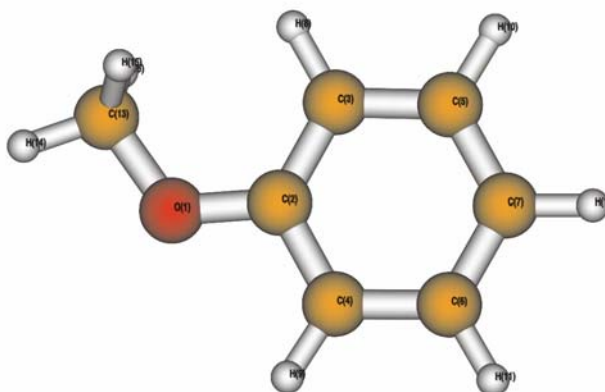


## B Berechnete Geometrien

### B.1 Anisol-h8 im S<sub>0</sub>-Zustand

B3LYP/6-31++g(d,p)

! R1	R(1,2)	1.3686	-DI		
! R2	R(1,13)	1.4216	-C		
! R3	R(2,3)	1.4007	-D		
! R4	R(2,4)	1.4039	-D		
! R5	R(3,5)	1.4011	-D		
! R6	R(3,8)	1.0834	-D		
! R7	R(4,6)	1.3916	-D		
! R8	R(4,9)	1.0852	-D		
! R9	R(5,7)	1.3939	-D		
! R10	R(5,10)	1.0865	-I		
! R11	R(6,7)	1.4015	-C		
! R12	R(6,11)	1.0863	-I		
! R13	R(7,12)	1.0855	-I		
! R14	R(13,14)	1.0907	-		
! R15	R(13,15)	1.0974	-DE/DX = 0.	!	
! R16	R(13,16)	1.0974	-DE/DX = 0.	!	
! A1	A(2,1,13)	118.5319	-DE/DX = 0.0001	!	
! A2	A(1,2,3)	124.4253	-DE/DX = 0.	!	
! A3	A(1,2,4)	115.6328	-DE/DX = 0.	!	
! A4	A(3,2,4)	119.9419	-DE/DX = -0.0001	!	
! A5	A(2,3,5)	119.3991	-DE/DX = 0.	!	
! A6	A(2,3,8)	121.1349	-DE/DX = 0.	!	
! A7	A(5,3,8)	119.466	-DE/DX = 0.	!	
! A8	A(2,4,6)	119.9419	-DE/DX = 0.	!	
! A9	A(2,4,9)	118.5992	-DE/DX = 0.	!	
! A10	A(6,4,9)	121.4589	-DE/DX = 0.	!	
! A11	A(3,5,7)	120.9552	-DE/DX = 0.	!	
! A12	A(3,5,10)	118.9771	-DE/DX = 0.	!	
! A13	A(7,5,10)	120.0677	-DE/DX = 0.	!	
! A14	A(4,6,7)	120.6046	-DE/DX = 0.	!	
! A15	A(4,6,11)	119.3333	-DE/DX = 0.	!	
! A16	A(7,6,11)	120.062	-DE/DX = 0.	!	
! A17	A(5,7,6)	119.1573	-DE/DX = 0.	!	
! A18	A(5,7,12)	120.421	-DE/DX = 0.	!	
! A19	A(6,7,12)	120.4217	-DE/DX = 0.	!	
! A20	A(1,13,14)	105.8006	-DE/DX = 0.0001	!	
! A21	A(1,13,15)	111.4147	-DE/DX = 0.	!	
! A22	A(1,13,16)	111.4147	-DE/DX = 0.	!	
! A23	A(14,13,15)	109.3559	-DE/DX = 0.	!	
! A24	A(14,13,16)	109.3559	-DE/DX = 0.	!	
! A25	A(15,13,16)	109.4136	-DE/DX = 0.	!	
! D1	D(13,1,2,3)	0.	-DE/DX = 0.	!	
! D2	D(13,1,2,4)	180.	-DE/DX = 0.	!	
! D3	D(2,1,13,14)	180.	-DE/DX = 0.	!	
! D4	D(2,1,13,15)	-61.2508	-DE/DX = 0.	!	
! D5	D(2,1,13,16)	61.2508	-DE/DX = 0.	!	
! D6	D(1,2,3,5)	180.	-DE/DX = 0.	!	

