0	!
! R51	R(36,38)	1.0773	-DE/DX = 0.0	!
! R52	R(36,39)	1.0807	-DE/DX = 0.0	!
! R53	R(40,41)	1.0706	-DE/DX = 0.0	!
! R54	R(40,59)	1.4054	-DE/DX = 0.0	!
! R55	R(42,43)	1.084	-DE/DX = 0.0	!
! R56	R(42,44)	1.0814	-DE/DX = 0.0	!
! R57	R(42,45)	1.0802	-DE/DX = 0.0	!
! R58	R(46,47)	1.0744	-DE/DX = 0.0	!
! R59	R(46,48)	1.5076	-DE/DX = 0.0	!

! R60	R(46,61)	1.4051	-DE/DX = 0.0	!
! R61	R(48,49)	1.0852	-DE/DX = 0.0	!
! R62	R(48,50)	1.0855	-DE/DX = 0.0	!
! R63	R(48,51)	1.5405	-DE/DX = 0.0	!
! R64	R(51,52)	1.0819	-DE/DX = 0.0	!
! R65	R(53,54)	1.0707	-DE/DX = 0.0	!
! R66	R(53,55)	1.3381	-DE/DX = 0.0	!
! R67	R(55,56)	1.0689	-DE/DX = 0.0	!
! R68	R(57,58)	1.0681	-DE/DX = 0.0	!
! R69	R(60,62)	1.3397	-DE/DX = 0.0	!
! R70	R(62,63)	1.503	-DE/DX = 0.0	!
! R71	R(62,65)	1.1873	-DE/DX = 0.0	!
! R72	R(63,64)	1.323	-DE/DX = 0.0	!
! R73	R(63,71)	1.5159	-DE/DX = 0.0	!
! R74	R(64,66)	1.0768	-DE/DX = 0.0	!
! R75	R(64,67)	1.5002	-DE/DX = 0.0	!
! R76	R(67,68)	1.0817	-DE/DX = 0.0	!
! R77	R(67,69)	1.0868	-DE/DX = 0.0	!
! R78	R(67,70)	1.0871	-DE/DX = 0.0	!
! R79	R(71,72)	1.083	-DE/DX = 0.0	!
! R80	R(71,73)	1.0857	-DE/DX = 0.0	!
! R81	R(71,74)	1.0821	-DE/DX = 0.0	!
! A1	A(2,1,3)	115.1538	-DE/DX = 0.0	!
! A2	A(2,1,20)	105.236	-DE/DX = 0.0	!
! A3	A(2,1,22)	104.8093	-DE/DX = 0.0	!
! A4	A(3,1,20)	104.9239	-DE/DX = 0.0	!
! A5	A(3,1,22)	110.4677	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.5134	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.1731	-DE/DX = 0.0	!
! A8	A(1,2,34)	119.0297	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.606	-DE/DX = 0.0	!
! A10	A(1,3,4)	117.2546	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.3391	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.6346	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.8618	-DE/DX = 0.0	!
! A14	A(4,3,59)	111.3348	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.0767	-DE/DX = 0.0	!
! A16	A(3,4,12)	116.9148	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.5825	-DE/DX = 0.0	!
! A18	A(5,4,12)	111.259	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.39	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.2361	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.516	-DE/DX = 0.0	!
! A22	A(4,5,46)	126.0858	-DE/DX = 0.0	!
! A23	A(4,5,61)	113.5947	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.4312	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.1575	-DE/DX = 0.0	!
! A26	A(5,6,26)	107.1323	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.8607	-DE/DX = 0.0	!
! A28	A(5,6,51)	101.883	-DE/DX = 0.0	!
! A29	A(26,6,42)	108.6162	-DE/DX = 0.0	!
! A30	A(26,6,51)	113.8653	-DE/DX = 0.0	!

! A31	A(42,6,51)	110.4727	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.8806	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.5431	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.4283	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.4321	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.2487	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.2659	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.5073	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.1246	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.4735	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.1065	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.1494	-DE/DX = 0.0	!
! A43	A(12,9,20)	109.4574	-DE/DX = 0.0	!
! A44	A(9,11,29)	111.2217	-DE/DX = 0.0	!
! A45	A(4,12,9)	110.6951	-DE/DX = 0.0	!
! A46	A(4,12,13)	106.8893	-DE/DX = 0.0	!
! A47	A(4,12,60)	111.457	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.1609	-DE/DX = 0.0	!
! A49	A(9,12,60)	108.7044	-DE/DX = 0.0	!
! A50	A(13,12,60)	108.9106	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.0928	-DE/DX = 0.0	!
! A52	A(51,14,57)	129.1716	-DE/DX = 0.0	!
! A53	A(53,14,57)	104.7043	-DE/DX = 0.0	!
! A54	A(55,15,57)	107.1499	-DE/DX = 0.0	!
! A55	A(8,16,17)	108.8652	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.4173	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.6197	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.5584	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.5116	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.6716	-DE/DX = 0.0	!
! A61	A(1,20,8)	121.0073	-DE/DX = 0.0	!
! A62	A(1,20,9)	118.522	-DE/DX = 0.0	!
! A63	A(1,20,21)	103.9894	-DE/DX = 0.0	!
! A64	A(8,20,9)	103.9439	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.9416	-DE/DX = 0.0	!
! A66	A(9,20,21)	104.1273	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.2058	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.4545	-DE/DX = 0.0	!
! A69	A(1,22,25)	109.2493	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.5329	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.5345	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.7106	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.5061	-DE/DX = 0.0	!
! A74	A(6,26,28)	110.915	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.6304	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.4709	-DE/DX = 0.0	!
! A77	A(27,26,40)	108.7293	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.4383	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.4819	-DE/DX = 0.0	!
! A80	A(8,29,30)	111.9908	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.6619	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.4335	-DE/DX = 0.0	!

! A83	A(11,29,31)	107.9166	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.1339	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.7061	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.4528	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.7329	-DE/DX = 0.0	!
! A88	A(2,34,32)	124.9802	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.7128	-DE/DX = 0.0	!
! A90	A(32,34,35)	121.1452	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.4219	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.9466	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.3694	-DE/DX = 0.0	!
! A94	A(37,36,38)	108.1825	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.2528	-DE/DX = 0.0	!
! A96	A(38,36,39)	108.5338	-DE/DX = 0.0	!
! A97	A(3,40,26)	125.1561	-DE/DX = 0.0	!
! A98	A(3,40,41)	116.9571	-DE/DX = 0.0	!
! A99	A(26,40,41)	114.4095	-DE/DX = 0.0	!
! A100	A(26,40,59)	115.9652	-DE/DX = 0.0	!
! A101	A(41,40,59)	112.7468	-DE/DX = 0.0	!
! A102	A(6,42,43)	108.5321	-DE/DX = 0.0	!
! A103	A(6,42,44)	112.5203	-DE/DX = 0.0	!
! A104	A(6,42,45)	112.1348	-DE/DX = 0.0	!
! A105	A(43,42,44)	107.9804	-DE/DX = 0.0	!
! A106	A(43,42,45)	107.8314	-DE/DX = 0.0	!
! A107	A(44,42,45)	107.6632	-DE/DX = 0.0	!
! A108	A(5,46,47)	123.9077	-DE/DX = 0.0	!
! A109	A(5,46,48)	110.0212	-DE/DX = 0.0	!
! A110	A(47,46,48)	120.8359	-DE/DX = 0.0	!
! A111	A(47,46,61)	115.2615	-DE/DX = 0.0	!
! A112	A(48,46,61)	111.5456	-DE/DX = 0.0	!
! A113	A(46,48,49)	112.3782	-DE/DX = 0.0	!
! A114	A(46,48,50)	109.4427	-DE/DX = 0.0	!
! A115	A(46,48,51)	102.7788	-DE/DX = 0.0	!
! A116	A(49,48,50)	107.9181	-DE/DX = 0.0	!
! A117	A(49,48,51)	111.9371	-DE/DX = 0.0	!
! A118	A(50,48,51)	112.383	-DE/DX = 0.0	!
! A119	A(6,51,14)	116.8705	-DE/DX = 0.0	!
! A120	A(6,51,48)	104.5425	-DE/DX = 0.0	!
! A121	A(6,51,52)	106.7389	-DE/DX = 0.0	!
! A122	A(14,51,48)	114.8714	-DE/DX = 0.0	!
! A123	A(14,51,52)	106.3982	-DE/DX = 0.0	!
! A124	A(48,51,52)	106.7767	-DE/DX = 0.0	!
! A125	A(14,53,54)	127.4942	-DE/DX = 0.0	!
! A126	A(14,53,55)	106.2381	-DE/DX = 0.0	!
! A127	A(54,53,55)	126.2662	-DE/DX = 0.0	!
! A128	A(15,55,53)	110.6455	-DE/DX = 0.0	!
! A129	A(15,55,56)	116.6182	-DE/DX = 0.0	!
! A130	A(53,55,56)	132.7354	-DE/DX = 0.0	!
! A131	A(14,57,15)	111.2607	-DE/DX = 0.0	!
! A132	A(14,57,58)	132.9729	-DE/DX = 0.0	!
! A133	A(15,57,58)	115.7663	-DE/DX = 0.0	!
! A134	A(12,60,62)	123.4264	-DE/DX = 0.0	!

! A135	A(60,62,63)	119.1473	-DE/DX = 0.0	!
! A136	A(60,62,65)	117.9395	-DE/DX = 0.0	!
! A137	A(63,62,65)	122.6884	-DE/DX = 0.0	!
! A138	A(62,63,64)	117.195	-DE/DX = 0.0	!
! A139	A(62,63,71)	117.3833	-DE/DX = 0.0	!
! A140	A(64,63,71)	125.2904	-DE/DX = 0.0	!
! A141	A(63,64,66)	117.5683	-DE/DX = 0.0	!
! A142	A(63,64,67)	127.2197	-DE/DX = 0.0	!
! A143	A(66,64,67)	115.2014	-DE/DX = 0.0	!
! A144	A(64,67,68)	113.1831	-DE/DX = 0.0	!
! A145	A(64,67,69)	109.7504	-DE/DX = 0.0	!
! A146	A(64,67,70)	109.9132	-DE/DX = 0.0	!
! A147	A(68,67,69)	108.2422	-DE/DX = 0.0	!
! A148	A(68,67,70)	108.5522	-DE/DX = 0.0	!
! A149	A(69,67,70)	106.9961	-DE/DX = 0.0	!
! A150	A(63,71,72)	110.8324	-DE/DX = 0.0	!
! A151	A(63,71,73)	112.5587	-DE/DX = 0.0	!
! A152	A(63,71,74)	110.3331	-DE/DX = 0.0	!
! A153	A(72,71,73)	108.0379	-DE/DX = 0.0	!
! A154	A(72,71,74)	107.2605	-DE/DX = 0.0	!
! A155	A(73,71,74)	107.6129	-DE/DX = 0.0	!
! D1	D(3,1,2,7)	-56.793	-DE/DX = 0.0	!
! D2	D(3,1,2,34)	128.3036	-DE/DX = 0.0	!
! D3	D(20,1,2,7)	-171.8032	-DE/DX = 0.0	!
! D4	D(20,1,2,34)	13.2934	-DE/DX = 0.0	!
! D5	D(22,1,2,7)	64.7902	-DE/DX = 0.0	!
! D6	D(22,1,2,34)	-110.1132	-DE/DX = 0.0	!
! D7	D(2,1,3,4)	-155.7271	-DE/DX = 0.0	!
! D8	D(2,1,3,40)	6.162	-DE/DX = 0.0	!
! D9	D(2,1,3,59)	72.0397	-DE/DX = 0.0	!
! D10	D(20,1,3,4)	-40.5374	-DE/DX = 0.0	!
! D11	D(20,1,3,40)	121.3518	-DE/DX = 0.0	!
! D12	D(20,1,3,59)	-172.7706	-DE/DX = 0.0	!
! D13	D(22,1,3,4)	85.8044	-DE/DX = 0.0	!
! D14	D(22,1,3,40)	-112.3065	-DE/DX = 0.0	!
! D15	D(22,1,3,59)	-46.4288	-DE/DX = 0.0	!
! D16	D(2,1,20,8)	-48.9288	-DE/DX = 0.0	!
! D17	D(2,1,20,9)	-179.2158	-DE/DX = 0.0	!
! D18	D(2,1,20,21)	65.8438	-DE/DX = 0.0	!
! D19	D(3,1,20,8)	-170.8333	-DE/DX = 0.0	!
! D20	D(3,1,20,9)	58.8797	-DE/DX = 0.0	!
! D21	D(3,1,20,21)	-56.0607	-DE/DX = 0.0	!
! D22	D(22,1,20,8)	66.6611	-DE/DX = 0.0	!
! D23	D(22,1,20,9)	-63.6259	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	-178.5662	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	38.7537	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	159.4171	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-79.7873	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	163.3617	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-75.9749	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	44.8208	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-77.074	-DE/DX = 0.0	!

! D32	D(20,1,22,24)	43.5894	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	164.385	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	9.9453	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-174.6536	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-165.1413	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	10.2598	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	161.7983	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	35.3967	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-81.3581	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-0.1811	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-126.5827	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	116.6625	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-64.9386	-DE/DX = 0.0	!
! D45	D(59,3,4,12)	168.6598	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	51.905	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-158.2857	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.5791	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	3.1327	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	160.8394	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-32.6051	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	169.1834	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	102.0716	-DE/DX = 0.0	!
! D54	D(12,4,5,6)	97.0322	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-61.1793	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-128.2911	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-148.9247	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	52.8638	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-14.2481	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-38.5421	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-158.5247	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	82.5767	-DE/DX = 0.0	!
! D63	D(5,4,12,9)	-163.3551	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	76.6623	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-42.2363	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	80.0326	-DE/DX = 0.0	!
! D67	D(36,4,12,13)	-39.95	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-158.8486	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-169.1227	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-49.1848	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	71.8302	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-52.4839	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	67.454	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-171.531	-DE/DX = 0.0	!
! D75	D(12,4,36,37)	66.107	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-173.9551	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-52.9401	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	59.6444	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-61.086	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	179.4798	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-138.788	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	100.4817	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-18.9526	-DE/DX = 0.0	!

! D84	D(61,5,6,26)	-76.738	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	162.5316	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	43.0974	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	4.0179	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	158.4761	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-156.7182	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-2.26	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-170.7155	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	70.2018	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-49.5776	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-46.1004	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-165.1831	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	75.0375	-DE/DX = 0.0	!
! D97	D(51,6,26,27)	77.4456	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-41.6371	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-161.4165	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-179.2159	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-59.7806	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	61.7706	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	60.8719	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.6927	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.1415	-DE/DX = 0.0	!
! D106	D(51,6,42,43)	-64.682	-DE/DX = 0.0	!
! D107	D(51,6,42,44)	54.7533	-DE/DX = 0.0	!
! D108	D(51,6,42,45)	176.3045	-DE/DX = 0.0	!
! D109	D(5,6,51,14)	160.9117	-DE/DX = 0.0	!
! D110	D(5,6,51,48)	32.7026	-DE/DX = 0.0	!
! D111	D(5,6,51,52)	-80.2152	-DE/DX = 0.0	!
! D112	D(26,6,51,14)	-84.1103	-DE/DX = 0.0	!
! D113	D(26,6,51,48)	147.6806	-DE/DX = 0.0	!
! D114	D(26,6,51,52)	34.7628	-DE/DX = 0.0	!
! D115	D(42,6,51,14)	38.4223	-DE/DX = 0.0	!
! D116	D(42,6,51,48)	-89.7868	-DE/DX = 0.0	!
! D117	D(42,6,51,52)	157.2954	-DE/DX = 0.0	!
! D118	D(20,8,16,17)	-173.6877	-DE/DX = 0.0	!
! D119	D(20,8,16,18)	-55.232	-DE/DX = 0.0	!
! D120	D(20,8,16,19)	67.1785	-DE/DX = 0.0	!
! D121	D(29,8,16,17)	-65.5602	-DE/DX = 0.0	!
! D122	D(29,8,16,18)	52.8955	-DE/DX = 0.0	!
! D123	D(29,8,16,19)	175.306	-DE/DX = 0.0	!
! D124	D(32,8,16,17)	64.8282	-DE/DX = 0.0	!
! D125	D(32,8,16,18)	-176.7161	-DE/DX = 0.0	!
! D126	D(32,8,16,19)	-54.3056	-DE/DX = 0.0	!
! D127	D(16,8,20,1)	-65.5414	-DE/DX = 0.0	!
! D128	D(16,8,20,9)	70.7821	-DE/DX = 0.0	!
! D129	D(16,8,20,21)	179.1488	-DE/DX = 0.0	!
! D130	D(29,8,20,1)	179.5167	-DE/DX = 0.0	!
! D131	D(29,8,20,9)	-44.1598	-DE/DX = 0.0	!
! D132	D(29,8,20,21)	64.2069	-DE/DX = 0.0	!
! D133	D(32,8,20,1)	57.562	-DE/DX = 0.0	!
! D134	D(32,8,20,9)	-166.1145	-DE/DX = 0.0	!
! D135	D(32,8,20,21)	-57.7478	-DE/DX = 0.0	!

