

原子编号:

29 44 45 46

29 44 45 46 (47 48)

charge

29 44 45 46

0.110 0.520 -0.760 -0.760

(0.110 0.050 0.090 0.090)

pair

44 0.070000000000000 3.56359487256136 0.070000000000000 3.56359487256136

45 0.120000000000000 3.02905564167715 0.120000000000000 3.02905564167715

46 0.120000000000000 3.02905564167715 0.120000000000000 3.02905564167715

44 0.056000000000000 3.58141284692416 0.010000000000000 3.38541512893329

45 0.035000000000000 2.38760856461611 0.035000000000000 2.38760856461611

46 0.035000000000000 2.38760856461611 0.035000000000000 2.38760856461611

bond 20 21

44 45 525.000 1.2600

44 46 525.000 1.2600

29 44 200.000 1.4800

44 45 309.000 1.1110

44 46 309.000 1.1110

29 44 222.500 1.4900

angle 40 40 41 42 43 44

29 44 45 40.00000 114.00000 50.00000 2.38800

29 44 46 40.00000 114.00000 50.00000 2.38800

45 44 46 100.00000 132.00000 70.00000 2.22500

30 29 44 50.00000 109.50000 0.00000 0.00000

31 29 44 45.00000 103.00000 0.00000 0.00000

40 29 44 52.00000 108.00000 0.00000 0.00000

29 44 45 33.43000 110.10000 22.53000 2.17900

29 44 46 33.43000 110.10000 22.53000 2.17900

45 44 46 75.70000 110.10000 0.00000 0.00000

30	29	44	34.50000	110.10000	22.53000	2.17900
31	29	44	45.00000	109.00000	0.00000	0.00000
40	29	44	58.35000	113.50000	11.16000	2.56100

dihedral 91 91 92 92 91 91

30	29	44	45	0.0500	6	180	1.00
30	29	44	46	0.0500	6	180	1.00
31	29	44	45	0.6400	2	180	1.00
31	29	44	46	0.6400	2	180	1.00
40	29	44	45	0.0500	6	180	1.00
40	29	44	46	0.0500	6	180	1.00

1	31	29	44	0.2000	3	0	1.00
36	40	29	44	0.2000	3	0	1.00
41	40	29	44	0.2000	3	0	1.00
42	40	29	44	0.2000	3	0	1.00

30	29	44	45	0.2000	3	0	1.00
30	29	44	46	0.2000	3	0	1.00
31	29	44	45	0.2000	3	0	1.00
31	29	44	46	0.2000	3	0	1.00
40	29	44	45	0.2000	3	0	1.00
40	29	44	46	0.2000	3	0	1.00

1	31	29	44	0.2000	3	0	1.00
36	40	29	44	0.2000	3	0	1.00
41	40	29	44	0.2000	3	0	1.00
42	40	29	44	0.2000	3	0	1.00

improper 1

44	29	46	45	96.000	0.00
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