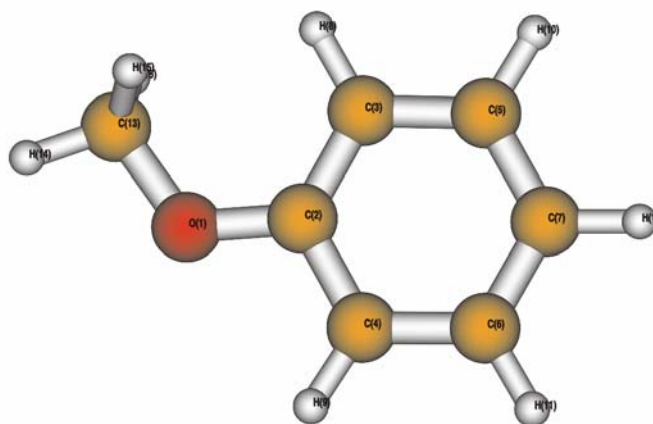


! D7	D(1,2,3,8)	0.	-DE/DX = 0.	!
! D8	D(4,2,3,5)	0.	-DE/DX = 0.	!
! D9	D(4,2,3,8)	180.	-DE/DX = 0.	!
! D10	D(1,2,4,6)	180.	-DE/DX = 0.	!
! D11	D(1,2,4,9)	0.	-DE/DX = 0.	!
! D12	D(3,2,4,6)	0.	-DE/DX = 0.	!
! D13	D(3,2,4,9)	180.	-DE/DX = 0.	!
! D14	D(2,3,5,7)	0.	-DE/DX = 0.	!
! D15	D(2,3,5,10)	180.	-DE/DX = 0.	!
! D16	D(8,3,5,7)	180.	-DE/DX = 0.	!
! D17	D(8,3,5,10)	0.	-DE/DX = 0.	!
! D18	D(2,4,6,7)	0.	-DE/DX = 0.	!
! D19	D(2,4,6,11)	180.	-DE/DX = 0.	!
! D20	D(9,4,6,7)	180.	-DE/DX = 0.	!
! D21	D(9,4,6,11)	0.	-DE/DX = 0.	!
! D22	D(3,5,7,6)	0.	-DE/DX = 0.	!
! D23	D(3,5,7,12)	180.	-DE/DX = 0.	!
! D24	D(10,5,7,6)	180.	-DE/DX = 0.	!
! D25	D(10,5,7,12)	0.	-DE/DX = 0.	!
! D26	D(4,6,7,5)	0.	-DE/DX = 0.	!
! D27	D(4,6,7,12)	180.	-DE/DX = 0.	!
! D28	D(11,6,7,5)	180.	-DE/DX = 0.	!
! D29	D(11,6,7,12)	0.	-DE/DX = 0.	!

B.2 Anisol-h8 im S<sub>1</sub>-Zustand

CIS/6-31g(d,p)