! D136 D(16,8,29,11)	-83.7169	-DE/DX = 0.0	!
! D137 D(16,8,29,30)	157.9304	-DE/DX = 0.0	!
! D138 D(16,8,29,31)	33.6742	-DE/DX = 0.0	!
! D139 D(20,8,29,11)	38.5711	-DE/DX = 0.0	!
! D140 D(20,8,29,30)	-79.7815	-DE/DX = 0.0	!
! D141 D(20,8,29,31)	155.9623	-DE/DX = 0.0	!
! D142 D(32,8,29,11)	150.9243	-DE/DX = 0.0	!
! D143 D(32,8,29,30)	32.5717	-DE/DX = 0.0	!
! D144 D(32,8,29,31)	-91.6845	-DE/DX = 0.0	!
! D145 D(16,8,32,33)	-76.2573	-DE/DX = 0.0	!
! D146 D(16,8,32,34)	99.952	-DE/DX = 0.0	!
! D147 D(20,8,32,33)	155.4781	-DE/DX = 0.0	!
! D148 D(20,8,32,34)	-28.3125	-DE/DX = 0.0	!
! D149 D(29,8,32,33)	48.6687	-DE/DX = 0.0	!
! D150 D(29,8,32,34)	-135.1219	-DE/DX = 0.0	!
! D151 D(10,9,11,29)	111.8478	-DE/DX = 0.0	!
! D152 D(12,9,11,29)	-126.924	-DE/DX = 0.0	!
! D153 D(20,9,11,29)	-8.7866	-DE/DX = 0.0	!
! D154 D(10,9,12,4)	-74.1898	-DE/DX = 0.0	!
! D155 D(10,9,12,13)	43.8143	-DE/DX = 0.0	!
! D156 D(10,9,12,60)	163.0762	-DE/DX = 0.0	!
! D157 D(11,9,12,4)	164.9314	-DE/DX = 0.0	!
! D158 D(11,9,12,13)	-77.0646	-DE/DX = 0.0	!
! D159 D(11,9,12,60)	42.1974	-DE/DX = 0.0	!
! D160 D(20,9,12,4)	50.5349	-DE/DX = 0.0	!
! D161 D(20,9,12,13)	168.5389	-DE/DX = 0.0	!
! D162 D(20,9,12,60)	-72.1991	-DE/DX = 0.0	!
! D163 D(10,9,20,1)	54.9534	-DE/DX = 0.0	!
! D164 D(10,9,20,8)	-82.6962	-DE/DX = 0.0	!
! D165 D(10,9,20,21)	169.8194	-DE/DX = 0.0	!
! D166 D(11,9,20,1)	172.1364	-DE/DX = 0.0	!
! D167 D(11,9,20,8)	34.4867	-DE/DX = 0.0	!
! D168 D(11,9,20,21)	-72.9976	-DE/DX = 0.0	!
! D169 D(12,9,20,1)	-67.203	-DE/DX = 0.0	!
! D170 D(12,9,20,8)	155.1473	-DE/DX = 0.0	!
! D171 D(12,9,20,21)	47.663	-DE/DX = 0.0	!
! D172 D(9,11,29,8)	-19.909	-DE/DX = 0.0	!
! D173 D(9,11,29,30)	100.1727	-DE/DX = 0.0	!
! D174 D(9,11,29,31)	-141.1836	-DE/DX = 0.0	!
! D175 D(4,12,60,62)	163.4066	-DE/DX = 0.0	!
! D176 D(9,12,60,62)	-74.3203	-DE/DX = 0.0	!
! D177 D(13,12,60,62)	45.721	-DE/DX = 0.0	!
! D178 D(53,14,51,6)	73.6315	-DE/DX = 0.0	!
! D179 D(53,14,51,48)	-163.3334	-DE/DX = 0.0	!
! D180 D(53,14,51,52)	-45.4248	-DE/DX = 0.0	!
! D181 D(57,14,51,6)	-108.7185	-DE/DX = 0.0	!
! D182 D(57,14,51,48)	14.3165	-DE/DX = 0.0	!
! D183 D(57,14,51,52)	132.2252	-DE/DX = 0.0	!
! D184 D(51,14,53,54)	-1.0996	-DE/DX = 0.0	!
! D185 D(51,14,53,55)	178.4808	-DE/DX = 0.0	!
! D186 D(57,14,53,54)	-179.2162	-DE/DX = 0.0	!
! D187 D(57,14,53,55)	0.3641	-DE/DX = 0.0	!

! D188	D(51,14,57,15)	-178.4028	-DE/DX = 0.0	!
! D189	D(51,14,57,58)	1.4817	-DE/DX = 0.0	!
! D190	D(53,14,57,15)	-0.3658	-DE/DX = 0.0	!
! D191	D(53,14,57,58)	179.5186	-DE/DX = 0.0	!
! D192	D(57,15,55,53)	0.0207	-DE/DX = 0.0	!
! D193	D(57,15,55,56)	179.7192	-DE/DX = 0.0	!
! D194	D(55,15,57,14)	0.2319	-DE/DX = 0.0	!
! D195	D(55,15,57,58)	-179.6742	-DE/DX = 0.0	!
! D196	D(6,26,40,3)	24.0065	-DE/DX = 0.0	!
! D197	D(6,26,40,41)	-134.1964	-DE/DX = 0.0	!
! D198	D(6,26,40,59)	91.9128	-DE/DX = 0.0	!
! D199	D(27,26,40,3)	146.1717	-DE/DX = 0.0	!
! D200	D(27,26,40,41)	-12.0311	-DE/DX = 0.0	!
! D201	D(27,26,40,59)	-145.922	-DE/DX = 0.0	!
! D202	D(28,26,40,3)	-97.8022	-DE/DX = 0.0	!
! D203	D(28,26,40,41)	103.995	-DE/DX = 0.0	!
! D204	D(28,26,40,59)	-29.8959	-DE/DX = 0.0	!
! D205	D(8,32,34,2)	-1.2518	-DE/DX = 0.0	!
! D206	D(8,32,34,35)	-176.3313	-DE/DX = 0.0	!
! D207	D(33,32,34,2)	174.9565	-DE/DX = 0.0	!
! D208	D(33,32,34,35)	-0.123	-DE/DX = 0.0	!
! D209	D(5,46,48,49)	143.5014	-DE/DX = 0.0	!
! D210	D(5,46,48,50)	-96.6197	-DE/DX = 0.0	!
! D211	D(5,46,48,51)	22.9935	-DE/DX = 0.0	!
! D212	D(47,46,48,49)	-61.1286	-DE/DX = 0.0	!
! D213	D(47,46,48,50)	58.7503	-DE/DX = 0.0	!
! D214	D(47,46,48,51)	178.3635	-DE/DX = 0.0	!
! D215	D(61,46,48,49)	79.2294	-DE/DX = 0.0	!
! D216	D(61,46,48,50)	-160.8917	-DE/DX = 0.0	!
! D217	D(61,46,48,51)	-41.2785	-DE/DX = 0.0	!
! D218	D(46,48,51,6)	-34.2585	-DE/DX = 0.0	!
! D219	D(46,48,51,14)	-163.6729	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	78.6323	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-155.0694	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	75.5162	-DE/DX = 0.0	!
! D223	D(49,48,51,52)	-42.1786	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	83.2921	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-46.1223	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-163.8171	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2397	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.8726	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.3474	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.2856	-DE/DX = 0.0	!
! D231	D(12,60,62,63)	-39.6919	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	145.6078	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	130.513	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-53.4296	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-55.0508	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	121.0066	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-2.5448	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	178.7043	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-178.2552	-DE/DX = 0.0	!

! D240	D(71,63,64,67)	2.9939	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-21.2499	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	99.8696	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-139.9074	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	154.4533	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-84.4272	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	35.7957	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	0.7973	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	121.8333	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-120.7542	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	-177.9789	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-56.9428	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	60.4696	-DE/DX = 0.0	!

3. opt=tight b3lyp/6-311++g(d,p) nosymm

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.5603	-DE/DX = 0.0	!
! R2	R(1,3)	1.5811	-DE/DX = 0.0	!
! R3	R(1,20)	1.5221	-DE/DX = 0.0	!
! R4	R(1,22)	1.551	-DE/DX = 0.0	!
! R5	R(2,7)	1.2167	-DE/DX = 0.0	!
! R6	R(2,34)	1.4966	-DE/DX = 0.0	!
! R7	R(3,4)	1.5973	-DE/DX = 0.0	!
! R8	R(3,40)	1.4972	-DE/DX = 0.0	!
! R9	R(3,59)	1.4311	-DE/DX = 0.0	!
! R10	R(4,5)	1.5549	-DE/DX = 0.0	!
! R11	R(4,12)	1.5756	-DE/DX = 0.0	!
! R12	R(4,36)	1.5543	-DE/DX = 0.0	!
! R13	R(5,6)	1.5477	-DE/DX = 0.0	!
! R14	R(5,46)	1.472	-DE/DX = 0.0	!
! R15	R(5,61)	1.4568	-DE/DX = 0.0	!
! R16	R(6,26)	1.5306	-DE/DX = 0.0	!
! R17	R(6,42)	1.5373	-DE/DX = 0.0	!
! R18	R(6,51)	1.581	-DE/DX = 0.0	!
! R19	R(8,16)	1.5477	-DE/DX = 0.0	!
! R20	R(8,20)	1.5348	-DE/DX = 0.0	!
! R21	R(8,29)	1.5479	-DE/DX = 0.0	!
! R22	R(8,32)	1.501	-DE/DX = 0.0	!
! R23	R(9,10)	1.0935	-DE/DX = 0.0	!
! R24	R(9,11)	1.4389	-DE/DX = 0.0	!
! R25	R(9,12)	1.5357	-DE/DX = 0.0	!
! R26	R(9,20)	1.5044	-DE/DX = 0.0	!
! R27	R(11,29)	1.453	-DE/DX = 0.0	!
! R28	R(12,13)	1.0914	-DE/DX = 0.0	!
! R29	R(12,60)	1.4339	-DE/DX = 0.0	!

! R30	R(14,51)	1.5003	-DE/DX = 0.0	!
! R31	R(14,53)	1.4428	-DE/DX = 0.0	!
! R32	R(14,57)	1.3621	-DE/DX = 0.0	!
! R33	R(15,55)	1.3609	-DE/DX = 0.0	!
! R34	R(15,57)	1.3659	-DE/DX = 0.0	!
! R35	R(16,17)	1.0941	-DE/DX = 0.0	!
! R36	R(16,18)	1.0926	-DE/DX = 0.0	!
! R37	R(16,19)	1.0884	-DE/DX = 0.0	!
! R38	R(20,21)	1.0979	-DE/DX = 0.0	!
! R39	R(22,23)	1.0902	-DE/DX = 0.0	!
! R40	R(22,24)	1.0907	-DE/DX = 0.0	!
! R41	R(22,25)	1.0894	-DE/DX = 0.0	!
! R42	R(26,27)	1.0937	-DE/DX = 0.0	!
! R43	R(26,28)	1.0944	-DE/DX = 0.0	!
! R44	R(26,40)	1.519	-DE/DX = 0.0	!
! R45	R(29,30)	1.095	-DE/DX = 0.0	!
! R46	R(29,31)	1.0914	-DE/DX = 0.0	!
! R47	R(32,33)	1.0881	-DE/DX = 0.0	!
! R48	R(32,34)	1.3431	-DE/DX = 0.0	!
! R49	R(34,35)	1.0852	-DE/DX = 0.0	!
! R50	R(36,37)	1.0911	-DE/DX = 0.0	!
! R51	R(36,38)	1.086	-DE/DX = 0.0	!
! R52	R(36,39)	1.0896	-DE/DX = 0.0	!
! R53	R(40,41)	1.0823	-DE/DX = 0.0	!
! R54	R(40,59)	1.4353	-DE/DX = 0.0	!
! R55	R(42,43)	1.0923	-DE/DX = 0.0	!
! R56	R(42,44)	1.0897	-DE/DX = 0.0	!
! R57	R(42,45)	1.0882	-DE/DX = 0.0	!
! R58	R(46,47)	1.0858	-DE/DX = 0.0	!
! R59	R(46,48)	1.5135	-DE/DX = 0.0	!
! R60	R(46,61)	1.4326	-DE/DX = 0.0	!
! R61	R(48,49)	1.0934	-DE/DX = 0.0	!
! R62	R(48,50)	1.0953	-DE/DX = 0.0	!
! R63	R(48,51)	1.5478	-DE/DX = 0.0	!
! R64	R(51,52)	1.0918	-DE/DX = 0.0	!
! R65	R(53,54)	1.079	-DE/DX = 0.0	!
! R66	R(53,55)	1.3567	-DE/DX = 0.0	!
! R67	R(55,56)	1.077	-DE/DX = 0.0	!
! R68	R(57,58)	1.0764	-DE/DX = 0.0	!
! R69	R(60,62)	1.3805	-DE/DX = 0.0	!
! R70	R(62,63)	1.4998	-DE/DX = 0.0	!
! R71	R(62,65)	1.2059	-DE/DX = 0.0	!
! R72	R(63,64)	1.3402	-DE/DX = 0.0	!
! R73	R(63,71)	1.5127	-DE/DX = 0.0	!
! R74	R(64,66)	1.0859	-DE/DX = 0.0	!
! R75	R(64,67)	1.4954	-DE/DX = 0.0	!
! R76	R(67,68)	1.0903	-DE/DX = 0.0	!
! R77	R(67,69)	1.0961	-DE/DX = 0.0	!
! R78	R(67,70)	1.0959	-DE/DX = 0.0	!
! R79	R(71,72)	1.0897	-DE/DX = 0.0	!
! R80	R(71,73)	1.0954	-DE/DX = 0.0	!
! R81	R(71,74)	1.0915	-DE/DX = 0.0	!

! A1	A(2,1,3)	115.3519	-DE/DX = 0.0	!
! A2	A(2,1,20)	104.8861	-DE/DX = 0.0	!
! A3	A(2,1,22)	104.8467	-DE/DX = 0.0	!
! A4	A(3,1,20)	106.0693	-DE/DX = 0.0	!
! A5	A(3,1,22)	109.3407	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.6409	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.589	-DE/DX = 0.0	!
! A8	A(1,2,34)	118.552	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.675	-DE/DX = 0.0	!
! A10	A(1,3,4)	117.5179	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.5229	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.2288	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.6777	-DE/DX = 0.0	!
! A14	A(4,3,59)	110.6687	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.5292	-DE/DX = 0.0	!
! A16	A(3,4,12)	116.6545	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.2145	-DE/DX = 0.0	!
! A18	A(5,4,12)	110.8879	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.2857	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.883	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.2095	-DE/DX = 0.0	!
! A22	A(4,5,46)	126.2488	-DE/DX = 0.0	!
! A23	A(4,5,61)	113.7382	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.2407	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.785	-DE/DX = 0.0	!
! A26	A(5,6,26)	107.1725	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.4807	-DE/DX = 0.0	!
! A28	A(5,6,51)	101.9281	-DE/DX = 0.0	!
! A29	A(26,6,42)	109.1102	-DE/DX = 0.0	!
! A30	A(26,6,51)	113.9931	-DE/DX = 0.0	!
! A31	A(42,6,51)	110.1102	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.522	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.4117	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.5034	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.6032	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.428	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.3155	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.1241	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.219	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.6829	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.2048	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.8285	-DE/DX = 0.0	!
! A43	A(12,9,20)	108.7908	-DE/DX = 0.0	!
! A44	A(9,11,29)	109.8976	-DE/DX = 0.0	!
! A45	A(4,12,9)	110.0123	-DE/DX = 0.0	!
! A46	A(4,12,13)	107.3123	-DE/DX = 0.0	!
! A47	A(4,12,60)	110.9644	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.4492	-DE/DX = 0.0	!
! A49	A(9,12,60)	108.7314	-DE/DX = 0.0	!
! A50	A(13,12,60)	109.3677	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.1043	-DE/DX = 0.0	!
! A52	A(51,14,57)	128.8385	-DE/DX = 0.0	!

! A53	A(53,14,57)	105.0493	-DE/DX = 0.0	!
! A54	A(55,15,57)	106.7602	-DE/DX = 0.0	!
! A55	A(8,16,17)	109.1935	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.1802	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.5413	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.4834	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.5463	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.7072	-DE/DX = 0.0	!
! A61	A(1,20,8)	120.9097	-DE/DX = 0.0	!
! A62	A(1,20,9)	118.7478	-DE/DX = 0.0	!
! A63	A(1,20,21)	103.9084	-DE/DX = 0.0	!
! A64	A(8,20,9)	104.2023	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.8345	-DE/DX = 0.0	!
! A66	A(9,20,21)	103.8017	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.5061	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.2128	-DE/DX = 0.0	!
! A69	A(1,22,25)	108.5736	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.8544	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.8603	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.7098	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.4015	-DE/DX = 0.0	!
! A74	A(6,26,28)	110.4847	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.4804	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.6552	-DE/DX = 0.0	!
! A77	A(27,26,40)	109.0851	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.6129	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.6594	-DE/DX = 0.0	!
! A80	A(8,29,30)	112.1608	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.6071	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.2789	-DE/DX = 0.0	!
! A83	A(11,29,31)	107.1977	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.6381	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.4842	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.5688	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.825	-DE/DX = 0.0	!
! A88	A(2,34,32)	125.5569	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.2158	-DE/DX = 0.0	!
! A90	A(32,34,35)	121.0796	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.6514	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.2611	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.4605	-DE/DX = 0.0	!
! A94	A(37,36,38)	107.9835	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.8359	-DE/DX = 0.0	!
! A96	A(38,36,39)	108.5364	-DE/DX = 0.0	!
! A97	A(3,40,26)	124.3752	-DE/DX = 0.0	!
! A98	A(3,40,41)	116.3572	-DE/DX = 0.0	!
! A99	A(26,40,41)	115.5633	-DE/DX = 0.0	!
! A100	A(26,40,59)	116.0868	-DE/DX = 0.0	!
! A101	A(41,40,59)	112.1713	-DE/DX = 0.0	!
! A102	A(6,42,43)	108.655	-DE/DX = 0.0	!
! A103	A(6,42,44)	112.5453	-DE/DX = 0.0	!
! A104	A(6,42,45)	112.3985	-DE/DX = 0.0	!

! A105 A(43,42,44)	107.8542	-DE/DX = 0.0	!
! A106 A(43,42,45)	108.1767	-DE/DX = 0.0	!
! A107 A(44,42,45)	107.0318	-DE/DX = 0.0	!
! A108 A(5,46,47)	123.3677	-DE/DX = 0.0	!
! A109 A(5,46,48)	109.8202	-DE/DX = 0.0	!
! A110 A(47,46,48)	121.1683	-DE/DX = 0.0	!
! A111 A(47,46,61)	115.1313	-DE/DX = 0.0	!
! A112 A(48,46,61)	111.7313	-DE/DX = 0.0	!
! A113 A(46,48,49)	112.6208	-DE/DX = 0.0	!
! A114 A(46,48,50)	109.5706	-DE/DX = 0.0	!
! A115 A(46,48,51)	102.857	-DE/DX = 0.0	!
! A116 A(49,48,50)	107.8033	-DE/DX = 0.0	!
! A117 A(49,48,51)	111.8888	-DE/DX = 0.0	!
! A118 A(50,48,51)	112.1114	-DE/DX = 0.0	!
! A119 A(6,51,14)	116.6829	-DE/DX = 0.0	!
! A120 A(6,51,48)	104.2867	-DE/DX = 0.0	!
! A121 A(6,51,52)	106.1393	-DE/DX = 0.0	!
! A122 A(14,51,48)	115.2826	-DE/DX = 0.0	!
! A123 A(14,51,52)	107.1892	-DE/DX = 0.0	!
! A124 A(48,51,52)	106.51	-DE/DX = 0.0	!
! A125 A(14,53,54)	126.9823	-DE/DX = 0.0	!
! A126 A(14,53,55)	106.7966	-DE/DX = 0.0	!
! A127 A(54,53,55)	126.2177	-DE/DX = 0.0	!
! A128 A(15,55,53)	110.3339	-DE/DX = 0.0	!
! A129 A(15,55,56)	116.0077	-DE/DX = 0.0	!
! A130 A(53,55,56)	133.6564	-DE/DX = 0.0	!
! A131 A(14,57,15)	111.0591	-DE/DX = 0.0	!
! A132 A(14,57,58)	133.6057	-DE/DX = 0.0	!
! A133 A(15,57,58)	115.3348	-DE/DX = 0.0	!
! A134 A(12,60,62)	122.452	-DE/DX = 0.0	!
! A135 A(60,62,63)	118.6681	-DE/DX = 0.0	!
! A136 A(60,62,65)	117.5454	-DE/DX = 0.0	!
! A137 A(63,62,65)	123.472	-DE/DX = 0.0	!
! A138 A(62,63,64)	116.2922	-DE/DX = 0.0	!
! A139 A(62,63,71)	119.4971	-DE/DX = 0.0	!
! A140 A(64,63,71)	124.1105	-DE/DX = 0.0	!
! A141 A(63,64,66)	116.9604	-DE/DX = 0.0	!
! A142 A(63,64,67)	127.2301	-DE/DX = 0.0	!
! A143 A(66,64,67)	115.8042	-DE/DX = 0.0	!
! A144 A(64,67,68)	113.4828	-DE/DX = 0.0	!
! A145 A(64,67,69)	110.1791	-DE/DX = 0.0	!
! A146 A(64,67,70)	110.3058	-DE/DX = 0.0	!
! A147 A(68,67,69)	107.9366	-DE/DX = 0.0	!
! A148 A(68,67,70)	108.3499	-DE/DX = 0.0	!
! A149 A(69,67,70)	106.3016	-DE/DX = 0.0	!
! A150 A(63,71,72)	110.9819	-DE/DX = 0.0	!
! A151 A(63,71,73)	112.869	-DE/DX = 0.0	!
! A152 A(63,71,74)	110.5308	-DE/DX = 0.0	!
! A153 A(72,71,73)	107.7057	-DE/DX = 0.0	!
! A154 A(72,71,74)	107.4152	-DE/DX = 0.0	!
! A155 A(73,71,74)	107.0977	-DE/DX = 0.0	!
! D1 D(3,1,2,7)	-51.4632	-DE/DX = 0.0	!

