**2/8/18: Initialized HF calculations**

5760489 mf\_nes2.8 mp2\_10B\_cc-pVTZ bdnguye2 R 3:05 1 c-8-20

5760490 mf\_nes2.8 mp2\_11B\_cc-pVTZ bdnguye2 R 3:05 1 c-8-19

5760491 mf\_nes2.8 mp2\_12B\_cc-pVTZ bdnguye2 R 3:05 1 c-8-18

5760494 mf\_nes2.8 mp2\_15B\_cc-pVTZ bdnguye2 R 3:05 1 c-6-234

5760495 mf\_nes2.8 mp2\_16B\_cc-pVTZ bdnguye2 R 3:05 1 c-6-232

5760499 mf\_nes2.8 mp2\_1B\_cc-pVTZ bdnguye2 R 3:05 1 c-5-24

5760500 mf\_nes2.8 mp2\_20B\_cc-pVTZ bdnguye2 R 3:05 1 c-3-343

5760501 mf\_nes2.8 mp2\_21B\_cc-pVTZ bdnguye2 R 3:05 1 c-3-342

5760502 mf\_nes2.8 mp2\_22B\_cc-pVTZ bdnguye2 R 3:05 1 c-3-341

5760503 mf\_i-b2.8 mp2\_23B\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760504 mf\_i-b2.8 mp2\_23-ciB\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760505 mf\_i-b2.8 mp2\_24B\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760506 mf\_i-b2.8 mp2\_24-ciB\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760507 mf\_i-b2.8 mp2\_25B\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760508 mf\_i-b2.8 mp2\_25-ciB\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760509 mf\_i-b2.8 mp2\_26B\_cc-pVTZ bdnguye2 R 3:05 1 c-9-413

5760510 mf\_i-b2.8 mp2\_26-ciB\_cc-pVTZ bdnguye2 R 3:02 1 c-9-413

5760520 mf\_i-b2.8 mp2\_3B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760521 mf\_i-b2.8 mp2\_4B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760522 mf\_i-b2.8 mp2\_5B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760523 mf\_i-b2.8 mp2\_6B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760524 mf\_i-b2.8 mp2\_7B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760525 mf\_i-b2.8 mp2\_8B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-371

5760526 mf\_i-b2.8 mp2\_9B\_cc-pVTZ bdnguye2 R 3:02 1 c-9-333

5760527 mf\_i-b2.8 mp2\_10B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760528 mf\_i-b2.8 mp2\_11B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760529 mf\_i-b2.8 mp2\_12B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760530 mf\_i-b2.8 mp2\_13B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760531 mf\_i-b2.8 mp2\_14B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760532 mf\_i-b2.8 mp2\_15B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760533 mf\_i-b2.8 mp2\_16B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-333

5760534 mf\_i-b2.8 mp2\_17B\_cc-pVQZ bdnguye2 R 3:02 1 c-9-332

5760535 mf\_i-b2.8 mp2\_18B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-332

5760536 mf\_i-b2.8 mp2\_19B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-332

5760537 mf\_i-b2.8 mp2\_1B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-332

5760538 mf\_i-b2.8 mp2\_20B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-332

5760539 mf\_i-b2.8 mp2\_21B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-331

5760540 mf\_i-b2.8 mp2\_22B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-331

5760541 mf\_i-b2.8 mp2\_23B\_cc-pVQZ bdnguye2 R 2:59 1 c-9-331

5760542 mf\_ilg2.3 mp2\_23-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-41

5760543 mf\_ilg2.3 mp2\_24B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-41

5760544 mf\_ilg2.3 mp2\_24-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-41

5760545 mf\_ilg2.3 mp2\_25B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-41

5760546 mf\_ilg2.3 mp2\_25-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-38

5760547 mf\_ilg2.3 mp2\_26B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-37

5760548 mf\_ilg2.3 mp2\_26-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-33

5760549 mf\_ilg2.3 mp2\_27B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-33

5760550 mf\_ilg2.3 mp2\_27-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-33

5760551 mf\_ilg2.3 mp2\_28B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-33

5760552 mf\_ilg2.3 mp2\_28-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-33

5760555 mf\_ilg2.3 mp2\_2B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-29

5760556 mf\_ilg2.3 mp2\_30B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-29

5760557 mf\_ilg2.3 mp2\_30-ciB\_cc-pVQZ bdnguye2 R 2:55 1 c-16-28

5760558 mf\_ilg2.3 mp2\_3B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-28