! R1	R(1,2)	1.3262	-]		
! R2	R(1,13)	1.406	-		
! R3	R(2,3)	1.417	-]		
! R4	R(2,4)	1.4199	-		
! R5	R(3,5)	1.4109	-		
! R6	R(3,8)	1.0705	-		
! R7	R(4,6)	1.4109	-		
! R8	R(4,9)	1.0721	-		
! R9	R(5,7)	1.4142	-		
! R10	R(5,10)	1.0732	-		
! R11	R(6,7)	1.416	-		
! R12	R(6,11)	1.0729	-		
! R13	R(7,12)	1.0752	-		
! R14	R(13,14)	1.0794	-DE/DX = 0.	!	
! R15	R(13,15)	1.0837	-DE/DX = 0.	!	
! R16	R(13,16)	1.0837	-DE/DX = 0.	!	
! A1	A(2,1,13)	121.1602	-DE/DX = 0.0001	!	
! A2	A(1,2,3)	123.3988	-DE/DX = 0.0001	!	
! A3	A(1,2,4)	114.5909	-DE/DX = 0.	!	
! A4	A(3,2,4)	122.0103	-DE/DX = 0.	!	
! A5	A(2,3,5)	118.138	-DE/DX = 0.	!	
! A6	A(2,3,8)	121.2929	-DE/DX = 0.	!	
! A7	A(5,3,8)	120.5691	-DE/DX = 0.	!	
! A8	A(2,4,6)	119.0397	-DE/DX = 0.	!	
! A9	A(2,4,9)	118.351	-DE/DX = 0.	!	
! A10	A(6,4,9)	122.6093	-DE/DX = 0.	!	
! A11	A(3,5,7)	120.0179	-DE/DX = 0.	!	
! A12	A(3,5,10)	120.0361	-DE/DX = 0.	!	
! A13	A(7,5,10)	119.9459	-DE/DX = 0.	!	
! A14	A(4,6,7)	119.2307	-DE/DX = 0.	!	
! A15	A(4,6,11)	120.449	-DE/DX = 0.	!	
! A16	A(7,6,11)	120.3204	-DE/DX = 0.	!	
! A17	A(5,7,6)	121.5635	-DE/DX = 0.	!	
! A18	A(5,7,12)	118.9883	-DE/DX = 0.	!	
! A19	A(6,7,12)	119.4482	-DE/DX = 0.	!	
! A20	A(1,13,14)	105.9947	-DE/DX = 0.	!	
! A21	A(1,13,15)	110.9977	-DE/DX = 0.	!	
! A22	A(1,13,16)	110.9977	-DE/DX = 0.	!	
! A23	A(14,13,15)	109.5309	-DE/DX = 0.	!	
! A24	A(14,13,16)	109.5309	-DE/DX = 0.	!	
! A25	A(15,13,16)	109.7133	-DE/DX = 0.	!	
! D1	D(13,1,2,3)	0.	-DE/DX = 0.	!	
! D2	D(13,1,2,4)	180.	-DE/DX = 0.	!	
! D3	D(2,1,13,14)	180.	-DE/DX = 0.	!	
! D4	D(2,1,13,15)	-61.1489	-DE/DX = 0.	!	
! D5	D(2,1,13,16)	61.1489	-DE/DX = 0.	!	
! D6	D(1,2,3,5)	180.	-DE/DX = 0.	!	
! D7	D(1,2,3,8)	0.	-DE/DX = 0.	!	
! D8	D(4,2,3,5)	0.	-DE/DX = 0.	!	
! D9	D(4,2,3,8)	180.	-DE/DX = 0.	!	



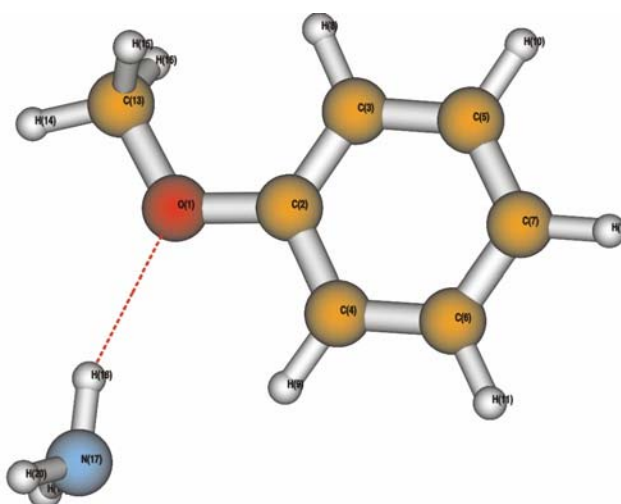
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! D10	D(1,2,4,6)	180.	-DE/DX = 0.	!
! D11	D(1,2,4,9)	0.	-DE/DX = 0.	!
! D12	D(3,2,4,6)	0.	-DE/DX = 0.	!
! D13	D(3,2,4,9)	180.	-DE/DX = 0.	!
! D14	D(2,3,5,7)	0.	-DE/DX = 0.	!
! D15	D(2,3,5,10)	180.	-DE/DX = 0.	!
! D16	D(8,3,5,7)	180.	-DE/DX = 0.	!
! D17	D(8,3,5,10)	0.	-DE/DX = 0.	!
! D18	D(2,4,6,7)	0.	-DE/DX = 0.	!
! D19	D(2,4,6,11)	180.	-DE/DX = 0.	!
! D20	D(9,4,6,7)	180.	-DE/DX = 0.	!
! D21	D(9,4,6,11)	0.	-DE/DX = 0.	!
! D22	D(3,5,7,6)	0.	-DE/DX = 0.	!
! D23	D(3,5,7,12)	180.	-DE/DX = 0.	!
! D24	D(10,5,7,6)	180.	-DE/DX = 0.	!
! D25	D(10,5,7,12)	0.	-DE/DX = 0.	!
! D26	D(4,6,7,5)	0.	-DE/DX = 0.	!
! D27	D(4,6,7,12)	180.	-DE/DX = 0.	!
! D28	D(11,6,7,5)	180.	-DE/DX = 0.	!
! D29	D(11,6,7,12)	0.	-DE/DX = 0.	!