! D2	D(3,1,2,34)	133.5355	-DE/DX = 0.0	!
! D3	D(20,1,2,7)	-167.7511	-DE/DX = 0.0	!
! D4	D(20,1,2,34)	17.2477	-DE/DX = 0.0	!
! D5	D(22,1,2,7)	68.8505	-DE/DX = 0.0	!
! D6	D(22,1,2,34)	-106.1507	-DE/DX = 0.0	!
! D7	D(2,1,3,4)	-152.0105	-DE/DX = 0.0	!
! D8	D(2,1,3,40)	10.7826	-DE/DX = 0.0	!
! D9	D(2,1,3,59)	76.9413	-DE/DX = 0.0	!
! D10	D(20,1,3,4)	-36.3958	-DE/DX = 0.0	!
! D11	D(20,1,3,40)	126.3972	-DE/DX = 0.0	!
! D12	D(20,1,3,59)	-167.444	-DE/DX = 0.0	!
! D13	D(22,1,3,4)	90.1627	-DE/DX = 0.0	!
! D14	D(22,1,3,40)	-107.0443	-DE/DX = 0.0	!
! D15	D(22,1,3,59)	-40.8855	-DE/DX = 0.0	!
! D16	D(2,1,20,8)	-51.1391	-DE/DX = 0.0	!
! D17	D(2,1,20,9)	177.9718	-DE/DX = 0.0	!
! D18	D(2,1,20,21)	63.3794	-DE/DX = 0.0	!
! D19	D(3,1,20,8)	-173.6616	-DE/DX = 0.0	!
! D20	D(3,1,20,9)	55.4493	-DE/DX = 0.0	!
! D21	D(3,1,20,21)	-59.1431	-DE/DX = 0.0	!
! D22	D(22,1,20,8)	64.3268	-DE/DX = 0.0	!
! D23	D(22,1,20,9)	-66.5623	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	178.8453	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	42.1086	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	163.2307	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-76.5876	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	166.3375	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-72.5404	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	47.6413	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-73.3793	-DE/DX = 0.0	!
! D32	D(20,1,22,24)	47.7429	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	167.9246	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	6.5901	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-177.8138	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-168.6099	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	6.9862	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	160.1013	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	34.0165	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-83.1376	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-2.8428	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-128.9276	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	113.9183	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-67.6895	-DE/DX = 0.0	!
! D45	D(59,3,4,12)	166.2257	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	49.0716	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-158.0127	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.7315	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	4.4115	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	161.6927	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-30.325	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	172.6592	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	105.242	-DE/DX = 0.0	!

! D54	D(12,4,5,6)	99.0448	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-57.971	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-125.3883	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-146.3957	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	56.5885	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-10.8288	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-41.522	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-161.7206	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	78.8455	-DE/DX = 0.0	!
! D63	D(5,4,12,9)	-166.4218	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	73.3796	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-46.0543	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	76.9048	-DE/DX = 0.0	!
! D67	D(36,4,12,13)	-43.2938	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-162.7277	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-172.2578	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-52.8623	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	67.7506	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-55.3366	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	64.0589	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-175.3282	-DE/DX = 0.0	!
! D75	D(12,4,36,37)	63.1111	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-177.4935	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-56.8806	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	59.6292	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-61.5164	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	179.6472	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-139.7346	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	99.1198	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-19.7165	-DE/DX = 0.0	!
! D84	D(61,5,6,26)	-77.4453	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	161.4092	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	42.5728	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	4.1793	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	157.8284	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-155.4639	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-1.8148	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-173.022	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	68.0065	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-51.6058	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-48.5441	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-167.5155	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	72.8722	-DE/DX = 0.0	!
! D97	D(51,6,26,27)	74.9951	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-43.9764	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-163.5887	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-178.7818	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-59.4065	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	61.5317	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	61.1459	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.4789	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.5407	-DE/DX = 0.0	!

! D106 D(51,6,42,43)	-64.6674	-DE/DX = 0.0	!
! D107 D(51,6,42,44)	54.7078	-DE/DX = 0.0	!
! D108 D(51,6,42,45)	175.646	-DE/DX = 0.0	!
! D109 D(5,6,51,14)	161.948	-DE/DX = 0.0	!
! D110 D(5,6,51,48)	33.5426	-DE/DX = 0.0	!
! D111 D(5,6,51,52)	-78.7275	-DE/DX = 0.0	!
! D112 D(26,6,51,14)	-82.944	-DE/DX = 0.0	!
! D113 D(26,6,51,48)	148.6506	-DE/DX = 0.0	!
! D114 D(26,6,51,52)	36.3805	-DE/DX = 0.0	!
! D115 D(42,6,51,14)	40.0521	-DE/DX = 0.0	!
! D116 D(42,6,51,48)	-88.3533	-DE/DX = 0.0	!
! D117 D(42,6,51,52)	159.3766	-DE/DX = 0.0	!
! D118 D(20,8,16,17)	-173.7189	-DE/DX = 0.0	!
! D119 D(20,8,16,18)	-55.2917	-DE/DX = 0.0	!
! D120 D(20,8,16,19)	66.9332	-DE/DX = 0.0	!
! D121 D(29,8,16,17)	-65.6529	-DE/DX = 0.0	!
! D122 D(29,8,16,18)	52.7743	-DE/DX = 0.0	!
! D123 D(29,8,16,19)	174.9992	-DE/DX = 0.0	!
! D124 D(32,8,16,17)	64.7569	-DE/DX = 0.0	!
! D125 D(32,8,16,18)	-176.816	-DE/DX = 0.0	!
! D126 D(32,8,16,19)	-54.591	-DE/DX = 0.0	!
! D127 D(16,8,20,1)	-66.2056	-DE/DX = 0.0	!
! D128 D(16,8,20,9)	70.6612	-DE/DX = 0.0	!
! D129 D(16,8,20,21)	178.7234	-DE/DX = 0.0	!
! D130 D(29,8,20,1)	179.0329	-DE/DX = 0.0	!
! D131 D(29,8,20,9)	-44.1003	-DE/DX = 0.0	!
! D132 D(29,8,20,21)	63.9619	-DE/DX = 0.0	!
! D133 D(32,8,20,1)	56.8957	-DE/DX = 0.0	!
! D134 D(32,8,20,9)	-166.2375	-DE/DX = 0.0	!
! D135 D(32,8,20,21)	-58.1754	-DE/DX = 0.0	!
! D136 D(16,8,29,11)	-82.4537	-DE/DX = 0.0	!
! D137 D(16,8,29,30)	159.1842	-DE/DX = 0.0	!
! D138 D(16,8,29,31)	34.1525	-DE/DX = 0.0	!
! D139 D(20,8,29,11)	39.4711	-DE/DX = 0.0	!
! D140 D(20,8,29,30)	-78.891	-DE/DX = 0.0	!
! D141 D(20,8,29,31)	156.0772	-DE/DX = 0.0	!
! D142 D(32,8,29,11)	152.1623	-DE/DX = 0.0	!
! D143 D(32,8,29,30)	33.8002	-DE/DX = 0.0	!
! D144 D(32,8,29,31)	-91.2316	-DE/DX = 0.0	!
! D145 D(16,8,32,33)	-74.4097	-DE/DX = 0.0	!
! D146 D(16,8,32,34)	101.5671	-DE/DX = 0.0	!
! D147 D(20,8,32,33)	157.6012	-DE/DX = 0.0	!
! D148 D(20,8,32,34)	-26.4219	-DE/DX = 0.0	!
! D149 D(29,8,32,33)	50.4411	-DE/DX = 0.0	!
! D150 D(29,8,32,34)	-133.5821	-DE/DX = 0.0	!
! D151 D(10,9,11,29)	113.8911	-DE/DX = 0.0	!
! D152 D(12,9,11,29)	-124.9661	-DE/DX = 0.0	!
! D153 D(20,9,11,29)	-7.1618	-DE/DX = 0.0	!
! D154 D(10,9,12,4)	-70.1426	-DE/DX = 0.0	!
! D155 D(10,9,12,13)	48.1393	-DE/DX = 0.0	!
! D156 D(10,9,12,60)	168.1503	-DE/DX = 0.0	!
! D157 D(11,9,12,4)	169.3346	-DE/DX = 0.0	!

! D158 D(11,9,12,13)	-72.3836	-DE/DX = 0.0	!
! D159 D(11,9,12,60)	47.6274	-DE/DX = 0.0	!
! D160 D(20,9,12,4)	54.4646	-DE/DX = 0.0	!
! D161 D(20,9,12,13)	172.7464	-DE/DX = 0.0	!
! D162 D(20,9,12,60)	-67.2426	-DE/DX = 0.0	!
! D163 D(10,9,20,1)	54.1742	-DE/DX = 0.0	!
! D164 D(10,9,20,8)	-83.8311	-DE/DX = 0.0	!
! D165 D(10,9,20,21)	168.824	-DE/DX = 0.0	!
! D166 D(11,9,20,1)	171.4187	-DE/DX = 0.0	!
! D167 D(11,9,20,8)	33.4134	-DE/DX = 0.0	!
! D168 D(11,9,20,21)	-73.9315	-DE/DX = 0.0	!
! D169 D(12,9,20,1)	-67.7589	-DE/DX = 0.0	!
! D170 D(12,9,20,8)	154.2358	-DE/DX = 0.0	!
! D171 D(12,9,20,21)	46.891	-DE/DX = 0.0	!
! D172 D(9,11,29,8)	-21.4745	-DE/DX = 0.0	!
! D173 D(9,11,29,30)	98.8278	-DE/DX = 0.0	!
! D174 D(9,11,29,31)	-142.4234	-DE/DX = 0.0	!
! D175 D(4,12,60,62)	171.0431	-DE/DX = 0.0	!
! D176 D(9,12,60,62)	-67.8322	-DE/DX = 0.0	!
! D177 D(13,12,60,62)	52.8479	-DE/DX = 0.0	!
! D178 D(53,14,51,6)	76.8263	-DE/DX = 0.0	!
! D179 D(53,14,51,48)	-160.2976	-DE/DX = 0.0	!
! D180 D(53,14,51,52)	-41.9322	-DE/DX = 0.0	!
! D181 D(57,14,51,6)	-104.3544	-DE/DX = 0.0	!
! D182 D(57,14,51,48)	18.5217	-DE/DX = 0.0	!
! D183 D(57,14,51,52)	136.8872	-DE/DX = 0.0	!
! D184 D(51,14,53,54)	-0.023	-DE/DX = 0.0	!
! D185 D(51,14,53,55)	179.3422	-DE/DX = 0.0	!
! D186 D(57,14,53,54)	-179.0707	-DE/DX = 0.0	!
! D187 D(57,14,53,55)	0.2945	-DE/DX = 0.0	!
! D188 D(51,14,57,15)	-179.2521	-DE/DX = 0.0	!
! D189 D(51,14,57,58)	0.5073	-DE/DX = 0.0	!
! D190 D(53,14,57,15)	-0.2399	-DE/DX = 0.0	!
! D191 D(53,14,57,58)	179.5195	-DE/DX = 0.0	!
! D192 D(57,15,55,53)	0.1047	-DE/DX = 0.0	!
! D193 D(57,15,55,56)	179.6613	-DE/DX = 0.0	!
! D194 D(55,15,57,14)	0.0948	-DE/DX = 0.0	!
! D195 D(55,15,57,58)	-179.7125	-DE/DX = 0.0	!
! D196 D(6,26,40,3)	25.0846	-DE/DX = 0.0	!
! D197 D(6,26,40,41)	-132.3578	-DE/DX = 0.0	!
! D198 D(6,26,40,59)	93.2174	-DE/DX = 0.0	!
! D199 D(27,26,40,3)	147.2629	-DE/DX = 0.0	!
! D200 D(27,26,40,41)	-10.1794	-DE/DX = 0.0	!
! D201 D(27,26,40,59)	-144.6043	-DE/DX = 0.0	!
! D202 D(28,26,40,3)	-96.2143	-DE/DX = 0.0	!
! D203 D(28,26,40,41)	106.3433	-DE/DX = 0.0	!
! D204 D(28,26,40,59)	-28.0816	-DE/DX = 0.0	!
! D205 D(8,32,34,2)	-1.2789	-DE/DX = 0.0	!
! D206 D(8,32,34,35)	-176.5525	-DE/DX = 0.0	!
! D207 D(33,32,34,2)	174.6843	-DE/DX = 0.0	!
! D208 D(33,32,34,35)	-0.5893	-DE/DX = 0.0	!
! D209 D(5,46,48,49)	143.7376	-DE/DX = 0.0	!

! D210	D(5,46,48,50)	-96.284	-DE/DX = 0.0	!
! D211	D(5,46,48,51)	23.1159	-DE/DX = 0.0	!
! D212	D(47,46,48,49)	-61.9356	-DE/DX = 0.0	!
! D213	D(47,46,48,50)	58.0428	-DE/DX = 0.0	!
! D214	D(47,46,48,51)	177.4427	-DE/DX = 0.0	!
! D215	D(61,46,48,49)	78.9059	-DE/DX = 0.0	!
! D216	D(61,46,48,50)	-161.1157	-DE/DX = 0.0	!
! D217	D(61,46,48,51)	-41.7158	-DE/DX = 0.0	!
! D218	D(46,48,51,6)	-34.8421	-DE/DX = 0.0	!
! D219	D(46,48,51,14)	-164.0955	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	77.1611	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-155.9649	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	74.7818	-DE/DX = 0.0	!
! D223	D(49,48,51,52)	-43.9616	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	82.7768	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-46.4765	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-165.22	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2497	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.6989	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.1218	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.3275	-DE/DX = 0.0	!
! D231	D(12,60,62,63)	-49.0612	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	137.1517	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	148.3287	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-35.1627	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-38.2768	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	138.2318	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-1.6992	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	179.1798	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-178.0287	-DE/DX = 0.0	!
! D240	D(71,63,64,67)	2.8503	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-20.0731	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	100.9422	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-139.1452	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	156.1459	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-82.8389	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	37.0738	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	-2.4028	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	118.7552	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-124.1891	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	178.4674	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-60.3746	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	56.6811	-DE/DX = 0.0	!

**4. opt=tight b3lyp/6-311++g(d,p) scrf=(cpcm,solvent=chloroform,read)
nosymm**

! Optimized Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
<hr/>				
! R1	R(1,2)	1.5583	-DE/DX = 0.0	!
! R2	R(1,3)	1.5777	-DE/DX = 0.0	!
! R3	R(1,20)	1.5215	-DE/DX = 0.0	!
! R4	R(1,22)	1.5509	-DE/DX = 0.0	!
! R5	R(2,7)	1.2213	-DE/DX = 0.0	!
! R6	R(2,34)	1.491	-DE/DX = 0.0	!
! R7	R(3,4)	1.5968	-DE/DX = 0.0	!
! R8	R(3,40)	1.4958	-DE/DX = 0.0	!
! R9	R(3,59)	1.4335	-DE/DX = 0.0	!
! R10	R(4,5)	1.5548	-DE/DX = 0.0	!
! R11	R(4,12)	1.5787	-DE/DX = 0.0	!
! R12	R(4,36)	1.5543	-DE/DX = 0.0	!
! R13	R(5,6)	1.5487	-DE/DX = 0.0	!
! R14	R(5,46)	1.4717	-DE/DX = 0.0	!
! R15	R(5,61)	1.459	-DE/DX = 0.0	!
! R16	R(6,26)	1.5307	-DE/DX = 0.0	!
! R17	R(6,42)	1.5373	-DE/DX = 0.0	!
! R18	R(6,51)	1.5814	-DE/DX = 0.0	!
! R19	R(8,16)	1.5481	-DE/DX = 0.0	!
! R20	R(8,20)	1.5335	-DE/DX = 0.0	!
! R21	R(8,29)	1.5468	-DE/DX = 0.0	!
! R22	R(8,32)	1.501	-DE/DX = 0.0	!
! R23	R(9,10)	1.0929	-DE/DX = 0.0	!
! R24	R(9,11)	1.4411	-DE/DX = 0.0	!
! R25	R(9,12)	1.5373	-DE/DX = 0.0	!
! R26	R(9,20)	1.5042	-DE/DX = 0.0	!
! R27	R(11,29)	1.4551	-DE/DX = 0.0	!
! R28	R(12,13)	1.0897	-DE/DX = 0.0	!
! R29	R(12,60)	1.4369	-DE/DX = 0.0	!
! R30	R(14,51)	1.501	-DE/DX = 0.0	!
! R31	R(14,53)	1.4438	-DE/DX = 0.0	!
! R32	R(14,57)	1.3619	-DE/DX = 0.0	!
! R33	R(15,55)	1.3638	-DE/DX = 0.0	!
! R34	R(15,57)	1.3686	-DE/DX = 0.0	!
! R35	R(16,17)	1.0935	-DE/DX = 0.0	!
! R36	R(16,18)	1.0924	-DE/DX = 0.0	!
! R37	R(16,19)	1.0884	-DE/DX = 0.0	!
! R38	R(20,21)	1.0982	-DE/DX = 0.0	!
! R39	R(22,23)	1.09	-DE/DX = 0.0	!
! R40	R(22,24)	1.0897	-DE/DX = 0.0	!
! R41	R(22,25)	1.0896	-DE/DX = 0.0	!
! R42	R(26,27)	1.0932	-DE/DX = 0.0	!
! R43	R(26,28)	1.0943	-DE/DX = 0.0	!
! R44	R(26,40)	1.5181	-DE/DX = 0.0	!
! R45	R(29,30)	1.0949	-DE/DX = 0.0	!
! R46	R(29,31)	1.0905	-DE/DX = 0.0	!
! R47	R(32,33)	1.0874	-DE/DX = 0.0	!
! R48	R(32,34)	1.3445	-DE/DX = 0.0	!
! R49	R(34,35)	1.0852	-DE/DX = 0.0	!
! R50	R(36,37)	1.0905	-DE/DX = 0.0	!