5760559 mf\_ilg2.3 mp2\_4B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-28

5760560 mf\_ilg2.3 mp2\_5B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-28

5760561 mf\_ilg2.3 mp2\_6B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-28

5760562 mf\_ilg2.3 mp2\_7B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-19

5760563 mf\_ilg2.3 mp2\_8B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-19

5760564 mf\_ilg2.3 mp2\_9B\_cc-pVQZ bdnguye2 R 2:55 1 c-16-19

5760565 mf\_ilg2.3 mp2\_10B\_def2-qzvp bdnguye2 R 2:55 1 c-16-19

5760566 mf\_ilg2.3 mp2\_11B\_def2-qzvp bdnguye2 R 2:55 1 c-16-19

5760567 mf\_ilg2.3 mp2\_12B\_def2-qzvp bdnguye2 R 2:55 1 c-15-41

5760568 mf\_ilg2.3 mp2\_13B\_def2-qzvp bdnguye2 R 2:55 1 c-15-41

5760569 mf\_ilg2.3 mp2\_14B\_def2-qzvp bdnguye2 R 2:55 1 c-15-41

5760570 mf\_ilg2.3 mp2\_15B\_def2-qzvp bdnguye2 R 2:55 1 c-15-41

5760571 mf\_ilg2.3 mp2\_16B\_def2-qzvp bdnguye2 R 2:55 1 c-15-41

5760572 mf\_ilg2.3 mp2\_17B\_def2-qzvp bdnguye2 R 2:55 1 c-15-38

5760573 mf\_ilg2.3 mp2\_18B\_def2-qzvp bdnguye2 R 2:54 1 c-15-37

5760575 mf\_i-b2.8 mp2\_1B\_def2-qzvp bdnguye2 R 2:49 1 c-9-411

5760576 mf\_i-b2.8 mp2\_20B\_def2-qzvp bdnguye2 R 2:45 1 c-9-411

5760577 mf\_i-b2.8 mp2\_21B\_def2-qzvp bdnguye2 R 2:29 1 c-9-412

5760578 mf\_i-b2.8 mp2\_22B\_def2-qzvp bdnguye2 R 2:29 1 c-9-411

5760579 mf\_nes2.8 mp2\_23B\_def2-qzvp bdnguye2 R 2:18 1 c-8-17

5760580 mf\_i-b2.8 mp2\_23-ciB\_def2-qzvp bdnguye2 R 2:05 1 c-9-412

5760581 mf\_nes2.8 mp2\_24B\_def2-qzvp bdnguye2 R 2:04 1 c-5-25

5760582 mf\_nes2.8 mp2\_24-ciB\_def2-qzvp bdnguye2 R 2:03 1 c-5-26

5760583 mf\_nes2.8 mp2\_25B\_def2-qzvp bdnguye2 R 1:55 1 c-7-21

5760584 mf\_ilg2.3 mp2\_25-ciB\_def2-qzvp bdnguye2 R 1:48 1 c-16-32

5760585 mf\_nes2.8 mp2\_26B\_def2-qzvp bdnguye2 R 1:43 1 c-6-231

5760586 mf\_i-b2.8 mp2\_26-ciB\_def2-qzvp bdnguye2 R 1:39 1 c-9-411

5760587 mf\_i-b2.8 mp2\_27B\_def2-qzvp bdnguye2 R 1:27 1 c-9-371

5760588 mf\_i-b2.8 mp2\_27-ciB\_def2-qzvp bdnguye2 R 0:38 1 c-9-371

5760589 mf\_ilg2.3 mp2\_28B\_def2-qzvp bdnguye2 R 0:12 1 c-16-29

5760590 mf\_i-b2.8 mp2\_28-ciB\_def2-qzvp bdnguye2 R 0:10 1 c-9-411

5760591 mf\_nes2.8 mp2\_29B\_def2-qzvp bdnguye2 PD 0:00 1 (Resources)

5760592 mf\_nes2.8 mp2\_29-ciB\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760593 mf\_nes2.8 mp2\_2B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760594 mf\_nes2.8 mp2\_30B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760595 mf\_nes2.8 mp2\_30-ciB\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760596 mf\_nes2.8 mp2\_3B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760597 mf\_nes2.8 mp2\_4B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760598 mf\_nes2.8 mp2\_5B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760599 mf\_nes2.8 mp2\_6B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760600 mf\_nes2.8 mp2\_7B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760601 mf\_nes2.8 mp2\_8B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760602 mf\_nes2.8 mp2\_9B\_def2-qzvp bdnguye2 PD 0:00 1 (Priority)