B.3 Anisol-h8/NH<sub>3</sub> im S<sub>0</sub>-Zustand

B3LYP/6-31++g(d,p)

! R1	R(1,2)	1.3761	-]		
! R2	R(1,13)	1.4224			
! R3	R(1,18)	2.2745			
! R4	R(2,3)	1.3998	-		
! R5	R(2,4)	1.4033	-		
! R6	R(3,5)	1.4013	-		
! R7	R(3,8)	1.0835	-		
! R8	R(4,6)	1.3923	-		
! R9	R(4,9)	1.086	-]		
! R10	R(5,7)	1.3937			
! R11	R(5,10)	1.0865			
! R12	R(6,7)	1.4012			
! R13	R(6,11)	1.0864			
! R14	R(7,12)	1.0856			
! R15	R(9,17)	2.636			
! R16	R(9,19)	3.3345			
! R17	R(9,20)	3.3345		-DE/DX = 0.	!
! R18	R(13,14)	1.091		-DE/DX = 0.	!
! R19	R(13,15)	1.0971		-DE/DX = 0.	!
! R20	R(13,16)	1.0971		-DE/DX = 0.	!
! R21	R(17,18)	1.0181		-DE/DX = 0.	!
! R22	R(17,19)	1.0161		-DE/DX = 0.	!
! R23	R(17,20)	1.0161		-DE/DX = 0.	!
! A1	A(2,1,13)	118.4996		-DE/DX = 0.	!
! A2	A(2,1,18)	116.5073		-DE/DX = 0.	!
! A3	A(13,1,18)	124.9931		-DE/DX = 0.	!
! A4	A(1,2,3)	123.9617		-DE/DX = 0.	!
! A5	A(1,2,4)	115.7264		-DE/DX = 0.	!
! A6	A(3,2,4)	120.3119		-DE/DX = 0.	!
! A7	A(2,3,5)	119.319		-DE/DX = 0.	!
! A8	A(2,3,8)	121.2832		-DE/DX = 0.	!
! A9	A(5,3,8)	119.3978		-DE/DX = 0.	!
! A10	A(2,4,6)	119.5175		-DE/DX = 0.	!
! A11	A(2,4,9)	119.0582		-DE/DX = 0.	!
! A12	A(6,4,9)	121.4243		-DE/DX = 0.	!
! A13	A(3,5,7)	120.8499		-DE/DX = 0.	!
! A14	A(3,5,10)	118.9933		-DE/DX = 0.	!
! A15	A(7,5,10)	120.1568		-DE/DX = 0.	!
! A16	A(4,6,7)	120.813		-DE/DX = 0.	!
! A17	A(4,6,11)	119.1408		-DE/DX = 0.	!
! A18	A(7,6,11)	120.0462		-DE/DX = 0.	!
! A19	A(5,7,6)	119.1888		-DE/DX = 0.	!
! A20	A(5,7,12)	120.3853		-DE/DX = 0.	!
! A21	A(6,7,12)	120.4259		-DE/DX = 0.	!
! A22	A(4,9,17)	145.1008		-DE/DX = 0.	!
! A23	A(4,9,19)	143.7199		-DE/DX = 0.	!
! A24	A(4,9,20)	143.7199		-DE/DX = 0.	!
! A25	A(19,9,20)	28.5015		-DE/DX = 0.	!
! A26	A(1,13,14)	105.9395		-DE/DX = 0.	!
! A27	A(1,13,15)	111.3712		-DE/DX = 0.	!
! A28	A(1,13,16)	111.3712		-DE/DX = 0.	!