! R51	R(36,38)	1.0862	-DE/DX = 0.0	!
! R52	R(36,39)	1.0892	-DE/DX = 0.0	!
! R53	R(40,41)	1.0822	-DE/DX = 0.0	!
! R54	R(40,59)	1.4395	-DE/DX = 0.0	!
! R55	R(42,43)	1.0924	-DE/DX = 0.0	!
! R56	R(42,44)	1.0895	-DE/DX = 0.0	!
! R57	R(42,45)	1.0885	-DE/DX = 0.0	!
! R58	R(46,47)	1.0847	-DE/DX = 0.0	!
! R59	R(46,48)	1.5123	-DE/DX = 0.0	!
! R60	R(46,61)	1.4376	-DE/DX = 0.0	!
! R61	R(48,49)	1.0932	-DE/DX = 0.0	!
! R62	R(48,50)	1.0947	-DE/DX = 0.0	!
! R63	R(48,51)	1.5475	-DE/DX = 0.0	!
! R64	R(51,52)	1.0918	-DE/DX = 0.0	!
! R65	R(53,54)	1.0791	-DE/DX = 0.0	!
! R66	R(53,55)	1.3567	-DE/DX = 0.0	!
! R67	R(55,56)	1.0772	-DE/DX = 0.0	!
! R68	R(57,58)	1.0766	-DE/DX = 0.0	!
! R69	R(60,62)	1.37	-DE/DX = 0.0	!
! R70	R(62,63)	1.5	-DE/DX = 0.0	!
! R71	R(62,65)	1.2113	-DE/DX = 0.0	!
! R72	R(63,64)	1.3403	-DE/DX = 0.0	!
! R73	R(63,71)	1.5135	-DE/DX = 0.0	!
! R74	R(64,66)	1.0862	-DE/DX = 0.0	!
! R75	R(64,67)	1.4959	-DE/DX = 0.0	!
! R76	R(67,68)	1.09	-DE/DX = 0.0	!
! R77	R(67,69)	1.0958	-DE/DX = 0.0	!
! R78	R(67,70)	1.0957	-DE/DX = 0.0	!
! R79	R(71,72)	1.0907	-DE/DX = 0.0	!
! R80	R(71,73)	1.0947	-DE/DX = 0.0	!
! R81	R(71,74)	1.0908	-DE/DX = 0.0	!
! A1	A(2,1,3)	115.0591	-DE/DX = 0.0	!
! A2	A(2,1,20)	105.3058	-DE/DX = 0.0	!
! A3	A(2,1,22)	105.0548	-DE/DX = 0.0	!
! A4	A(3,1,20)	105.3428	-DE/DX = 0.0	!
! A5	A(3,1,22)	109.9326	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.416	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.0461	-DE/DX = 0.0	!
! A8	A(1,2,34)	118.858	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.9135	-DE/DX = 0.0	!
! A10	A(1,3,4)	117.3499	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.3696	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.4708	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.7275	-DE/DX = 0.0	!
! A14	A(4,3,59)	111.0566	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.302	-DE/DX = 0.0	!
! A16	A(3,4,12)	116.8466	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.389	-DE/DX = 0.0	!
! A18	A(5,4,12)	111.1131	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.5557	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.2585	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.2513	-DE/DX = 0.0	!

! A22	A(4,5,46)	126.1993	-DE/DX = 0.0	!
! A23	A(4,5,61)	113.6922	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.2667	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.6384	-DE/DX = 0.0	!
! A26	A(5,6,26)	107.3025	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.5006	-DE/DX = 0.0	!
! A28	A(5,6,51)	102.0115	-DE/DX = 0.0	!
! A29	A(26,6,42)	108.9149	-DE/DX = 0.0	!
! A30	A(26,6,51)	114.0014	-DE/DX = 0.0	!
! A31	A(42,6,51)	110.0888	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.5381	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.5195	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.3293	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.6193	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.3876	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.42	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.0925	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.175	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.7144	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.206	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.6622	-DE/DX = 0.0	!
! A43	A(12,9,20)	108.9954	-DE/DX = 0.0	!
! A44	A(9,11,29)	109.9018	-DE/DX = 0.0	!
! A45	A(4,12,9)	110.398	-DE/DX = 0.0	!
! A46	A(4,12,13)	107.0937	-DE/DX = 0.0	!
! A47	A(4,12,60)	111.4849	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.5238	-DE/DX = 0.0	!
! A49	A(9,12,60)	108.2508	-DE/DX = 0.0	!
! A50	A(13,12,60)	109.0922	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.1692	-DE/DX = 0.0	!
! A52	A(51,14,57)	128.6558	-DE/DX = 0.0	!
! A53	A(53,14,57)	105.1666	-DE/DX = 0.0	!
! A54	A(55,15,57)	106.8013	-DE/DX = 0.0	!
! A55	A(8,16,17)	109.074	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.1961	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.4813	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.6466	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.6132	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.6534	-DE/DX = 0.0	!
! A61	A(1,20,8)	120.7705	-DE/DX = 0.0	!
! A62	A(1,20,9)	118.3732	-DE/DX = 0.0	!
! A63	A(1,20,21)	104.0202	-DE/DX = 0.0	!
! A64	A(8,20,9)	104.36	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.9435	-DE/DX = 0.0	!
! A66	A(9,20,21)	104.0736	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.4272	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.3187	-DE/DX = 0.0	!
! A69	A(1,22,25)	108.9347	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.6204	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.7097	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.6917	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.4903	-DE/DX = 0.0	!

! A74	A(6,26,28)	110.5815	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.5216	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.3854	-DE/DX = 0.0	!
! A77	A(27,26,40)	108.978	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.75	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.594	-DE/DX = 0.0	!
! A80	A(8,29,30)	112.0162	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.7035	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.3815	-DE/DX = 0.0	!
! A83	A(11,29,31)	107.3691	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.503	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.5162	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.4387	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.8989	-DE/DX = 0.0	!
! A88	A(2,34,32)	125.2584	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.7016	-DE/DX = 0.0	!
! A90	A(32,34,35)	120.833	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.4906	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.5298	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.4425	-DE/DX = 0.0	!
! A94	A(37,36,38)	108.1527	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.6004	-DE/DX = 0.0	!
! A96	A(38,36,39)	108.5092	-DE/DX = 0.0	!
! A97	A(3,40,26)	124.7373	-DE/DX = 0.0	!
! A98	A(3,40,41)	116.3885	-DE/DX = 0.0	!
! A99	A(26,40,41)	115.2071	-DE/DX = 0.0	!
! A100	A(26,40,59)	116.0753	-DE/DX = 0.0	!
! A101	A(41,40,59)	112.2757	-DE/DX = 0.0	!
! A102	A(6,42,43)	108.5191	-DE/DX = 0.0	!
! A103	A(6,42,44)	112.4207	-DE/DX = 0.0	!
! A104	A(6,42,45)	112.2378	-DE/DX = 0.0	!
! A105	A(43,42,44)	108.0579	-DE/DX = 0.0	!
! A106	A(43,42,45)	108.0197	-DE/DX = 0.0	!
! A107	A(44,42,45)	107.4199	-DE/DX = 0.0	!
! A108	A(5,46,47)	123.4126	-DE/DX = 0.0	!
! A109	A(5,46,48)	109.8537	-DE/DX = 0.0	!
! A110	A(47,46,48)	121.1461	-DE/DX = 0.0	!
! A111	A(47,46,61)	115.0803	-DE/DX = 0.0	!
! A112	A(48,46,61)	111.7203	-DE/DX = 0.0	!
! A113	A(46,48,49)	112.5105	-DE/DX = 0.0	!
! A114	A(46,48,50)	109.3906	-DE/DX = 0.0	!
! A115	A(46,48,51)	103.0253	-DE/DX = 0.0	!
! A116	A(49,48,50)	107.7377	-DE/DX = 0.0	!
! A117	A(49,48,51)	111.9812	-DE/DX = 0.0	!
! A118	A(50,48,51)	112.2078	-DE/DX = 0.0	!
! A119	A(6,51,14)	116.6156	-DE/DX = 0.0	!
! A120	A(6,51,48)	104.3539	-DE/DX = 0.0	!
! A121	A(6,51,52)	106.1635	-DE/DX = 0.0	!
! A122	A(14,51,48)	115.1809	-DE/DX = 0.0	!
! A123	A(14,51,52)	107.0351	-DE/DX = 0.0	!
! A124	A(48,51,52)	106.7881	-DE/DX = 0.0	!
! A125	A(14,53,54)	127.0085	-DE/DX = 0.0	!

! A126 A(14,53,55)	106.8606	-DE/DX = 0.0	!
! A127 A(54,53,55)	126.1289	-DE/DX = 0.0	!
! A128 A(15,55,53)	110.235	-DE/DX = 0.0	!
! A129 A(15,55,56)	116.0609	-DE/DX = 0.0	!
! A130 A(53,55,56)	133.7024	-DE/DX = 0.0	!
! A131 A(14,57,15)	110.9356	-DE/DX = 0.0	!
! A132 A(14,57,58)	133.6488	-DE/DX = 0.0	!
! A133 A(15,57,58)	115.4153	-DE/DX = 0.0	!
! A134 A(12,60,62)	122.2629	-DE/DX = 0.0	!
! A135 A(60,62,63)	119.4932	-DE/DX = 0.0	!
! A136 A(60,62,65)	117.1467	-DE/DX = 0.0	!
! A137 A(63,62,65)	123.0718	-DE/DX = 0.0	!
! A138 A(62,63,64)	116.7661	-DE/DX = 0.0	!
! A139 A(62,63,71)	118.5815	-DE/DX = 0.0	!
! A140 A(64,63,71)	124.5124	-DE/DX = 0.0	!
! A141 A(63,64,66)	117.2641	-DE/DX = 0.0	!
! A142 A(63,64,67)	127.2514	-DE/DX = 0.0	!
! A143 A(66,64,67)	115.47	-DE/DX = 0.0	!
! A144 A(64,67,68)	113.4659	-DE/DX = 0.0	!
! A145 A(64,67,69)	110.1136	-DE/DX = 0.0	!
! A146 A(64,67,70)	110.2071	-DE/DX = 0.0	!
! A147 A(68,67,69)	108.0324	-DE/DX = 0.0	!
! A148 A(68,67,70)	108.4587	-DE/DX = 0.0	!
! A149 A(69,67,70)	106.2837	-DE/DX = 0.0	!
! A150 A(63,71,72)	111.0742	-DE/DX = 0.0	!
! A151 A(63,71,73)	112.906	-DE/DX = 0.0	!
! A152 A(63,71,74)	110.4081	-DE/DX = 0.0	!
! A153 A(72,71,73)	107.7672	-DE/DX = 0.0	!
! A154 A(72,71,74)	107.3475	-DE/DX = 0.0	!
! A155 A(73,71,74)	107.0925	-DE/DX = 0.0	!
! D1 D(3,1,2,7)	-55.1299	-DE/DX = 0.0	!
! D2 D(3,1,2,34)	129.834	-DE/DX = 0.0	!
! D3 D(20,1,2,7)	-170.6476	-DE/DX = 0.0	!
! D4 D(20,1,2,34)	14.3163	-DE/DX = 0.0	!
! D5 D(22,1,2,7)	65.8994	-DE/DX = 0.0	!
! D6 D(22,1,2,34)	-109.1366	-DE/DX = 0.0	!
! D7 D(2,1,3,4)	-154.3084	-DE/DX = 0.0	!
! D8 D(2,1,3,40)	7.5273	-DE/DX = 0.0	!
! D9 D(2,1,3,59)	73.9645	-DE/DX = 0.0	!
! D10 D(20,1,3,4)	-38.8119	-DE/DX = 0.0	!
! D11 D(20,1,3,40)	123.0237	-DE/DX = 0.0	!
! D12 D(20,1,3,59)	-170.5391	-DE/DX = 0.0	!
! D13 D(22,1,3,4)	87.3609	-DE/DX = 0.0	!
! D14 D(22,1,3,40)	-110.8035	-DE/DX = 0.0	!
! D15 D(22,1,3,59)	-44.3663	-DE/DX = 0.0	!
! D16 D(2,1,20,8)	-49.39	-DE/DX = 0.0	!
! D17 D(2,1,20,9)	-179.9046	-DE/DX = 0.0	!
! D18 D(2,1,20,21)	65.2788	-DE/DX = 0.0	!
! D19 D(3,1,20,8)	-171.4256	-DE/DX = 0.0	!
! D20 D(3,1,20,9)	58.0598	-DE/DX = 0.0	!
! D21 D(3,1,20,21)	-56.7569	-DE/DX = 0.0	!
! D22 D(22,1,20,8)	66.4997	-DE/DX = 0.0	!

! D23	D(22,1,20,9)	-64.0149	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	-178.8315	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	40.8735	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	161.7122	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-77.8187	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	165.2131	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-73.9482	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	46.5209	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-75.1561	-DE/DX = 0.0	!
! D32	D(20,1,22,24)	45.6826	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	166.1517	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	9.2672	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-175.9511	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-165.9264	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	8.8552	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	160.7282	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	34.3829	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-82.2187	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-1.2289	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-127.5742	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	115.8242	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-66.4573	-DE/DX = 0.0	!
! D45	D(59,3,4,12)	167.1974	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	50.5958	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-157.7032	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.3982	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	3.7028	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	161.0078	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-31.7632	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	171.1527	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	103.5411	-DE/DX = 0.0	!
! D54	D(12,4,5,6)	97.8506	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-59.2335	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-126.8452	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-148.063	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	54.8529	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-12.7587	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-39.4947	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-159.8721	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	80.8661	-DE/DX = 0.0	!
! D63	D(5,4,12,9)	-164.4355	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	75.1871	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-44.0747	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	78.8147	-DE/DX = 0.0	!
! D67	D(36,4,12,13)	-41.5626	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-160.8244	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-170.4551	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-50.7795	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	69.969	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-53.5681	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	66.1075	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-173.144	-DE/DX = 0.0	!

! D75	D(12,4,36,37)	64.944	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-175.3804	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-54.6319	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	59.8821	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-61.1217	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	-179.9952	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-139.4408	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	99.5555	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-19.3181	-DE/DX = 0.0	!
! D84	D(61,5,6,26)	-76.9735	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	162.0227	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	43.1492	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	4.0084	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	157.7738	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-155.7011	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-1.9358	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-171.9656	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	69.2803	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-50.5963	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-47.501	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-166.2551	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	73.8683	-DE/DX = 0.0	!
! D97	D(51,6,26,27)	75.8675	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-42.8866	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-162.7632	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-178.8413	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-59.3795	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	61.857	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	61.0481	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.4901	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.2536	-DE/DX = 0.0	!
! D106	D(51,6,42,43)	-64.6245	-DE/DX = 0.0	!
! D107	D(51,6,42,44)	54.8373	-DE/DX = 0.0	!
! D108	D(51,6,42,45)	176.0738	-DE/DX = 0.0	!
! D109	D(5,6,51,14)	161.2716	-DE/DX = 0.0	!
! D110	D(5,6,51,48)	32.9937	-DE/DX = 0.0	!
! D111	D(5,6,51,52)	-79.6239	-DE/DX = 0.0	!
! D112	D(26,6,51,14)	-83.4137	-DE/DX = 0.0	!
! D113	D(26,6,51,48)	148.3084	-DE/DX = 0.0	!
! D114	D(26,6,51,52)	35.6908	-DE/DX = 0.0	!
! D115	D(42,6,51,14)	39.3158	-DE/DX = 0.0	!
! D116	D(42,6,51,48)	-88.962	-DE/DX = 0.0	!
! D117	D(42,6,51,52)	158.4203	-DE/DX = 0.0	!
! D118	D(20,8,16,17)	-173.8232	-DE/DX = 0.0	!
! D119	D(20,8,16,18)	-55.2606	-DE/DX = 0.0	!
! D120	D(20,8,16,19)	66.863	-DE/DX = 0.0	!
! D121	D(29,8,16,17)	-65.6579	-DE/DX = 0.0	!
! D122	D(29,8,16,18)	52.9047	-DE/DX = 0.0	!
! D123	D(29,8,16,19)	175.0283	-DE/DX = 0.0	!
! D124	D(32,8,16,17)	64.8388	-DE/DX = 0.0	!
! D125	D(32,8,16,18)	-176.5985	-DE/DX = 0.0	!
! D126	D(32,8,16,19)	-54.475	-DE/DX = 0.0	!