5760603 mf\_nes2.8 mp2\_10AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760604 mf\_nes2.8 mp2\_11AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760605 mf\_nes2.8 mp2\_12AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760606 mf\_nes2.8 mp2\_13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760607 mf\_nes2.8 mp2\_14AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760608 mf\_nes2.8 mp2\_15AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760609 mf\_nes2.8 mp2\_16AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760610 mf\_nes2.8 mp2\_17AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760611 mf\_nes2.8 mp2\_18AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760612 mf\_nes2.8 mp2\_19AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760613 mf\_nes2.8 mp2\_1AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760614 mf\_nes2.8 mp2\_20AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760615 mf\_nes2.8 mp2\_21AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760616 mf\_nes2.8 mp2\_22AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5760617 mf\_nes2.8 mp2\_23AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760618 mf\_nes2.8 mp2\_23-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760619 mf\_nes2.8 mp2\_24AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760620 mf\_nes2.8 mp2\_24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760621 mf\_nes2.8 mp2\_25AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760622 mf\_nes2.8 mp2\_25-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760623 mf\_nes2.8 mp2\_26AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760624 mf\_nes2.8 mp2\_26-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760625 mf\_nes2.8 mp2\_27AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760626 mf\_nes2.8 mp2\_27-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760627 mf\_nes2.8 mp2\_28AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760628 mf\_nes2.8 mp2\_28-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760629 mf\_nes2.8 mp2\_29AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760630 mf\_nes2.8 mp2\_29-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760631 mf\_nes2.8 mp2\_2AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760632 mf\_nes2.8 mp2\_30AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760633 mf\_nes2.8 mp2\_30-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760634 mf\_nes2.8 mp2\_3AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760635 mf\_nes2.8 mp2\_4AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760636 mf\_nes2.8 mp2\_5AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760637 mf\_nes2.8 mp2\_6AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760638 mf\_nes2.8 mp2\_7AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760639 mf\_nes2.8 mp2\_8AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760640 mf\_nes2.8 mp2\_9AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760641 mf\_nes2.8 mp2\_10AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760642 mf\_nes2.8 mp2\_11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760643 mf\_nes2.8 mp2\_12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760644 mf\_nes2.8 mp2\_13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760645 mf\_nes2.8 mp2\_14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760646 mf\_nes2.8 mp2\_15AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760647 mf\_nes2.8 mp2\_16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760648 mf\_nes2.8 mp2\_17AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760649 mf\_nes2.8 mp2\_18AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760650 mf\_nes2.8 mp2\_19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760651 mf\_nes2.8 mp2\_1AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760652 mf\_nes2.8 mp2\_20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760653 mf\_nes2.8 mp2\_21AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760654 mf\_nes2.8 mp2\_22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760655 mf\_nes2.8 mp2\_23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760656 mf\_nes2.8 mp2\_23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760657 mf\_nes2.8 mp2\_24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760658 mf\_nes2.8 mp2\_24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760659 mf\_nes2.8 mp2\_25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760660 mf\_nes2.8 mp2\_25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760661 mf\_nes2.8 mp2\_26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760662 mf\_nes2.8 mp2\_26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760663 mf\_nes2.8 mp2\_27AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760664 mf\_nes2.8 mp2\_27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760665 mf\_nes2.8 mp2\_28AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760666 mf\_nes2.8 mp2\_28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760667 mf\_nes2.8 mp2\_29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760668 mf\_nes2.8 mp2\_29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760669 mf\_nes2.8 mp2\_2AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760670 mf\_nes2.8 mp2\_30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760671 mf\_nes2.8 mp2\_30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760672 mf\_nes2.8 mp2\_3AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760673 mf\_nes2.8 mp2\_4AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760674 mf\_nes2.8 mp2\_5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760675 mf\_nes2.8 mp2\_6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760676 mf\_nes2.8 mp2\_7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760677 mf\_nes2.8 mp2\_8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760678 mf\_nes2.8 mp2\_9AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760679 mf\_nes2.8 mp2\_10AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760680 mf\_nes2.8 mp2\_11AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760681 mf\_nes2.8 mp2\_12AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760682 mf\_nes2.8 mp2\_13AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760683 mf\_nes2.8 mp2\_14AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760684 mf\_nes2.8 mp2\_15AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760685 mf\_nes2.8 mp2\_16AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760686 mf\_nes2.8 mp2\_17AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760687 mf\_nes2.8 mp2\_18AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760688 mf\_nes2.8 mp2\_19AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760689 mf\_nes2.8 mp2\_1AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760690 mf\_nes2.8 mp2\_20AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760691 mf\_nes2.8 mp2\_21AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760692 mf\_nes2.8 mp2\_22AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760693 mf\_nes2.8 mp2\_23AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760694 mf\_nes2.8 mp2\_23-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760695 