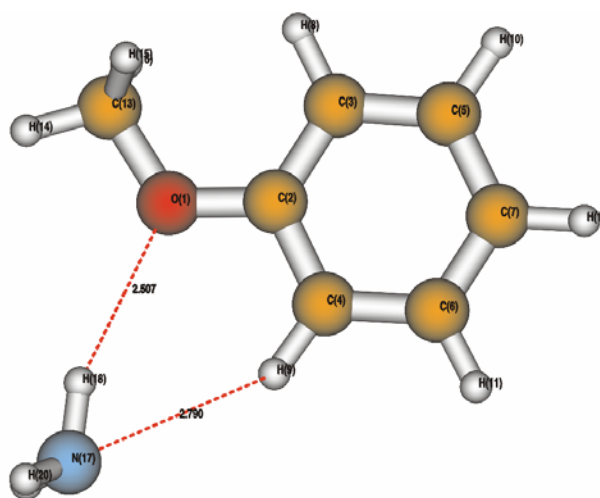


! A29	A(14,13,15)	109.304	-DE/DX = 0.	!
! A30	A(14,13,16)	109.304	-DE/DX = 0.	!
! A31	A(15,13,16)	109.4649	-DE/DX = 0.	!
! A32	A(9,17,18)	64.2116	-DE/DX = 0.	!
! A33	A(18,17,19)	108.2772	-DE/DX = 0.	!
! A34	A(18,17,20)	108.2772	-DE/DX = 0.	!
! A35	A(19,17,20)	107.7707	-DE/DX = 0.	!
! A36	A(1,18,17)	159.3956	-DE/DX = 0.	!
! D1	D(13,1,2,3)	0.	-DE/DX = 0.	!
! D2	D(13,1,2,4)	180.	-DE/DX = 0.	!
! D3	D(18,1,2,3)	180.	-DE/DX = 0.	!
! D4	D(18,1,2,4)	0.	-DE/DX = 0.	!
! D5	D(2,1,13,14)	180.	-DE/DX = 0.	!
! D6	D(2,1,13,15)	-61.2529	-DE/DX = 0.	!
! D7	D(2,1,13,16)	61.2529	-DE/DX = 0.	!
! D8	D(18,1,13,14)	0.	-DE/DX = 0.	!
! D9	D(18,1,13,15)	118.7471	-DE/DX = 0.	!
! D10	D(18,1,13,16)	-118.7471	-DE/DX = 0.	!
! D11	D(2,1,18,17)	0.	-DE/DX = 0.	!
! D12	D(13,1,18,17)	179.9999	-DE/DX = 0.	!
! D13	D(1,2,3,5)	-180.	-DE/DX = 0.	!
! D14	D(1,2,3,8)	0.	-DE/DX = 0.	!
! D15	D(4,2,3,5)	0.	-DE/DX = 0.	!
! D16	D(4,2,3,8)	-180.	-DE/DX = 0.	!
! D17	D(1,2,4,6)	180.	-DE/DX = 0.	!
! D18	D(1,2,4,9)	0.	-DE/DX = 0.	!
! D19	D(3,2,4,6)	0.	-DE/DX = 0.	!
! D20	D(3,2,4,9)	180.	-DE/DX = 0.	!
! D21	D(2,3,5,7)	0.	-DE/DX = 0.	!
! D22	D(2,3,5,10)	180.	-DE/DX = 0.	!
! D23	D(8,3,5,7)	180.	-DE/DX = 0.	!
! D24	D(8,3,5,10)	0.	-DE/DX = 0.	!
! D25	D(2,4,6,7)	0.	-DE/DX = 0.	!
! D26	D(2,4,6,11)	180.	-DE/DX = 0.	!
! D27	D(9,4,6,7)	-180.	-DE/DX = 0.	!
! D28	D(9,4,6,11)	0.	-DE/DX = 0.	!
! D29	D(2,4,9,17)	0.	-DE/DX = 0.	!
! D30	D(2,4,9,19)	24.5829	-DE/DX = 0.	!
! D31	D(2,4,9,20)	-24.5828	-DE/DX = 0.	!
! D32	D(6,4,9,17)	-180.	-DE/DX = 0.	!
! D33	D(6,4,9,19)	-155.4171	-DE/DX = 0.	!
! D34	D(6,4,9,20)	155.4172	-DE/DX = 0.	!
! D35	D(3,5,7,6)	0.	-DE/DX = 0.	!
! D36	D(3,5,7,12)	180.	-DE/DX = 0.	!
! D37	D(10,5,7,6)	180.	-DE/DX = 0.	!
! D38	D(10,5,7,12)	0.	-DE/DX = 0.	!
! D39	D(4,6,7,5)	0.	-DE/DX = 0.	!
! D40	D(4,6,7,12)	-180.	-DE/DX = 0.	!
! D41	D(11,6,7,5)	180.	-DE/DX = 0.	!
! D42	D(11,6,7,12)	0.	-DE/DX = 0.	!
! D43	D(4,9,17,18)	-0.0001	-DE/DX = 0.	!
! D44	D(9,17,18,1)	0.0001	-DE/DX = 0.	!
! D45	D(19,17,18,1)	-121.7055	-DE/DX = 0.	!
! D46	D(20,17,18,1)	121.7057	-DE/DX = 0.	!