! D127 D(16,8,20,1)	-65.648	-DE/DX = 0.0	!
! D128 D(16,8,20,9)	70.6834	-DE/DX = 0.0	!
! D129 D(16,8,20,21)	179.1283	-DE/DX = 0.0	!
! D130 D(29,8,20,1)	179.4465	-DE/DX = 0.0	!
! D131 D(29,8,20,9)	-44.2221	-DE/DX = 0.0	!
! D132 D(29,8,20,21)	64.2228	-DE/DX = 0.0	!
! D133 D(32,8,20,1)	57.2016	-DE/DX = 0.0	!
! D134 D(32,8,20,9)	-166.4671	-DE/DX = 0.0	!
! D135 D(32,8,20,21)	-58.0221	-DE/DX = 0.0	!
! D136 D(16,8,29,11)	-82.4567	-DE/DX = 0.0	!
! D137 D(16,8,29,30)	159.1726	-DE/DX = 0.0	!
! D138 D(16,8,29,31)	34.3648	-DE/DX = 0.0	!
! D139 D(20,8,29,11)	39.5306	-DE/DX = 0.0	!
! D140 D(20,8,29,30)	-78.8401	-DE/DX = 0.0	!
! D141 D(20,8,29,31)	156.3522	-DE/DX = 0.0	!
! D142 D(32,8,29,11)	152.2207	-DE/DX = 0.0	!
! D143 D(32,8,29,30)	33.85	-DE/DX = 0.0	!
! D144 D(32,8,29,31)	-90.9578	-DE/DX = 0.0	!
! D145 D(16,8,32,33)	-75.4269	-DE/DX = 0.0	!
! D146 D(16,8,32,34)	100.1753	-DE/DX = 0.0	!
! D147 D(20,8,32,33)	156.7041	-DE/DX = 0.0	!
! D148 D(20,8,32,34)	-27.6937	-DE/DX = 0.0	!
! D149 D(29,8,32,33)	49.501	-DE/DX = 0.0	!
! D150 D(29,8,32,34)	-134.8968	-DE/DX = 0.0	!
! D151 D(10,9,11,29)	113.928	-DE/DX = 0.0	!
! D152 D(12,9,11,29)	-125.0061	-DE/DX = 0.0	!
! D153 D(20,9,11,29)	-7.0581	-DE/DX = 0.0	!
! D154 D(10,9,12,4)	-72.3446	-DE/DX = 0.0	!
! D155 D(10,9,12,13)	45.9537	-DE/DX = 0.0	!
! D156 D(10,9,12,60)	165.3737	-DE/DX = 0.0	!
! D157 D(11,9,12,4)	167.2029	-DE/DX = 0.0	!
! D158 D(11,9,12,13)	-74.4988	-DE/DX = 0.0	!
! D159 D(11,9,12,60)	44.9212	-DE/DX = 0.0	!
! D160 D(20,9,12,4)	52.408	-DE/DX = 0.0	!
! D161 D(20,9,12,13)	170.7062	-DE/DX = 0.0	!
! D162 D(20,9,12,60)	-69.8737	-DE/DX = 0.0	!
! D163 D(10,9,20,1)	53.8703	-DE/DX = 0.0	!
! D164 D(10,9,20,8)	-83.7312	-DE/DX = 0.0	!
! D165 D(10,9,20,21)	168.658	-DE/DX = 0.0	!
! D166 D(11,9,20,1)	170.9896	-DE/DX = 0.0	!
! D167 D(11,9,20,8)	33.3881	-DE/DX = 0.0	!
! D168 D(11,9,20,21)	-74.2227	-DE/DX = 0.0	!
! D169 D(12,9,20,1)	-68.1772	-DE/DX = 0.0	!
! D170 D(12,9,20,8)	154.2213	-DE/DX = 0.0	!
! D171 D(12,9,20,21)	46.6105	-DE/DX = 0.0	!
! D172 D(9,11,29,8)	-21.5706	-DE/DX = 0.0	!
! D173 D(9,11,29,30)	98.5772	-DE/DX = 0.0	!
! D174 D(9,11,29,31)	-142.6814	-DE/DX = 0.0	!
! D175 D(4,12,60,62)	164.8348	-DE/DX = 0.0	!
! D176 D(9,12,60,62)	-73.5505	-DE/DX = 0.0	!
! D177 D(13,12,60,62)	46.7674	-DE/DX = 0.0	!
! D178 D(53,14,51,6)	76.1367	-DE/DX = 0.0	!

! D179	D(53,14,51,48)	-161.0426	-DE/DX = 0.0	!
! D180	D(53,14,51,52)	-42.4965	-DE/DX = 0.0	!
! D181	D(57,14,51,6)	-105.0756	-DE/DX = 0.0	!
! D182	D(57,14,51,48)	17.7451	-DE/DX = 0.0	!
! D183	D(57,14,51,52)	136.2913	-DE/DX = 0.0	!
! D184	D(51,14,53,54)	-0.1703	-DE/DX = 0.0	!
! D185	D(51,14,53,55)	179.3248	-DE/DX = 0.0	!
! D186	D(57,14,53,54)	-179.1895	-DE/DX = 0.0	!
! D187	D(57,14,53,55)	0.3056	-DE/DX = 0.0	!
! D188	D(51,14,57,15)	-179.2387	-DE/DX = 0.0	!
! D189	D(51,14,57,58)	0.5377	-DE/DX = 0.0	!
! D190	D(53,14,57,15)	-0.2526	-DE/DX = 0.0	!
! D191	D(53,14,57,58)	179.5238	-DE/DX = 0.0	!
! D192	D(57,15,55,53)	0.1015	-DE/DX = 0.0	!
! D193	D(57,15,55,56)	179.6907	-DE/DX = 0.0	!
! D194	D(55,15,57,14)	0.105	-DE/DX = 0.0	!
! D195	D(55,15,57,58)	-179.7159	-DE/DX = 0.0	!
! D196	D(6,26,40,3)	24.4084	-DE/DX = 0.0	!
! D197	D(6,26,40,41)	-133.1341	-DE/DX = 0.0	!
! D198	D(6,26,40,59)	92.6964	-DE/DX = 0.0	!
! D199	D(27,26,40,3)	146.6525	-DE/DX = 0.0	!
! D200	D(27,26,40,41)	-10.89	-DE/DX = 0.0	!
! D201	D(27,26,40,59)	-145.0595	-DE/DX = 0.0	!
! D202	D(28,26,40,3)	-97.1256	-DE/DX = 0.0	!
! D203	D(28,26,40,41)	105.3319	-DE/DX = 0.0	!
! D204	D(28,26,40,59)	-28.8376	-DE/DX = 0.0	!
! D205	D(8,32,34,2)	-1.5171	-DE/DX = 0.0	!
! D206	D(8,32,34,35)	-175.9514	-DE/DX = 0.0	!
! D207	D(33,32,34,2)	174.0683	-DE/DX = 0.0	!
! D208	D(33,32,34,35)	-0.366	-DE/DX = 0.0	!
! D209	D(5,46,48,49)	143.696	-DE/DX = 0.0	!
! D210	D(5,46,48,50)	-96.6023	-DE/DX = 0.0	!
! D211	D(5,46,48,51)	22.9159	-DE/DX = 0.0	!
! D212	D(47,46,48,49)	-61.8438	-DE/DX = 0.0	!
! D213	D(47,46,48,50)	57.8579	-DE/DX = 0.0	!
! D214	D(47,46,48,51)	177.3762	-DE/DX = 0.0	!
! D215	D(61,46,48,49)	78.8596	-DE/DX = 0.0	!
! D216	D(61,46,48,50)	-161.4387	-DE/DX = 0.0	!
! D217	D(61,46,48,51)	-41.9204	-DE/DX = 0.0	!
! D218	D(46,48,51,6)	-34.3925	-DE/DX = 0.0	!
! D219	D(46,48,51,14)	-163.5395	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	77.7768	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-155.5334	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	75.3196	-DE/DX = 0.0	!
! D223	D(49,48,51,52)	-43.3642	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	83.1574	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-45.9895	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-164.6733	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2541	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.7436	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.2466	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.2429	-DE/DX = 0.0	!

! D231	D(12,60,62,63)	-40.5681	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	145.4084	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	138.214	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-45.8923	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-48.1339	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	127.7598	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-2.7197	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	178.7359	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-178.3431	-DE/DX = 0.0	!
! D240	D(71,63,64,67)	3.1125	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-23.6737	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	97.514	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-142.6411	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	151.8762	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-86.936	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	32.9089	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	-2.6458	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	118.5765	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-124.4883	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	178.7874	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-59.9903	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	56.9449	-DE/DX = 0.0	!

5. opt=tight b3pw91/6-311++g(d,p) nosymm

! Optimized Parameters !				
! (Angstroms and Degrees) !				

! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.5521	-DE/DX = 0.0	!
! R2	R(1,3)	1.5719	-DE/DX = 0.0	!
! R3	R(1,20)	1.5153	-DE/DX = 0.0	!
! R4	R(1,22)	1.5439	-DE/DX = 0.0	!
! R5	R(2,7)	1.2152	-DE/DX = 0.0	!
! R6	R(2,34)	1.492	-DE/DX = 0.0	!
! R7	R(3,4)	1.5866	-DE/DX = 0.0	!
! R8	R(3,40)	1.4931	-DE/DX = 0.0	!
! R9	R(3,59)	1.4236	-DE/DX = 0.0	!
! R10	R(4,5)	1.5473	-DE/DX = 0.0	!
! R11	R(4,12)	1.5676	-DE/DX = 0.0	!
! R12	R(4,36)	1.5471	-DE/DX = 0.0	!
! R13	R(5,6)	1.5401	-DE/DX = 0.0	!
! R14	R(5,46)	1.4686	-DE/DX = 0.0	!
! R15	R(5,61)	1.4473	-DE/DX = 0.0	!
! R16	R(6,26)	1.5246	-DE/DX = 0.0	!
! R17	R(6,42)	1.5298	-DE/DX = 0.0	!
! R18	R(6,51)	1.5724	-DE/DX = 0.0	!
! R19	R(8,16)	1.5405	-DE/DX = 0.0	!
! R20	R(8,20)	1.5276	-DE/DX = 0.0	!

! R21	R(8,29)	1.5416	-DE/DX = 0.0	!
! R22	R(8,32)	1.4958	-DE/DX = 0.0	!
! R23	R(9,10)	1.0952	-DE/DX = 0.0	!
! R24	R(9,11)	1.4304	-DE/DX = 0.0	!
! R25	R(9,12)	1.5311	-DE/DX = 0.0	!
! R26	R(9,20)	1.4999	-DE/DX = 0.0	!
! R27	R(11,29)	1.4438	-DE/DX = 0.0	!
! R28	R(12,13)	1.0936	-DE/DX = 0.0	!
! R29	R(12,60)	1.4255	-DE/DX = 0.0	!
! R30	R(14,51)	1.4953	-DE/DX = 0.0	!
! R31	R(14,53)	1.4387	-DE/DX = 0.0	!
! R32	R(14,57)	1.3614	-DE/DX = 0.0	!
! R33	R(15,55)	1.3548	-DE/DX = 0.0	!
! R34	R(15,57)	1.3592	-DE/DX = 0.0	!
! R35	R(16,17)	1.0947	-DE/DX = 0.0	!
! R36	R(16,18)	1.0933	-DE/DX = 0.0	!
! R37	R(16,19)	1.0893	-DE/DX = 0.0	!
! R38	R(20,21)	1.1004	-DE/DX = 0.0	!
! R39	R(22,23)	1.0912	-DE/DX = 0.0	!
! R40	R(22,24)	1.0915	-DE/DX = 0.0	!
! R41	R(22,25)	1.0905	-DE/DX = 0.0	!
! R42	R(26,27)	1.0944	-DE/DX = 0.0	!
! R43	R(26,28)	1.0953	-DE/DX = 0.0	!
! R44	R(26,40)	1.5137	-DE/DX = 0.0	!
! R45	R(29,30)	1.0964	-DE/DX = 0.0	!
! R46	R(29,31)	1.0926	-DE/DX = 0.0	!
! R47	R(32,33)	1.0891	-DE/DX = 0.0	!
! R48	R(32,34)	1.3422	-DE/DX = 0.0	!
! R49	R(34,35)	1.0862	-DE/DX = 0.0	!
! R50	R(36,37)	1.0921	-DE/DX = 0.0	!
! R51	R(36,38)	1.0872	-DE/DX = 0.0	!
! R52	R(36,39)	1.0906	-DE/DX = 0.0	!
! R53	R(40,41)	1.084	-DE/DX = 0.0	!
! R54	R(40,59)	1.4282	-DE/DX = 0.0	!
! R55	R(42,43)	1.0934	-DE/DX = 0.0	!
! R56	R(42,44)	1.0906	-DE/DX = 0.0	!
! R57	R(42,45)	1.0894	-DE/DX = 0.0	!
! R58	R(46,47)	1.087	-DE/DX = 0.0	!
! R59	R(46,48)	1.5088	-DE/DX = 0.0	!
! R60	R(46,61)	1.4254	-DE/DX = 0.0	!
! R61	R(48,49)	1.094	-DE/DX = 0.0	!
! R62	R(48,50)	1.0961	-DE/DX = 0.0	!
! R63	R(48,51)	1.5408	-DE/DX = 0.0	!
! R64	R(51,52)	1.0933	-DE/DX = 0.0	!
! R65	R(53,54)	1.0799	-DE/DX = 0.0	!
! R66	R(53,55)	1.3559	-DE/DX = 0.0	!
! R67	R(55,56)	1.0781	-DE/DX = 0.0	!
! R68	R(57,58)	1.0776	-DE/DX = 0.0	!
! R69	R(60,62)	1.3743	-DE/DX = 0.0	!
! R70	R(62,63)	1.4956	-DE/DX = 0.0	!
! R71	R(62,65)	1.2046	-DE/DX = 0.0	!
! R72	R(63,64)	1.3394	-DE/DX = 0.0	!

! R73	R(63,71)	1.5071	-DE/DX = 0.0	!
! R74	R(64,66)	1.0869	-DE/DX = 0.0	!
! R75	R(64,67)	1.4898	-DE/DX = 0.0	!
! R76	R(67,68)	1.091	-DE/DX = 0.0	!
! R77	R(67,69)	1.0964	-DE/DX = 0.0	!
! R78	R(67,70)	1.0963	-DE/DX = 0.0	!
! R79	R(71,72)	1.09	-DE/DX = 0.0	!
! R80	R(71,73)	1.096	-DE/DX = 0.0	!
! R81	R(71,74)	1.0928	-DE/DX = 0.0	!
! A1	A(2,1,3)	115.3042	-DE/DX = 0.0	!
! A2	A(2,1,20)	105.0195	-DE/DX = 0.0	!
! A3	A(2,1,22)	104.7619	-DE/DX = 0.0	!
! A4	A(3,1,20)	105.9491	-DE/DX = 0.0	!
! A5	A(3,1,22)	109.4774	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.6212	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.6012	-DE/DX = 0.0	!
! A8	A(1,2,34)	118.5112	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.6899	-DE/DX = 0.0	!
! A10	A(1,3,4)	117.4703	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.4781	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.274	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.7605	-DE/DX = 0.0	!
! A14	A(4,3,59)	110.7288	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.446	-DE/DX = 0.0	!
! A16	A(3,4,12)	116.8336	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.2213	-DE/DX = 0.0	!
! A18	A(5,4,12)	111.031	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.089	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.7988	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.2181	-DE/DX = 0.0	!
! A22	A(4,5,46)	126.1315	-DE/DX = 0.0	!
! A23	A(4,5,61)	114.0173	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.2513	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.6935	-DE/DX = 0.0	!
! A26	A(5,6,26)	107.1359	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.5313	-DE/DX = 0.0	!
! A28	A(5,6,51)	101.8916	-DE/DX = 0.0	!
! A29	A(26,6,42)	109.1443	-DE/DX = 0.0	!
! A30	A(26,6,51)	113.9406	-DE/DX = 0.0	!
! A31	A(42,6,51)	110.1443	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.3986	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.527	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.619	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.4146	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.432	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.3462	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.3478	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.3648	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.6017	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.1493	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.8971	-DE/DX = 0.0	!
! A43	A(12,9,20)	108.4814	-DE/DX = 0.0	!

! A44	A(9,11,29)	109.819	-DE/DX = 0.0	!
! A45	A(4,12,9)	109.811	-DE/DX = 0.0	!
! A46	A(4,12,13)	107.1958	-DE/DX = 0.0	!
! A47	A(4,12,60)	111.3257	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.5701	-DE/DX = 0.0	!
! A49	A(9,12,60)	108.4512	-DE/DX = 0.0	!
! A50	A(13,12,60)	109.4933	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.2986	-DE/DX = 0.0	!
! A52	A(51,14,57)	128.7371	-DE/DX = 0.0	!
! A53	A(53,14,57)	104.9597	-DE/DX = 0.0	!
! A54	A(55,15,57)	106.8133	-DE/DX = 0.0	!
! A55	A(8,16,17)	109.2938	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.1021	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.5088	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.4736	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.5375	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.7389	-DE/DX = 0.0	!
! A61	A(1,20,8)	120.9914	-DE/DX = 0.0	!
! A62	A(1,20,9)	118.6818	-DE/DX = 0.0	!
! A63	A(1,20,21)	104.0531	-DE/DX = 0.0	!
! A64	A(8,20,9)	104.0389	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.8796	-DE/DX = 0.0	!
! A66	A(9,20,21)	103.7827	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.5209	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.2616	-DE/DX = 0.0	!
! A69	A(1,22,25)	108.5112	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.8623	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.7517	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.8058	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.3925	-DE/DX = 0.0	!
! A74	A(6,26,28)	110.4568	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.4199	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.6919	-DE/DX = 0.0	!
! A77	A(27,26,40)	109.2051	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.5575	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.6712	-DE/DX = 0.0	!
! A80	A(8,29,30)	112.0231	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.5599	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.4555	-DE/DX = 0.0	!
! A83	A(11,29,31)	107.3042	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.5579	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.6059	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.4312	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.8398	-DE/DX = 0.0	!
! A88	A(2,34,32)	125.5114	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.2668	-DE/DX = 0.0	!
! A90	A(32,34,35)	121.0488	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.6524	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.1988	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.5392	-DE/DX = 0.0	!
! A94	A(37,36,38)	107.9713	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.8241	-DE/DX = 0.0	!