mf\_nes2.8 mp2\_24AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760696 mf\_nes2.8 mp2\_24-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760697 mf\_nes2.8 mp2\_25AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760698 mf\_nes2.8 mp2\_25-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760699 mf\_nes2.8 mp2\_26AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760700 mf\_nes2.8 mp2\_26-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760701 mf\_nes2.8 mp2\_27AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760702 mf\_nes2.8 mp2\_27-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760703 mf\_nes2.8 mp2\_28AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760704 mf\_nes2.8 mp2\_28-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760705 mf\_nes2.8 mp2\_29AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760706 mf\_nes2.8 mp2\_29-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760707 mf\_nes2.8 mp2\_2AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760708 mf\_nes2.8 mp2\_30AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760709 mf\_nes2.8 mp2\_30-ciAB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760710 mf\_nes2.8 mp2\_3AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760711 mf\_nes2.8 mp2\_4AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760712 mf\_nes2.8 mp2\_5AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760713 mf\_nes2.8 mp2\_6AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760714 mf\_nes2.8 mp2\_7AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760715 mf\_nes2.8 mp2\_8AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760716 mf\_nes2.8 mp2\_9AB\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760726 mf\_nes2.8 mp2\_1A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760727 mf\_nes2.8 mp2\_1A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760728 mf\_nes2.8 mp2\_1A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760729 mf\_nes2.8 mp2\_3A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760730 mf\_nes2.8 mp2\_3A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760731 mf\_nes2.8 mp2\_3A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760732 mf\_nes2.8 mp2\_5A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760733 mf\_nes2.8 mp2\_5A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760734 mf\_nes2.8 mp2\_5A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760735 mf\_nes2.8 mp2\_7A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760736 mf\_nes2.8 mp2\_7A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760737 mf\_nes2.8 mp2\_7A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760738 mf\_nes2.8 mp2\_8A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760739 mf\_nes2.8 mp2\_8A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760740 mf\_nes2.8 mp2\_8A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760741 mf\_nes2.8 mp2\_9A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760742 mf\_nes2.8 mp2\_9A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760743 mf\_nes2.8 mp2\_9A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760744 mf\_nes2.8 mp2\_11A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760745 mf\_nes2.8 mp2\_11A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760746 mf\_nes2.8 mp2\_11A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760747 mf\_nes2.8 mp2\_13A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760748 mf\_nes2.8 mp2\_13A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760749 mf\_nes2.8 mp2\_13A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760750 mf\_nes2.8 mp2\_15A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760751 mf\_nes2.8 mp2\_15A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760752 mf\_nes2.8 mp2\_15A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760753 mf\_nes2.8 mp2\_17A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760754 mf\_nes2.8 mp2\_17A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760755 mf\_nes2.8 mp2\_17A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760756 mf\_nes2.8 mp2\_19A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760757 mf\_nes2.8 mp2\_19A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760758 mf\_nes2.8 mp2\_19A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760759 mf\_nes2.8 mp2\_21A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760760 mf\_nes2.8 mp2\_21A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760761 mf\_nes2.8 mp2\_21A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760762 mf\_nes2.8 mp2\_22A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760763 mf\_nes2.8 mp2\_22A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760764 mf\_nes2.8 mp2\_22A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760765 mf\_nes2.8 mp2\_23A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760766 mf\_nes2.8 mp2\_23A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760767 mf\_nes2.8 mp2\_23A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760768 mf\_nes2.8 mp2\_24A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760769 mf\_nes2.8 mp2\_24A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760770 mf\_nes2.8 mp2\_24A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760771 mf\_nes2.8 mp2\_25A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760772 mf\_nes2.8 mp2\_25A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760773 mf\_nes2.8 mp2\_25A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760774 mf\_nes2.8 mp2\_27A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760775 mf\_nes2.8 mp2\_27A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760776 mf\_nes2.8 mp2\_27A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760777 mf\_nes2.8 mp2\_29A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760778 mf\_nes2.8 mp2\_29A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760779 mf\_nes2.8 mp2\_29A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760780 mf\_nes2.8 mp2\_30A\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760781 mf\_nes2.8 mp2\_30A\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760782 mf\_nes2.8 mp2\_30A\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760783 mf\_nes2.8 mp2\_23-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760784 mf\_nes2.8 mp2\_23-ciA\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760785 mf\_nes2.8 mp2\_23-ciA\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760786 mf\_nes2.8 mp2\_24-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760787 mf\_nes2.8 mp2\_24-ciA\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760788 mf\_nes2.8 mp2\_24-ciA\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760789 mf\_nes2.8 mp2\_25-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760790 mf\_nes2.8 mp2\_25-ciA\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760791 mf\_nes2.8 mp2\_25-ciA\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760792 mf\_nes2.8 mp2\_27-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760793 mf\_nes2.8 mp2\_27-ciA\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760794 mf\_nes2.8 mp2\_27-ciA\_def2-qzvp bdnguye2 PD 0:00 1 (None)