B.4 Anisol-h8/NH<sub>3</sub> im S<sub>1</sub>-Zustand

CIS/6-31g(d,p)

! R1	R(1,2)	1.3326	-]		
! R2	R(1,13)	1.4062			
! R3	R(1,18)	2.5066			
! R4	R(2,3)	1.418	-]		
! R5	R(2,4)	1.4179	-		
! R6	R(3,5)	1.4108	-		
! R7	R(3,8)	1.0703	-		
! R8	R(4,6)	1.412	-]		
! R9	R(4,9)	1.0724	-		
! R10	R(5,7)	1.4141			
! R11	R(5,10)	1.0733			
! R12	R(6,7)	1.4062			
! R13	R(6,11)	1.0728			
! R14	R(7,12)	1.0751			
! R15	R(9,17)	2.7902			
! R16	R(9,19)	3.4751			
! R17	R(9,20)	3.4751			
! R18	R(13,14)	1.0797		-DE/DX = 0.	!
! R19	R(13,15)	1.0836		-DE/DX = 0.	!
! R20	R(13,16)	1.0836		-DE/DX = 0.	!
! R21	R(17,18)	1.0009		-DE/DX = 0.	!
! R22	R(17,19)	1.0007		-DE/DX = 0.	!
! R23	R(17,20)	1.0007		-DE/DX = 0.	!
! A1	A(2,1,13)	120.9645		-DE/DX = 0.	!
! A2	A(2,1,18)	116.97		-DE/DX = 0.	!
! A3	A(13,1,18)	122.0656		-DE/DX = 0.	!
! A4	A(1,2,3)	123.0139		-DE/DX = 0.	!
! A5	A(1,2,4)	114.8317		-DE/DX = 0.	!
! A6	A(3,2,4)	122.1545		-DE/DX = 0.	!
! A7	A(2,3,5)	118.0736		-DE/DX = 0.	!
! A8	A(2,3,8)	121.4308		-DE/DX = 0.	!
! A9	A(5,3,8)	120.4957		-DE/DX = 0.	!
! A10	A(2,4,6)	118.8733		-DE/DX = 0.	!
! A11	A(2,4,9)	118.7732		-DE/DX = 0.	!
! A12	A(6,4,9)	122.3535		-DE/DX = 0.	!
! A13	A(3,5,7)	120.0677		-DE/DX = 0.	!
! A14	A(3,5,10)	119.981		-DE/DX = 0.	!
! A15	A(7,5,10)	119.9513		-DE/DX = 0.	!
! A16	A(4,6,7)	119.389		-DE/DX = 0.	!
! A17	A(4,6,11)	120.242		-DE/DX = 0.	!
! A18	A(7,6,11)	120.369		-DE/DX = 0.	!
! A19	A(5,7,6)	121.4419		-DE/DX = 0.	!
! A20	A(5,7,12)	119.024		-DE/DX = 0.	!
! A21	A(6,7,12)	119.5341		-DE/DX = 0.	!
! A22	A(4,9,17)	149.0349		-DE/DX = 0.	!
! A23	A(4,9,19)	146.6066		-DE/DX = 0.	!
! A24	A(4,9,20)	146.6054		-DE/DX = 0.	!
! A25	A(19,9,20)	26.909		-DE/DX = 0.	!
! A26	A(1,13,14)	106.0795		-DE/DX = 0.	!
! A27	A(1,13,15)	111.0194		-DE/DX = 0.	!
! A28	A(1,13,16)	111.0193		-DE/DX = 0.	!