! A96 A(38,36,39)	108.5417	-DE/DX = 0.0	!
! A97 A(3,40,26)	124.3541	-DE/DX = 0.0	!
! A98 A(3,40,41)	116.2163	-DE/DX = 0.0	!
! A99 A(26,40,41)	115.7399	-DE/DX = 0.0	!
! A100 A(26,40,59)	115.9905	-DE/DX = 0.0	!
! A101 A(41,40,59)	112.2124	-DE/DX = 0.0	!
! A102 A(6,42,43)	108.6051	-DE/DX = 0.0	!
! A103 A(6,42,44)	112.5355	-DE/DX = 0.0	!
! A104 A(6,42,45)	112.3143	-DE/DX = 0.0	!
! A105 A(43,42,44)	107.8578	-DE/DX = 0.0	!
! A106 A(43,42,45)	108.2575	-DE/DX = 0.0	!
! A107 A(44,42,45)	107.0996	-DE/DX = 0.0	!
! A108 A(5,46,47)	123.2612	-DE/DX = 0.0	!
! A109 A(5,46,48)	109.643	-DE/DX = 0.0	!
! A110 A(47,46,48)	121.3794	-DE/DX = 0.0	!
! A111 A(47,46,61)	115.0785	-DE/DX = 0.0	!
! A112 A(48,46,61)	111.8859	-DE/DX = 0.0	!
! A113 A(46,48,49)	112.8301	-DE/DX = 0.0	!
! A114 A(46,48,50)	109.4774	-DE/DX = 0.0	!
! A115 A(46,48,51)	102.6915	-DE/DX = 0.0	!
! A116 A(49,48,50)	107.8282	-DE/DX = 0.0	!
! A117 A(49,48,51)	111.9797	-DE/DX = 0.0	!
! A118 A(50,48,51)	112.0371	-DE/DX = 0.0	!
! A119 A(6,51,14)	116.3993	-DE/DX = 0.0	!
! A120 A(6,51,48)	104.3511	-DE/DX = 0.0	!
! A121 A(6,51,52)	106.1769	-DE/DX = 0.0	!
! A122 A(14,51,48)	115.2757	-DE/DX = 0.0	!
! A123 A(14,51,52)	107.3745	-DE/DX = 0.0	!
! A124 A(48,51,52)	106.535	-DE/DX = 0.0	!
! A125 A(14,53,54)	127.1029	-DE/DX = 0.0	!
! A126 A(14,53,55)	106.6618	-DE/DX = 0.0	!
! A127 A(54,53,55)	126.2308	-DE/DX = 0.0	!
! A128 A(15,55,53)	110.4305	-DE/DX = 0.0	!
! A129 A(15,55,56)	116.0171	-DE/DX = 0.0	!
! A130 A(53,55,56)	133.5502	-DE/DX = 0.0	!
! A131 A(14,57,15)	111.1339	-DE/DX = 0.0	!
! A132 A(14,57,58)	133.4899	-DE/DX = 0.0	!
! A133 A(15,57,58)	115.3757	-DE/DX = 0.0	!
! A134 A(12,60,62)	121.8099	-DE/DX = 0.0	!
! A135 A(60,62,63)	118.6273	-DE/DX = 0.0	!
! A136 A(60,62,65)	117.6414	-DE/DX = 0.0	!
! A137 A(63,62,65)	123.4069	-DE/DX = 0.0	!
! A138 A(62,63,64)	116.1754	-DE/DX = 0.0	!
! A139 A(62,63,71)	119.7175	-DE/DX = 0.0	!
! A140 A(64,63,71)	123.9876	-DE/DX = 0.0	!
! A141 A(63,64,66)	116.884	-DE/DX = 0.0	!
! A142 A(63,64,67)	126.9123	-DE/DX = 0.0	!
! A143 A(66,64,67)	116.1995	-DE/DX = 0.0	!
! A144 A(64,67,68)	113.384	-DE/DX = 0.0	!
! A145 A(64,67,69)	110.2417	-DE/DX = 0.0	!
! A146 A(64,67,70)	110.3442	-DE/DX = 0.0	!
! A147 A(68,67,69)	107.9748	-DE/DX = 0.0	!

! A148	A(68,67,70)	108.3647	-DE/DX = 0.0	!
! A149	A(69,67,70)	106.2482	-DE/DX = 0.0	!
! A150	A(63,71,72)	110.9096	-DE/DX = 0.0	!
! A151	A(63,71,73)	112.8938	-DE/DX = 0.0	!
! A152	A(63,71,74)	110.479	-DE/DX = 0.0	!
! A153	A(72,71,73)	107.8382	-DE/DX = 0.0	!
! A154	A(72,71,74)	107.3662	-DE/DX = 0.0	!
! A155	A(73,71,74)	107.1166	-DE/DX = 0.0	!
! D1	D(3,1,2,7)	-52.1399	-DE/DX = 0.0	!
! D2	D(3,1,2,34)	133.0409	-DE/DX = 0.0	!
! D3	D(20,1,2,7)	-168.343	-DE/DX = 0.0	!
! D4	D(20,1,2,34)	16.8378	-DE/DX = 0.0	!
! D5	D(22,1,2,7)	68.2573	-DE/DX = 0.0	!
! D6	D(22,1,2,34)	-106.5619	-DE/DX = 0.0	!
! D7	D(2,1,3,4)	-152.287	-DE/DX = 0.0	!
! D8	D(2,1,3,40)	10.4851	-DE/DX = 0.0	!
! D9	D(2,1,3,59)	76.5738	-DE/DX = 0.0	!
! D10	D(20,1,3,4)	-36.6134	-DE/DX = 0.0	!
! D11	D(20,1,3,40)	126.1587	-DE/DX = 0.0	!
! D12	D(20,1,3,59)	-167.7526	-DE/DX = 0.0	!
! D13	D(22,1,3,4)	89.9272	-DE/DX = 0.0	!
! D14	D(22,1,3,40)	-107.3006	-DE/DX = 0.0	!
! D15	D(22,1,3,59)	-41.2119	-DE/DX = 0.0	!
! D16	D(2,1,20,8)	-51.0631	-DE/DX = 0.0	!
! D17	D(2,1,20,9)	178.308	-DE/DX = 0.0	!
! D18	D(2,1,20,21)	63.6703	-DE/DX = 0.0	!
! D19	D(3,1,20,8)	-173.5387	-DE/DX = 0.0	!
! D20	D(3,1,20,9)	55.8324	-DE/DX = 0.0	!
! D21	D(3,1,20,21)	-58.8053	-DE/DX = 0.0	!
! D22	D(22,1,20,8)	64.3781	-DE/DX = 0.0	!
! D23	D(22,1,20,9)	-66.2508	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	179.1115	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	41.1651	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	162.3426	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-77.3669	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	165.362	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-73.4605	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	46.8299	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-74.4197	-DE/DX = 0.0	!
! D32	D(20,1,22,24)	46.7579	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	167.0483	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	7.1404	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-177.626	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-167.8848	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	7.3488	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	160.656	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	34.3075	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-82.8529	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-2.2448	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-128.5932	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	114.2464	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-67.0511	-DE/DX = 0.0	!

! D45	D(59,3,4,12)	166.6004	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	49.44	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-158.1356	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.7744	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	4.2444	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	161.6055	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-31.1026	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	172.2038	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	104.6945	-DE/DX = 0.0	!
! D54	D(12,4,5,6)	98.5443	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-58.1493	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-125.6586	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-147.0327	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	56.2737	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-11.2357	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-41.8273	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-161.9872	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	78.29	-DE/DX = 0.0	!
! D63	D(5,4,12,9)	-166.885	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	72.9551	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-46.7677	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	76.6506	-DE/DX = 0.0	!
! D67	D(36,4,12,13)	-43.5093	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-163.2322	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-171.7666	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-52.4256	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	68.2038	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-55.0403	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	64.3008	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-175.0698	-DE/DX = 0.0	!
! D75	D(12,4,36,37)	63.435	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-177.2239	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-56.5945	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	60.0752	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-61.1197	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	-179.9989	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-139.5873	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	99.2179	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-19.6614	-DE/DX = 0.0	!
! D84	D(61,5,6,26)	-77.3616	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	161.4436	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	42.5644	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	3.648	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	157.1961	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-155.7142	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-2.1661	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-172.9046	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	68.1018	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-51.383	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-48.367	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-167.3606	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	73.1546	-DE/DX = 0.0	!

! D97	D(51,6,26,27)	75.2055	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-43.788	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-163.2729	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-178.6306	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-59.2902	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	61.6678	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	61.2856	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.374	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.4161	-DE/DX = 0.0	!
! D106	D(51,6,42,43)	-64.5087	-DE/DX = 0.0	!
! D107	D(51,6,42,44)	54.8317	-DE/DX = 0.0	!
! D108	D(51,6,42,45)	175.7897	-DE/DX = 0.0	!
! D109	D(5,6,51,14)	162.1009	-DE/DX = 0.0	!
! D110	D(5,6,51,48)	33.855	-DE/DX = 0.0	!
! D111	D(5,6,51,52)	-78.4847	-DE/DX = 0.0	!
! D112	D(26,6,51,14)	-82.8788	-DE/DX = 0.0	!
! D113	D(26,6,51,48)	148.8753	-DE/DX = 0.0	!
! D114	D(26,6,51,52)	36.5356	-DE/DX = 0.0	!
! D115	D(42,6,51,14)	40.1503	-DE/DX = 0.0	!
! D116	D(42,6,51,48)	-88.0956	-DE/DX = 0.0	!
! D117	D(42,6,51,52)	159.5647	-DE/DX = 0.0	!
! D118	D(20,8,16,17)	-173.769	-DE/DX = 0.0	!
! D119	D(20,8,16,18)	-55.3381	-DE/DX = 0.0	!
! D120	D(20,8,16,19)	66.8474	-DE/DX = 0.0	!
! D121	D(29,8,16,17)	-65.9257	-DE/DX = 0.0	!
! D122	D(29,8,16,18)	52.5051	-DE/DX = 0.0	!
! D123	D(29,8,16,19)	174.6907	-DE/DX = 0.0	!
! D124	D(32,8,16,17)	64.6965	-DE/DX = 0.0	!
! D125	D(32,8,16,18)	-176.8727	-DE/DX = 0.0	!
! D126	D(32,8,16,19)	-54.6872	-DE/DX = 0.0	!
! D127	D(16,8,20,1)	-66.2059	-DE/DX = 0.0	!
! D128	D(16,8,20,9)	70.4547	-DE/DX = 0.0	!
! D129	D(16,8,20,21)	178.459	-DE/DX = 0.0	!
! D130	D(29,8,20,1)	179.0589	-DE/DX = 0.0	!
! D131	D(29,8,20,9)	-44.2806	-DE/DX = 0.0	!
! D132	D(29,8,20,21)	63.7238	-DE/DX = 0.0	!
! D133	D(32,8,20,1)	56.9661	-DE/DX = 0.0	!
! D134	D(32,8,20,9)	-166.3733	-DE/DX = 0.0	!
! D135	D(32,8,20,21)	-58.369	-DE/DX = 0.0	!
! D136	D(16,8,29,11)	-81.6974	-DE/DX = 0.0	!
! D137	D(16,8,29,30)	159.7934	-DE/DX = 0.0	!
! D138	D(16,8,29,31)	35.0202	-DE/DX = 0.0	!
! D139	D(20,8,29,11)	40.0424	-DE/DX = 0.0	!
! D140	D(20,8,29,30)	-78.4667	-DE/DX = 0.0	!
! D141	D(20,8,29,31)	156.7601	-DE/DX = 0.0	!
! D142	D(32,8,29,11)	152.6299	-DE/DX = 0.0	!
! D143	D(32,8,29,30)	34.1207	-DE/DX = 0.0	!
! D144	D(32,8,29,31)	-90.6525	-DE/DX = 0.0	!
! D145	D(16,8,32,33)	-74.3947	-DE/DX = 0.0	!
! D146	D(16,8,32,34)	101.566	-DE/DX = 0.0	!
! D147	D(20,8,32,33)	157.6919	-DE/DX = 0.0	!
! D148	D(20,8,32,34)	-26.3474	-DE/DX = 0.0	!

! D149	D(29,8,32,33)	50.7468	-DE/DX = 0.0	!
! D150	D(29,8,32,34)	-133.2925	-DE/DX = 0.0	!
! D151	D(10,9,11,29)	114.3675	-DE/DX = 0.0	!
! D152	D(12,9,11,29)	-124.1843	-DE/DX = 0.0	!
! D153	D(20,9,11,29)	-6.7367	-DE/DX = 0.0	!
! D154	D(10,9,12,4)	-69.7594	-DE/DX = 0.0	!
! D155	D(10,9,12,13)	48.3285	-DE/DX = 0.0	!
! D156	D(10,9,12,60)	168.3913	-DE/DX = 0.0	!
! D157	D(11,9,12,4)	169.3668	-DE/DX = 0.0	!
! D158	D(11,9,12,13)	-72.5453	-DE/DX = 0.0	!
! D159	D(11,9,12,60)	47.5175	-DE/DX = 0.0	!
! D160	D(20,9,12,4)	54.6383	-DE/DX = 0.0	!
! D161	D(20,9,12,13)	172.7262	-DE/DX = 0.0	!
! D162	D(20,9,12,60)	-67.211	-DE/DX = 0.0	!
! D163	D(10,9,20,1)	53.7167	-DE/DX = 0.0	!
! D164	D(10,9,20,8)	-84.1675	-DE/DX = 0.0	!
! D165	D(10,9,20,21)	168.5	-DE/DX = 0.0	!
! D166	D(11,9,20,1)	171.2318	-DE/DX = 0.0	!
! D167	D(11,9,20,8)	33.3476	-DE/DX = 0.0	!
! D168	D(11,9,20,21)	-73.9849	-DE/DX = 0.0	!
! D169	D(12,9,20,1)	-68.1242	-DE/DX = 0.0	!
! D170	D(12,9,20,8)	153.9916	-DE/DX = 0.0	!
! D171	D(12,9,20,21)	46.6591	-DE/DX = 0.0	!
! D172	D(9,11,29,8)	-22.1046	-DE/DX = 0.0	!
! D173	D(9,11,29,30)	98.1321	-DE/DX = 0.0	!
! D174	D(9,11,29,31)	-143.0574	-DE/DX = 0.0	!
! D175	D(4,12,60,62)	170.8473	-DE/DX = 0.0	!
! D176	D(9,12,60,62)	-68.2352	-DE/DX = 0.0	!
! D177	D(13,12,60,62)	52.4968	-DE/DX = 0.0	!
! D178	D(53,14,51,6)	76.9234	-DE/DX = 0.0	!
! D179	D(53,14,51,48)	-160.3657	-DE/DX = 0.0	!
! D180	D(53,14,51,52)	-41.8421	-DE/DX = 0.0	!
! D181	D(57,14,51,6)	-103.9733	-DE/DX = 0.0	!
! D182	D(57,14,51,48)	18.7377	-DE/DX = 0.0	!
! D183	D(57,14,51,52)	137.2612	-DE/DX = 0.0	!
! D184	D(51,14,53,54)	0.286	-DE/DX = 0.0	!
! D185	D(51,14,53,55)	179.5522	-DE/DX = 0.0	!
! D186	D(57,14,53,54)	-178.9901	-DE/DX = 0.0	!
! D187	D(57,14,53,55)	0.2761	-DE/DX = 0.0	!
! D188	D(51,14,57,15)	-179.4681	-DE/DX = 0.0	!
! D189	D(51,14,57,58)	0.2747	-DE/DX = 0.0	!
! D190	D(53,14,57,15)	-0.216	-DE/DX = 0.0	!
! D191	D(53,14,57,58)	179.5268	-DE/DX = 0.0	!
! D192	D(57,15,55,53)	0.1139	-DE/DX = 0.0	!
! D193	D(57,15,55,56)	179.6478	-DE/DX = 0.0	!
! D194	D(55,15,57,14)	0.0735	-DE/DX = 0.0	!
! D195	D(55,15,57,58)	-179.72	-DE/DX = 0.0	!
! D196	D(6,26,40,3)	24.8161	-DE/DX = 0.0	!
! D197	D(6,26,40,41)	-132.6417	-DE/DX = 0.0	!
! D198	D(6,26,40,59)	92.7744	-DE/DX = 0.0	!
! D199	D(27,26,40,3)	147.0253	-DE/DX = 0.0	!
! D200	D(27,26,40,41)	-10.4324	-DE/DX = 0.0	!

! D201	D(27,26,40,59)	-145.0163	-DE/DX = 0.0	!
! D202	D(28,26,40,3)	-96.3755	-DE/DX = 0.0	!
! D203	D(28,26,40,41)	106.1668	-DE/DX = 0.0	!
! D204	D(28,26,40,59)	-28.4172	-DE/DX = 0.0	!
! D205	D(8,32,34,2)	-1.6292	-DE/DX = 0.0	!
! D206	D(8,32,34,35)	-176.5172	-DE/DX = 0.0	!
! D207	D(33,32,34,2)	174.322	-DE/DX = 0.0	!
! D208	D(33,32,34,35)	-0.566	-DE/DX = 0.0	!
! D209	D(5,46,48,49)	144.3189	-DE/DX = 0.0	!
! D210	D(5,46,48,50)	-95.5989	-DE/DX = 0.0	!
! D211	D(5,46,48,51)	23.5839	-DE/DX = 0.0	!
! D212	D(47,46,48,49)	-61.5482	-DE/DX = 0.0	!
! D213	D(47,46,48,50)	58.534	-DE/DX = 0.0	!
! D214	D(47,46,48,51)	177.7168	-DE/DX = 0.0	!
! D215	D(61,46,48,49)	79.7163	-DE/DX = 0.0	!
! D216	D(61,46,48,50)	-160.2016	-DE/DX = 0.0	!
! D217	D(61,46,48,51)	-41.0187	-DE/DX = 0.0	!
! D218	D(46,48,51,6)	-35.3362	-DE/DX = 0.0	!
! D219	D(46,48,51,14)	-164.264	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	76.7461	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-156.6541	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	74.4181	-DE/DX = 0.0	!
! D223	D(49,48,51,52)	-44.5718	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	82.0433	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-46.8845	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-165.8744	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2444	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.6665	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.03	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.3921	-DE/DX = 0.0	!
! D231	D(12,60,62,63)	-47.9376	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	138.3764	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	148.8655	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-34.9505	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-37.8366	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	138.3474	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-1.8572	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	178.9249	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-177.86	-DE/DX = 0.0	!
! D240	D(71,63,64,67)	2.9222	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-15.2702	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	105.8814	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-134.2014	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	160.5991	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-78.2493	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	41.6678	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	-2.3627	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	118.8218	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-124.1271	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	178.4147	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-60.4007	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	56.6504	-DE/DX = 0.0	!

6. opt=tight b3pw91/6-311++g(d,p) scrf=(cpcm,solvent=chloroform) nosymm

! Optimized Parameters !				
! (Angstroms and Degrees) !				

! Name	Definition	Value	Derivative Info.	!

! R1	R(1,2)	1.55	-DE/DX = 0.0	!
! R2	R(1,3)	1.5684	-DE/DX = 0.0	!
! R3	R(1,20)	1.5147	-DE/DX = 0.0	!
! R4	R(1,22)	1.5438	-DE/DX = 0.0	!
! R5	R(2,7)	1.2197	-DE/DX = 0.0	!
! R6	R(2,34)	1.4867	-DE/DX = 0.0	!
! R7	R(3,4)	1.586	-DE/DX = 0.0	!
! R8	R(3,40)	1.4918	-DE/DX = 0.0	!
! R9	R(3,59)	1.4256	-DE/DX = 0.0	!
! R10	R(4,5)	1.5471	-DE/DX = 0.0	!
! R11	R(4,12)	1.5707	-DE/DX = 0.0	!
! R12	R(4,36)	1.5472	-DE/DX = 0.0	!
! R13	R(5,6)	1.541	-DE/DX = 0.0	!
! R14	R(5,46)	1.4684	-DE/DX = 0.0	!
! R15	R(5,61)	1.4492	-DE/DX = 0.0	!
! R16	R(6,26)	1.5248	-DE/DX = 0.0	!
! R17	R(6,42)	1.5298	-DE/DX = 0.0	!
! R18	R(6,51)	1.5728	-DE/DX = 0.0	!
! R19	R(8,16)	1.5408	-DE/DX = 0.0	!
! R20	R(8,20)	1.5264	-DE/DX = 0.0	!
! R21	R(8,29)	1.5406	-DE/DX = 0.0	!
! R22	R(8,32)	1.496	-DE/DX = 0.0	!
! R23	R(9,10)	1.0945	-DE/DX = 0.0	!
! R24	R(9,11)	1.4324	-DE/DX = 0.0	!
! R25	R(9,12)	1.5329	-DE/DX = 0.0	!
! R26	R(9,20)	1.4998	-DE/DX = 0.0	!
! R27	R(11,29)	1.4457	-DE/DX = 0.0	!
! R28	R(12,13)	1.092	-DE/DX = 0.0	!
! R29	R(12,60)	1.4283	-DE/DX = 0.0	!
! R30	R(14,51)	1.4959	-DE/DX = 0.0	!
! R31	R(14,53)	1.4397	-DE/DX = 0.0	!
! R32	R(14,57)	1.3614	-DE/DX = 0.0	!
! R33	R(15,55)	1.3574	-DE/DX = 0.0	!
! R34	R(15,57)	1.3616	-DE/DX = 0.0	!
! R35	R(16,17)	1.094	-DE/DX = 0.0	!
! R36	R(16,18)	1.0931	-DE/DX = 0.0	!
! R37	R(16,19)	1.0894	-DE/DX = 0.0	!
! R38	R(20,21)	1.1006	-DE/DX = 0.0	!
! R39	R(22,23)	1.0911	-DE/DX = 0.0	!
! R40	R(22,24)	1.0906	-DE/DX = 0.0	!
! R41	R(22,25)	1.0906	-DE/DX = 0.0	!
! R42	R(26,27)	1.094	-DE/DX = 0.0	!

! R43	R(26,28)	1.0952	-DE/DX = 0.0	!
! R44	R(26,40)	1.5129	-DE/DX = 0.0	!
! R45	R(29,30)	1.0963	-DE/DX = 0.0	!
! R46	R(29,31)	1.0917	-DE/DX = 0.0	!
! R47	R(32,33)	1.0884	-DE/DX = 0.0	!
! R48	R(32,34)	1.3436	-DE/DX = 0.0	!
! R49	R(34,35)	1.0862	-DE/DX = 0.0	!
! R50	R(36,37)	1.0916	-DE/DX = 0.0	!
! R51	R(36,38)	1.0874	-DE/DX = 0.0	!
! R52	R(36,39)	1.0902	-DE/DX = 0.0	!
! R53	R(40,41)	1.0839	-DE/DX = 0.0	!
! R54	R(40,59)	1.432	-DE/DX = 0.0	!
! R55	R(42,43)	1.0934	-DE/DX = 0.0	!
! R56	R(42,44)	1.0904	-DE/DX = 0.0	!
! R57	R(42,45)	1.0897	-DE/DX = 0.0	!
! R58	R(46,47)	1.0861	-DE/DX = 0.0	!
! R59	R(46,48)	1.5077	-DE/DX = 0.0	!
! R60	R(46,61)	1.4297	-DE/DX = 0.0	!
! R61	R(48,49)	1.0938	-DE/DX = 0.0	!
! R62	R(48,50)	1.0954	-DE/DX = 0.0	!
! R63	R(48,51)	1.5405	-DE/DX = 0.0	!
! R64	R(51,52)	1.0933	-DE/DX = 0.0	!
! R65	R(53,54)	1.08	-DE/DX = 0.0	!
! R66	R(53,55)	1.3559	-DE/DX = 0.0	!
! R67	R(55,56)	1.0784	-DE/DX = 0.0	!
! R68	R(57,58)	1.0779	-DE/DX = 0.0	!
! R69	R(60,62)	1.365	-DE/DX = 0.0	!
! R70	R(62,63)	1.4952	-DE/DX = 0.0	!
! R71	R(62,65)	1.2098	-DE/DX = 0.0	!
! R72	R(63,64)	1.3398	-DE/DX = 0.0	!
! R73	R(63,71)	1.5083	-DE/DX = 0.0	!
! R74	R(64,66)	1.0872	-DE/DX = 0.0	!
! R75	R(64,67)	1.4901	-DE/DX = 0.0	!
! R76	R(67,68)	1.0907	-DE/DX = 0.0	!
! R77	R(67,69)	1.0963	-DE/DX = 0.0	!
! R78	R(67,70)	1.0961	-DE/DX = 0.0	!
! R79	R(71,72)	1.0902	-DE/DX = 0.0	!
! R80	R(71,73)	1.0954	-DE/DX = 0.0	!
! R81	R(71,74)	1.0923	-DE/DX = 0.0	!
! A1	A(2,1,3)	114.9661	-DE/DX = 0.0	!
! A2	A(2,1,20)	105.4353	-DE/DX = 0.0	!
! A3	A(2,1,22)	105.0065	-DE/DX = 0.0	!
! A4	A(3,1,20)	105.1727	-DE/DX = 0.0	!
! A5	A(3,1,22)	110.1062	-DE/DX = 0.0	!
! A6	A(20,1,22)	116.4196	-DE/DX = 0.0	!
! A7	A(1,2,7)	122.0599	-DE/DX = 0.0	!
! A8	A(1,2,34)	118.8095	-DE/DX = 0.0	!
! A9	A(7,2,34)	118.9368	-DE/DX = 0.0	!
! A10	A(1,3,4)	117.2908	-DE/DX = 0.0	!
! A11	A(1,3,40)	120.3201	-DE/DX = 0.0	!
! A12	A(1,3,59)	113.5007	-DE/DX = 0.0	!
! A13	A(4,3,40)	119.8264	-DE/DX = 0.0	!

! A14	A(4,3,59)	111.1433	-DE/DX = 0.0	!
! A15	A(3,4,5)	108.1898	-DE/DX = 0.0	!
! A16	A(3,4,12)	117.026	-DE/DX = 0.0	!
! A17	A(3,4,36)	107.382	-DE/DX = 0.0	!
! A18	A(5,4,12)	111.3284	-DE/DX = 0.0	!
! A19	A(5,4,36)	108.3471	-DE/DX = 0.0	!
! A20	A(12,4,36)	104.153	-DE/DX = 0.0	!
! A21	A(4,5,6)	122.2697	-DE/DX = 0.0	!
! A22	A(4,5,46)	126.0739	-DE/DX = 0.0	!
! A23	A(4,5,61)	113.9553	-DE/DX = 0.0	!
! A24	A(6,5,46)	108.29	-DE/DX = 0.0	!
! A25	A(6,5,61)	109.5481	-DE/DX = 0.0	!
! A26	A(5,6,26)	107.2931	-DE/DX = 0.0	!
! A27	A(5,6,42)	114.5541	-DE/DX = 0.0	!
! A28	A(5,6,51)	101.9777	-DE/DX = 0.0	!
! A29	A(26,6,42)	108.9314	-DE/DX = 0.0	!
! A30	A(26,6,51)	113.9367	-DE/DX = 0.0	!
! A31	A(42,6,51)	110.1222	-DE/DX = 0.0	!
! A32	A(16,8,20)	117.3974	-DE/DX = 0.0	!
! A33	A(16,8,29)	108.6672	-DE/DX = 0.0	!
! A34	A(16,8,32)	109.4415	-DE/DX = 0.0	!
! A35	A(20,8,29)	96.4285	-DE/DX = 0.0	!
! A36	A(20,8,32)	106.3732	-DE/DX = 0.0	!
! A37	A(29,8,32)	118.4575	-DE/DX = 0.0	!
! A38	A(10,9,11)	108.2933	-DE/DX = 0.0	!
! A39	A(10,9,12)	109.3298	-DE/DX = 0.0	!
! A40	A(10,9,20)	113.6397	-DE/DX = 0.0	!
! A41	A(11,9,12)	113.1724	-DE/DX = 0.0	!
! A42	A(11,9,20)	103.7399	-DE/DX = 0.0	!
! A43	A(12,9,20)	108.664	-DE/DX = 0.0	!
! A44	A(9,11,29)	109.8362	-DE/DX = 0.0	!
! A45	A(4,12,9)	110.1418	-DE/DX = 0.0	!
! A46	A(4,12,13)	106.9483	-DE/DX = 0.0	!
! A47	A(4,12,60)	111.9073	-DE/DX = 0.0	!
! A48	A(9,12,13)	110.6773	-DE/DX = 0.0	!
! A49	A(9,12,60)	107.9972	-DE/DX = 0.0	!
! A50	A(13,12,60)	109.1839	-DE/DX = 0.0	!
! A51	A(51,14,53)	126.3771	-DE/DX = 0.0	!
! A52	A(51,14,57)	128.5448	-DE/DX = 0.0	!
! A53	A(53,14,57)	105.0728	-DE/DX = 0.0	!
! A54	A(55,15,57)	106.8678	-DE/DX = 0.0	!
! A55	A(8,16,17)	109.185	-DE/DX = 0.0	!
! A56	A(8,16,18)	111.126	-DE/DX = 0.0	!
! A57	A(8,16,19)	112.439	-DE/DX = 0.0	!
! A58	A(17,16,18)	107.6381	-DE/DX = 0.0	!
! A59	A(17,16,19)	107.6018	-DE/DX = 0.0	!
! A60	A(18,16,19)	108.6775	-DE/DX = 0.0	!
! A61	A(1,20,8)	120.8439	-DE/DX = 0.0	!
! A62	A(1,20,9)	118.2898	-DE/DX = 0.0	!
! A63	A(1,20,21)	104.1437	-DE/DX = 0.0	!
! A64	A(8,20,9)	104.2216	-DE/DX = 0.0	!
! A65	A(8,20,21)	102.9989	-DE/DX = 0.0	!

! A66	A(9,20,21)	104.0705	-DE/DX = 0.0	!
! A67	A(1,22,23)	111.4305	-DE/DX = 0.0	!
! A68	A(1,22,24)	112.3866	-DE/DX = 0.0	!
! A69	A(1,22,25)	108.909	-DE/DX = 0.0	!
! A70	A(23,22,24)	107.6008	-DE/DX = 0.0	!
! A71	A(23,22,25)	107.625	-DE/DX = 0.0	!
! A72	A(24,22,25)	108.7458	-DE/DX = 0.0	!
! A73	A(6,26,27)	110.4776	-DE/DX = 0.0	!
! A74	A(6,26,28)	110.5612	-DE/DX = 0.0	!
! A75	A(6,26,40)	111.4969	-DE/DX = 0.0	!
! A76	A(27,26,28)	107.4002	-DE/DX = 0.0	!
! A77	A(27,26,40)	109.0884	-DE/DX = 0.0	!
! A78	A(28,26,40)	107.6844	-DE/DX = 0.0	!
! A79	A(8,29,11)	104.6043	-DE/DX = 0.0	!
! A80	A(8,29,30)	111.8561	-DE/DX = 0.0	!
! A81	A(8,29,31)	113.664	-DE/DX = 0.0	!
! A82	A(11,29,30)	109.5654	-DE/DX = 0.0	!
! A83	A(11,29,31)	107.4753	-DE/DX = 0.0	!
! A84	A(30,29,31)	109.4315	-DE/DX = 0.0	!
! A85	A(8,32,33)	119.6454	-DE/DX = 0.0	!
! A86	A(8,32,34)	120.2925	-DE/DX = 0.0	!
! A87	A(33,32,34)	119.9151	-DE/DX = 0.0	!
! A88	A(2,34,32)	125.1913	-DE/DX = 0.0	!
! A89	A(2,34,35)	113.7738	-DE/DX = 0.0	!
! A90	A(32,34,35)	120.7951	-DE/DX = 0.0	!
! A91	A(4,36,37)	110.4909	-DE/DX = 0.0	!
! A92	A(4,36,38)	110.4816	-DE/DX = 0.0	!
! A93	A(4,36,39)	111.5229	-DE/DX = 0.0	!
! A94	A(37,36,38)	108.1437	-DE/DX = 0.0	!
! A95	A(37,36,39)	107.5633	-DE/DX = 0.0	!
! A96	A(38,36,39)	108.5211	-DE/DX = 0.0	!
! A97	A(3,40,26)	124.7241	-DE/DX = 0.0	!
! A98	A(3,40,41)	116.2636	-DE/DX = 0.0	!
! A99	A(26,40,41)	115.3689	-DE/DX = 0.0	!
! A100	A(26,40,59)	115.9607	-DE/DX = 0.0	!
! A101	A(41,40,59)	112.3428	-DE/DX = 0.0	!
! A102	A(6,42,43)	108.4621	-DE/DX = 0.0	!
! A103	A(6,42,44)	112.4084	-DE/DX = 0.0	!
! A104	A(6,42,45)	112.1483	-DE/DX = 0.0	!
! A105	A(43,42,44)	108.0604	-DE/DX = 0.0	!
! A106	A(43,42,45)	108.1044	-DE/DX = 0.0	!
! A107	A(44,42,45)	107.4994	-DE/DX = 0.0	!
! A108	A(5,46,47)	123.3004	-DE/DX = 0.0	!
! A109	A(5,46,48)	109.6699	-DE/DX = 0.0	!
! A110	A(47,46,48)	121.3626	-DE/DX = 0.0	!
! A111	A(47,46,61)	115.0468	-DE/DX = 0.0	!
! A112	A(48,46,61)	111.8641	-DE/DX = 0.0	!
! A113	A(46,48,49)	112.7003	-DE/DX = 0.0	!
! A114	A(46,48,50)	109.3216	-DE/DX = 0.0	!
! A115	A(46,48,51)	102.8703	-DE/DX = 0.0	!
! A116	A(49,48,50)	107.7497	-DE/DX = 0.0	!
! A117	A(49,48,51)	112.0831	-DE/DX = 0.0	!

! A118	A(50,48,51)	112.1217	-DE/DX = 0.0	!
! A119	A(6,51,14)	116.3329	-DE/DX = 0.0	!
! A120	A(6,51,48)	104.4332	-DE/DX = 0.0	!
! A121	A(6,51,52)	106.194	-DE/DX = 0.0	!
! A122	A(14,51,48)	115.1468	-DE/DX = 0.0	!
! A123	A(14,51,52)	107.2279	-DE/DX = 0.0	!
! A124	A(48,51,52)	106.8251	-DE/DX = 0.0	!
! A125	A(14,53,54)	127.1394	-DE/DX = 0.0	!
! A126	A(14,53,55)	106.7168	-DE/DX = 0.0	!
! A127	A(54,53,55)	126.1409	-DE/DX = 0.0	!
! A128	A(15,55,53)	110.3331	-DE/DX = 0.0	!
! A129	A(15,55,56)	116.0722	-DE/DX = 0.0	!
! A130	A(53,55,56)	133.5928	-DE/DX = 0.0	!
! A131	A(14,57,15)	111.0086	-DE/DX = 0.0	!
! A132	A(14,57,58)	133.5343	-DE/DX = 0.0	!
! A133	A(15,57,58)	115.4567	-DE/DX = 0.0	!
! A134	A(12,60,62)	121.592	-DE/DX = 0.0	!
! A135	A(60,62,63)	119.3485	-DE/DX = 0.0	!
! A136	A(60,62,65)	117.2568	-DE/DX = 0.0	!
! A137	A(63,62,65)	123.1015	-DE/DX = 0.0	!
! A138	A(62,63,64)	116.6519	-DE/DX = 0.0	!
! A139	A(62,63,71)	119.0158	-DE/DX = 0.0	!
! A140	A(64,63,71)	124.1815	-DE/DX = 0.0	!
! A141	A(63,64,66)	117.2759	-DE/DX = 0.0	!
! A142	A(63,64,67)	126.7855	-DE/DX = 0.0	!
! A143	A(66,64,67)	115.926	-DE/DX = 0.0	!
! A144	A(64,67,68)	113.3371	-DE/DX = 0.0	!
! A145	A(64,67,69)	110.1895	-DE/DX = 0.0	!
! A146	A(64,67,70)	110.2552	-DE/DX = 0.0	!
! A147	A(68,67,69)	108.0877	-DE/DX = 0.0	!
! A148	A(68,67,70)	108.4872	-DE/DX = 0.0	!
! A149	A(69,67,70)	106.2069	-DE/DX = 0.0	!
! A150	A(63,71,72)	111.1008	-DE/DX = 0.0	!
! A151	A(63,71,73)	112.9413	-DE/DX = 0.0	!
! A152	A(63,71,74)	110.2752	-DE/DX = 0.0	!
! A153	A(72,71,73)	107.9503	-DE/DX = 0.0	!
! A154	A(72,71,74)	107.2375	-DE/DX = 0.0	!
! A155	A(73,71,74)	107.0873	-DE/DX = 0.0	!
! D1	D(3,1,2,7)	-55.9515	-DE/DX = 0.0	!
! D2	D(3,1,2,34)	129.1634	-DE/DX = 0.0	!
! D3	D(20,1,2,7)	-171.2961	-DE/DX = 0.0	!
! D4	D(20,1,2,34)	13.8188	-DE/DX = 0.0	!
! D5	D(22,1,2,7)	65.206	-DE/DX = 0.0	!
! D6	D(22,1,2,34)	-109.6791	-DE/DX = 0.0	!
! D7	D(2,1,3,4)	-154.6058	-DE/DX = 0.0	!
! D8	D(2,1,3,40)	7.2149	-DE/DX = 0.0	!
! D9	D(2,1,3,59)	73.5634	-DE/DX = 0.0	!
! D10	D(20,1,3,4)	-39.1099	-DE/DX = 0.0	!
! D11	D(20,1,3,40)	122.7108	-DE/DX = 0.0	!
! D12	D(20,1,3,59)	-170.9408	-DE/DX = 0.0	!
! D13	D(22,1,3,4)	87.0615	-DE/DX = 0.0	!
! D14	D(22,1,3,40)	-111.1178	-DE/DX = 0.0	!