! A29	A(14,13,15)	109.4577	-DE/DX = 0.	!
! A30	A(14,13,16)	109.4575	-DE/DX = 0.	!
! A31	A(15,13,16)	109.7296	-DE/DX = 0.	!
! A32	A(9,17,18)	58.9372	-DE/DX = 0.	!
! A33	A(18,17,19)	108.031	-DE/DX = 0.	!
! A34	A(18,17,20)	108.0311	-DE/DX = 0.	!
! A35	A(19,17,20)	107.8023	-DE/DX = 0.	!
! A36	A(1,18,17)	161.4531	-DE/DX = 0.	!
! D1	D(13,1,2,3)	-0.0005	-DE/DX = 0.	!
! D2	D(13,1,2,4)	-179.9988	-DE/DX = 0.	!
! D3	D(18,1,2,3)	-179.9984	-DE/DX = 0.	!
! D4	D(18,1,2,4)	0.0032	-DE/DX = 0.	!
! D5	D(2,1,13,14)	-179.9993	-DE/DX = 0.	!
! D6	D(2,1,13,15)	-61.1736	-DE/DX = 0.	!
! D7	D(2,1,13,16)	61.1753	-DE/DX = 0.	!
! D8	D(18,1,13,14)	-0.0015	-DE/DX = 0.	!
! D9	D(18,1,13,15)	118.8242	-DE/DX = 0.	!
! D10	D(18,1,13,16)	-118.8269	-DE/DX = 0.	!
! D11	D(2,1,18,17)	-0.0036	-DE/DX = 0.	!
! D12	D(13,1,18,17)	179.9985	-DE/DX = 0.	!
! D13	D(1,2,3,5)	-179.999	-DE/DX = 0.	!
! D14	D(1,2,3,8)	0.0016	-DE/DX = 0.	!
! D15	D(4,2,3,5)	-0.0008	-DE/DX = 0.	!
! D16	D(4,2,3,8)	179.9998	-DE/DX = 0.	!
! D17	D(1,2,4,6)	179.9991	-DE/DX = 0.	!
! D18	D(1,2,4,9)	-0.0014	-DE/DX = 0.	!
! D19	D(3,2,4,6)	0.0008	-DE/DX = 0.	!
! D20	D(3,2,4,9)	-179.9998	-DE/DX = 0.	!
! D21	D(2,3,5,7)	0.0001	-DE/DX = 0.	!
! D22	D(2,3,5,10)	-179.9998	-DE/DX = 0.	!
! D23	D(8,3,5,7)	179.9995	-DE/DX = 0.	!
! D24	D(8,3,5,10)	-0.0004	-DE/DX = 0.	!
! D25	D(2,4,6,7)	0.	-DE/DX = 0.	!
! D26	D(2,4,6,11)	179.9991	-DE/DX = 0.	!
! D27	D(9,4,6,7)	-179.9994	-DE/DX = 0.	!
! D28	D(9,4,6,11)	-0.0003	-DE/DX = 0.	!
! D29	D(2,4,9,17)	-0.0028	-DE/DX = 0.	!
! D30	D(2,4,9,19)	25.0048	-DE/DX = 0.	!
! D31	D(2,4,9,20)	-25.0105	-DE/DX = 0.	!
! D32	D(6,4,9,17)	179.9966	-DE/DX = 0.	!
! D33	D(6,4,9,19)	-154.9958	-DE/DX = 0.	!
! D34	D(6,4,9,20)	154.9889	-DE/DX = 0.	!
! D35	D(3,5,7,6)	0.0007	-DE/DX = 0.	!
! D36	D(3,5,7,12)	179.9999	-DE/DX = 0.	!
! D37	D(10,5,7,6)	-179.9994	-DE/DX = 0.	!
! D38	D(10,5,7,12)	-0.0002	-DE/DX = 0.	!
! D39	D(4,6,7,5)	-0.0007	-DE/DX = 0.	!
! D40	D(4,6,7,12)	-179.9999	-DE/DX = 0.	!
! D41	D(11,6,7,5)	-179.9999	-DE/DX = 0.	!
! D42	D(11,6,7,12)	0.001	-DE/DX = 0.	!
! D43	D(4,9,17,18)	0.003	-DE/DX = 0.	!
! D44	D(9,17,18,1)	0.0008	-DE/DX = 0.	!
! D45	D(19,17,18,1)	-121.8179	-DE/DX = 0.	!
! D46	D(20,17,18,1)	121.8168	-DE/DX = 0.	!