! D15	D(22,1,3,59)	-44.7694	-DE/DX = 0.0	!
! D16	D(2,1,20,8)	-49.3101	-DE/DX = 0.0	!
! D17	D(2,1,20,9)	-179.5774	-DE/DX = 0.0	!
! D18	D(2,1,20,21)	65.566	-DE/DX = 0.0	!
! D19	D(3,1,20,8)	-171.2187	-DE/DX = 0.0	!
! D20	D(3,1,20,9)	58.514	-DE/DX = 0.0	!
! D21	D(3,1,20,21)	-56.3426	-DE/DX = 0.0	!
! D22	D(22,1,20,8)	66.6104	-DE/DX = 0.0	!
! D23	D(22,1,20,9)	-63.6569	-DE/DX = 0.0	!
! D24	D(22,1,20,21)	-178.5136	-DE/DX = 0.0	!
! D25	D(2,1,22,23)	39.7858	-DE/DX = 0.0	!
! D26	D(2,1,22,24)	160.6493	-DE/DX = 0.0	!
! D27	D(2,1,22,25)	-78.7877	-DE/DX = 0.0	!
! D28	D(3,1,22,23)	164.0823	-DE/DX = 0.0	!
! D29	D(3,1,22,24)	-75.0542	-DE/DX = 0.0	!
! D30	D(3,1,22,25)	45.5089	-DE/DX = 0.0	!
! D31	D(20,1,22,23)	-76.3735	-DE/DX = 0.0	!
! D32	D(20,1,22,24)	44.49	-DE/DX = 0.0	!
! D33	D(20,1,22,25)	165.0531	-DE/DX = 0.0	!
! D34	D(1,2,34,32)	9.9246	-DE/DX = 0.0	!
! D35	D(1,2,34,35)	-175.692	-DE/DX = 0.0	!
! D36	D(7,2,34,32)	-165.1226	-DE/DX = 0.0	!
! D37	D(7,2,34,35)	9.2609	-DE/DX = 0.0	!
! D38	D(1,3,4,5)	161.476	-DE/DX = 0.0	!
! D39	D(1,3,4,12)	34.793	-DE/DX = 0.0	!
! D40	D(1,3,4,36)	-81.7775	-DE/DX = 0.0	!
! D41	D(40,3,4,5)	-0.4383	-DE/DX = 0.0	!
! D42	D(40,3,4,12)	-127.1213	-DE/DX = 0.0	!
! D43	D(40,3,4,36)	116.3082	-DE/DX = 0.0	!
! D44	D(59,3,4,5)	-65.6316	-DE/DX = 0.0	!
! D45	D(59,3,4,12)	167.6854	-DE/DX = 0.0	!
! D46	D(59,3,4,36)	51.1149	-DE/DX = 0.0	!
! D47	D(1,3,40,26)	-157.8875	-DE/DX = 0.0	!
! D48	D(1,3,40,41)	-0.4783	-DE/DX = 0.0	!
! D49	D(4,3,40,26)	3.4738	-DE/DX = 0.0	!
! D50	D(4,3,40,41)	160.8831	-DE/DX = 0.0	!
! D51	D(3,4,5,6)	-32.71	-DE/DX = 0.0	!
! D52	D(3,4,5,46)	170.479	-DE/DX = 0.0	!
! D53	D(3,4,5,61)	102.8153	-DE/DX = 0.0	!
! D54	D(12,4,5,6)	97.2133	-DE/DX = 0.0	!
! D55	D(12,4,5,46)	-59.5978	-DE/DX = 0.0	!
! D56	D(12,4,5,61)	-127.2615	-DE/DX = 0.0	!
! D57	D(36,4,5,6)	-148.8308	-DE/DX = 0.0	!
! D58	D(36,4,5,46)	54.3582	-DE/DX = 0.0	!
! D59	D(36,4,5,61)	-13.3055	-DE/DX = 0.0	!
! D60	D(3,4,12,9)	-39.8954	-DE/DX = 0.0	!
! D61	D(3,4,12,13)	-160.2238	-DE/DX = 0.0	!
! D62	D(3,4,12,60)	80.2507	-DE/DX = 0.0	!
! D63	D(5,4,12,9)	-165.0208	-DE/DX = 0.0	!
! D64	D(5,4,12,13)	74.6508	-DE/DX = 0.0	!
! D65	D(5,4,12,60)	-44.8747	-DE/DX = 0.0	!
! D66	D(36,4,12,9)	78.4308	-DE/DX = 0.0	!

! D67	D(36,4,12,13)	-41.8977	-DE/DX = 0.0	!
! D68	D(36,4,12,60)	-161.4231	-DE/DX = 0.0	!
! D69	D(3,4,36,37)	-169.8096	-DE/DX = 0.0	!
! D70	D(3,4,36,38)	-50.1759	-DE/DX = 0.0	!
! D71	D(3,4,36,39)	70.6086	-DE/DX = 0.0	!
! D72	D(5,4,36,37)	-53.1664	-DE/DX = 0.0	!
! D73	D(5,4,36,38)	66.4673	-DE/DX = 0.0	!
! D74	D(5,4,36,39)	-172.7482	-DE/DX = 0.0	!
! D75	D(12,4,36,37)	65.4416	-DE/DX = 0.0	!
! D76	D(12,4,36,38)	-174.9247	-DE/DX = 0.0	!
! D77	D(12,4,36,39)	-54.1402	-DE/DX = 0.0	!
! D78	D(4,5,6,26)	60.3171	-DE/DX = 0.0	!
! D79	D(4,5,6,42)	-60.7349	-DE/DX = 0.0	!
! D80	D(4,5,6,51)	-179.6536	-DE/DX = 0.0	!
! D81	D(46,5,6,26)	-139.2675	-DE/DX = 0.0	!
! D82	D(46,5,6,42)	99.6806	-DE/DX = 0.0	!
! D83	D(46,5,6,51)	-19.2382	-DE/DX = 0.0	!
! D84	D(61,5,6,26)	-76.8855	-DE/DX = 0.0	!
! D85	D(61,5,6,42)	162.0625	-DE/DX = 0.0	!
! D86	D(61,5,6,51)	43.1438	-DE/DX = 0.0	!
! D87	D(4,5,46,47)	3.5359	-DE/DX = 0.0	!
! D88	D(4,5,46,48)	157.1851	-DE/DX = 0.0	!
! D89	D(6,5,46,47)	-155.9363	-DE/DX = 0.0	!
! D90	D(6,5,46,48)	-2.2872	-DE/DX = 0.0	!
! D91	D(5,6,26,27)	-171.6867	-DE/DX = 0.0	!
! D92	D(5,6,26,28)	69.5617	-DE/DX = 0.0	!
! D93	D(5,6,26,40)	-50.2025	-DE/DX = 0.0	!
! D94	D(42,6,26,27)	-47.1525	-DE/DX = 0.0	!
! D95	D(42,6,26,28)	-165.9041	-DE/DX = 0.0	!
! D96	D(42,6,26,40)	74.3317	-DE/DX = 0.0	!
! D97	D(51,6,26,27)	76.2264	-DE/DX = 0.0	!
! D98	D(51,6,26,28)	-42.5251	-DE/DX = 0.0	!
! D99	D(51,6,26,40)	-162.2894	-DE/DX = 0.0	!
! D100	D(5,6,42,43)	-178.6711	-DE/DX = 0.0	!
! D101	D(5,6,42,44)	-59.2515	-DE/DX = 0.0	!
! D102	D(5,6,42,45)	62.0143	-DE/DX = 0.0	!
! D103	D(26,6,42,43)	61.1831	-DE/DX = 0.0	!
! D104	D(26,6,42,44)	-179.3973	-DE/DX = 0.0	!
! D105	D(26,6,42,45)	-58.1315	-DE/DX = 0.0	!
! D106	D(51,6,42,43)	-64.442	-DE/DX = 0.0	!
! D107	D(51,6,42,44)	54.9776	-DE/DX = 0.0	!
! D108	D(51,6,42,45)	176.2434	-DE/DX = 0.0	!
! D109	D(5,6,51,14)	161.3618	-DE/DX = 0.0	!
! D110	D(5,6,51,48)	33.2661	-DE/DX = 0.0	!
! D111	D(5,6,51,52)	-79.4383	-DE/DX = 0.0	!
! D112	D(26,6,51,14)	-83.3834	-DE/DX = 0.0	!
! D113	D(26,6,51,48)	148.5209	-DE/DX = 0.0	!
! D114	D(26,6,51,52)	35.8165	-DE/DX = 0.0	!
! D115	D(42,6,51,14)	39.3466	-DE/DX = 0.0	!
! D116	D(42,6,51,48)	-88.7491	-DE/DX = 0.0	!
! D117	D(42,6,51,52)	158.5465	-DE/DX = 0.0	!
! D118	D(20,8,16,17)	-173.7904	-DE/DX = 0.0	!

! D119	D(20,8,16,18)	-55.2108	-DE/DX = 0.0	!
! D120	D(20,8,16,19)	66.8626	-DE/DX = 0.0	!
! D121	D(29,8,16,17)	-65.8388	-DE/DX = 0.0	!
! D122	D(29,8,16,18)	52.7408	-DE/DX = 0.0	!
! D123	D(29,8,16,19)	174.8141	-DE/DX = 0.0	!
! D124	D(32,8,16,17)	64.9012	-DE/DX = 0.0	!
! D125	D(32,8,16,18)	-176.5192	-DE/DX = 0.0	!
! D126	D(32,8,16,19)	-54.4459	-DE/DX = 0.0	!
! D127	D(16,8,20,1)	-65.5483	-DE/DX = 0.0	!
! D128	D(16,8,20,9)	70.5722	-DE/DX = 0.0	!
! D129	D(16,8,20,21)	178.9877	-DE/DX = 0.0	!
! D130	D(29,8,20,1)	179.5424	-DE/DX = 0.0	!
! D131	D(29,8,20,9)	-44.3372	-DE/DX = 0.0	!
! D132	D(29,8,20,21)	64.0783	-DE/DX = 0.0	!
! D133	D(32,8,20,1)	57.3411	-DE/DX = 0.0	!
! D134	D(32,8,20,9)	-166.5384	-DE/DX = 0.0	!
! D135	D(32,8,20,21)	-58.123	-DE/DX = 0.0	!
! D136	D(16,8,29,11)	-81.6855	-DE/DX = 0.0	!
! D137	D(16,8,29,30)	159.8003	-DE/DX = 0.0	!
! D138	D(16,8,29,31)	35.2503	-DE/DX = 0.0	!
! D139	D(20,8,29,11)	40.1074	-DE/DX = 0.0	!
! D140	D(20,8,29,30)	-78.4069	-DE/DX = 0.0	!
! D141	D(20,8,29,31)	157.0432	-DE/DX = 0.0	!
! D142	D(32,8,29,11)	152.6723	-DE/DX = 0.0	!
! D143	D(32,8,29,30)	34.1581	-DE/DX = 0.0	!
! D144	D(32,8,29,31)	-90.3918	-DE/DX = 0.0	!
! D145	D(16,8,32,33)	-75.498	-DE/DX = 0.0	!
! D146	D(16,8,32,34)	100.0917	-DE/DX = 0.0	!
! D147	D(20,8,32,33)	156.7449	-DE/DX = 0.0	!
! D148	D(20,8,32,34)	-27.6653	-DE/DX = 0.0	!
! D149	D(29,8,32,33)	49.7686	-DE/DX = 0.0	!
! D150	D(29,8,32,34)	-134.6417	-DE/DX = 0.0	!
! D151	D(10,9,11,29)	114.5235	-DE/DX = 0.0	!
! D152	D(12,9,11,29)	-124.0959	-DE/DX = 0.0	!
! D153	D(20,9,11,29)	-6.5142	-DE/DX = 0.0	!
! D154	D(10,9,12,4)	-71.8878	-DE/DX = 0.0	!
! D155	D(10,9,12,13)	46.1662	-DE/DX = 0.0	!
! D156	D(10,9,12,60)	165.632	-DE/DX = 0.0	!
! D157	D(11,9,12,4)	167.3172	-DE/DX = 0.0	!
! D158	D(11,9,12,13)	-74.6288	-DE/DX = 0.0	!
! D159	D(11,9,12,60)	44.8371	-DE/DX = 0.0	!
! D160	D(20,9,12,4)	52.6543	-DE/DX = 0.0	!
! D161	D(20,9,12,13)	170.7083	-DE/DX = 0.0	!
! D162	D(20,9,12,60)	-69.8258	-DE/DX = 0.0	!
! D163	D(10,9,20,1)	53.3238	-DE/DX = 0.0	!
! D164	D(10,9,20,8)	-84.1575	-DE/DX = 0.0	!
! D165	D(10,9,20,21)	168.2201	-DE/DX = 0.0	!
! D166	D(11,9,20,1)	170.6951	-DE/DX = 0.0	!
! D167	D(11,9,20,8)	33.2137	-DE/DX = 0.0	!
! D168	D(11,9,20,21)	-74.4087	-DE/DX = 0.0	!
! D169	D(12,9,20,1)	-68.6299	-DE/DX = 0.0	!
! D170	D(12,9,20,8)	153.8888	-DE/DX = 0.0	!

! D171	D(12,9,20,21)	46.2664	-DE/DX = 0.0	!
! D172	D(9,11,29,8)	-22.2826	-DE/DX = 0.0	!
! D173	D(9,11,29,30)	97.776	-DE/DX = 0.0	!
! D174	D(9,11,29,31)	-143.4053	-DE/DX = 0.0	!
! D175	D(4,12,60,62)	165.3141	-DE/DX = 0.0	!
! D176	D(9,12,60,62)	-73.2945	-DE/DX = 0.0	!
! D177	D(13,12,60,62)	47.1118	-DE/DX = 0.0	!
! D178	D(53,14,51,6)	75.9894	-DE/DX = 0.0	!
! D179	D(53,14,51,48)	-161.3562	-DE/DX = 0.0	!
! D180	D(53,14,51,52)	-42.6486	-DE/DX = 0.0	!
! D181	D(57,14,51,6)	-104.9674	-DE/DX = 0.0	!
! D182	D(57,14,51,48)	17.687	-DE/DX = 0.0	!
! D183	D(57,14,51,52)	136.3945	-DE/DX = 0.0	!
! D184	D(51,14,53,54)	0.1119	-DE/DX = 0.0	!
! D185	D(51,14,53,55)	179.5167	-DE/DX = 0.0	!
! D186	D(57,14,53,54)	-179.1131	-DE/DX = 0.0	!
! D187	D(57,14,53,55)	0.2917	-DE/DX = 0.0	!
! D188	D(51,14,57,15)	-179.4346	-DE/DX = 0.0	!
! D189	D(51,14,57,58)	0.3052	-DE/DX = 0.0	!
! D190	D(53,14,57,15)	-0.2325	-DE/DX = 0.0	!
! D191	D(53,14,57,58)	179.5074	-DE/DX = 0.0	!
! D192	D(57,15,55,53)	0.1125	-DE/DX = 0.0	!
! D193	D(57,15,55,56)	179.6827	-DE/DX = 0.0	!
! D194	D(55,15,57,14)	0.085	-DE/DX = 0.0	!
! D195	D(55,15,57,58)	-179.7061	-DE/DX = 0.0	!
! D196	D(6,26,40,3)	24.0031	-DE/DX = 0.0	!
! D197	D(6,26,40,41)	-133.5854	-DE/DX = 0.0	!
! D198	D(6,26,40,59)	92.0837	-DE/DX = 0.0	!
! D199	D(27,26,40,3)	146.2906	-DE/DX = 0.0	!
! D200	D(27,26,40,41)	-11.298	-DE/DX = 0.0	!
! D201	D(27,26,40,59)	-145.6288	-DE/DX = 0.0	!
! D202	D(28,26,40,3)	-97.4474	-DE/DX = 0.0	!
! D203	D(28,26,40,41)	104.964	-DE/DX = 0.0	!
! D204	D(28,26,40,59)	-29.3668	-DE/DX = 0.0	!
! D205	D(8,32,34,2)	-1.8958	-DE/DX = 0.0	!
! D206	D(8,32,34,35)	-175.9109	-DE/DX = 0.0	!
! D207	D(33,32,34,2)	173.682	-DE/DX = 0.0	!
! D208	D(33,32,34,35)	-0.3331	-DE/DX = 0.0	!
! D209	D(5,46,48,49)	144.2637	-DE/DX = 0.0	!
! D210	D(5,46,48,50)	-95.9444	-DE/DX = 0.0	!
! D211	D(5,46,48,51)	23.3598	-DE/DX = 0.0	!
! D212	D(47,46,48,49)	-61.4875	-DE/DX = 0.0	!
! D213	D(47,46,48,50)	58.3044	-DE/DX = 0.0	!
! D214	D(47,46,48,51)	177.6086	-DE/DX = 0.0	!
! D215	D(61,46,48,49)	79.6635	-DE/DX = 0.0	!
! D216	D(61,46,48,50)	-160.5446	-DE/DX = 0.0	!
! D217	D(61,46,48,51)	-41.2403	-DE/DX = 0.0	!
! D218	D(46,48,51,6)	-34.85	-DE/DX = 0.0	!
! D219	D(46,48,51,14)	-163.6658	-DE/DX = 0.0	!
! D220	D(46,48,51,52)	77.4024	-DE/DX = 0.0	!
! D221	D(49,48,51,6)	-156.1751	-DE/DX = 0.0	!
! D222	D(49,48,51,14)	75.009	-DE/DX = 0.0	!

! D223	D(49,48,51,52)	-43.9227	-DE/DX = 0.0	!
! D224	D(50,48,51,6)	82.4886	-DE/DX = 0.0	!
! D225	D(50,48,51,14)	-46.3273	-DE/DX = 0.0	!
! D226	D(50,48,51,52)	-165.2591	-DE/DX = 0.0	!
! D227	D(14,53,55,15)	-0.2529	-DE/DX = 0.0	!
! D228	D(14,53,55,56)	-179.7198	-DE/DX = 0.0	!
! D229	D(54,53,55,15)	179.1596	-DE/DX = 0.0	!
! D230	D(54,53,55,56)	-0.3074	-DE/DX = 0.0	!
! D231	D(12,60,62,63)	-40.2659	-DE/DX = 0.0	!
! D232	D(12,60,62,65)	145.7581	-DE/DX = 0.0	!
! D233	D(60,62,63,64)	140.2804	-DE/DX = 0.0	!
! D234	D(60,62,63,71)	-43.9959	-DE/DX = 0.0	!
! D235	D(65,62,63,64)	-46.1138	-DE/DX = 0.0	!
! D236	D(65,62,63,71)	129.6099	-DE/DX = 0.0	!
! D237	D(62,63,64,66)	-2.7304	-DE/DX = 0.0	!
! D238	D(62,63,64,67)	178.6178	-DE/DX = 0.0	!
! D239	D(71,63,64,66)	-178.2095	-DE/DX = 0.0	!
! D240	D(71,63,64,67)	3.1387	-DE/DX = 0.0	!
! D241	D(62,63,71,72)	-15.9666	-DE/DX = 0.0	!
! D242	D(62,63,71,73)	105.503	-DE/DX = 0.0	!
! D243	D(62,63,71,74)	-134.7282	-DE/DX = 0.0	!
! D244	D(64,63,71,72)	159.4127	-DE/DX = 0.0	!
! D245	D(64,63,71,73)	-79.1178	-DE/DX = 0.0	!
! D246	D(64,63,71,74)	40.6511	-DE/DX = 0.0	!
! D247	D(63,64,67,68)	-2.7844	-DE/DX = 0.0	!
! D248	D(63,64,67,69)	118.4754	-DE/DX = 0.0	!
! D249	D(63,64,67,70)	-124.6089	-DE/DX = 0.0	!
! D250	D(66,64,67,68)	178.548	-DE/DX = 0.0	!
! D251	D(66,64,67,69)	-60.1923	-DE/DX = 0.0	!
! D252	D(66,64,67,70)	56.7234	-DE/DX = 0.0	!