5760795 mf\_nes2.8 mp2\_29-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

5760796 mf\_nes2.8 mp2\_29-ciA\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

5760797 mf\_nes2.8 mp2\_29-ciA\_def2-qzvp bdnguye2 PD 0:00 1 (None)

**2/12/18:**

gplogin2: dscf\_MPI calculations

5003 nes2.8 mp2\_3AB\_cc-pVTZ bdnguye2 R 1:24:43 4 c-12-[11-14]

5009 nes2.8 mp2\_8AB\_cc-pVTZ bdnguye2 R 39:12 4 c-12-[17-18,21-22]

5010 nes2.8 mp2\_9AB\_cc-pVTZ bdnguye2 R 30:57 4 c-12-[251,253-254],c-13-11

5011 nes2.8 mp2\_10AB\_cc-pVTZ bdnguye2 R 26:23 4 c-13-[12-15]

5014 nes2.8 mp2\_13AB\_cc-pVTZ bdnguye2 R 15:48 4 c-5-10,c-13-[222-224]

5016 nes2.8 mp2\_17AB\_cc-pVTZ bdnguye2 R 13:17 4 c-13-[16-18,221]

5017 nes2.8 mp2\_18AB\_cc-pVTZ bdnguye2 PD 0:00 4 (Resources)

5018 nes2.8 mp2\_19AB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5023 nes2.8 mp2\_24AB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5024 nes2.8 mp2\_25AB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5030 nes2.8 mp2\_23-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5031 nes2.8 mp2\_24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5032 nes2.8 mp2\_25-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5033 nes2.8 mp2\_26-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5034 nes2.8 mp2\_27-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5035 nes2.8 mp2\_28-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5036 nes2.8 mp2\_29-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5037 nes2.8 mp2\_30-ciAB\_cc-pVTZ bdnguye2 PD 0:00 4 (Priority)

5043 nes2.8 mp2\_7AB\_cc-pVTZ bdnguye2 R 42:27 8 c-17-[4-11]

5044 nes2.8 mp2\_28AB\_cc-pVTZ bdnguye2 R 37:56 4 c-17-[12-14,16]

5047 nes2.8 mp2\_30AB\_cc-pVTZ bdnguye2 R 31:25 4 c-17-[17-18,22-23]

5048 nes2.8 mp2\_27AB\_cc-pVTZ bdnguye2 R 29:25 4 c-17-[24-27]

5050 nes2.8 mp2\_26AB\_cc-pVTZ bdnguye2 R 26:55 3 c-3-38,c-17-[28-29]

5051 has2.5 mp2\_14AB\_cc-pVTZ bdnguye2 R 7:01 4 c-19-[291-294]

5052 ilg2.3 mp2\_20AB\_cc-pVTZ bdnguye2 R 4:24 4 c-13-[32-33,37-38]

5054 ilg2.3 mp2\_21AB\_cc-pVTZ bdnguye2 R 1:51 4 c-14-[37,42],c-15-[18-19]

5056 ilg2.3 mp2\_22AB\_cc-pVTZ bdnguye2 R 0:45 3 c-13-42,c-15-[24-25]

**02/28/18: Running MP2 and dscf calculations**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

5899 nes2.8 mp2\_9AB\_cc-pVTZ bdnguye2 R 3-03:45:46 4 c-12-254,c-13-[11-13]

5991 nes2.8 mp2\_17A\_def2-qzvp bdnguye2 R 1-21:32:58 2 c-17-[16-17]

6004 nes2.8 mp2\_28-ciA\_def2-qzvp bdnguye2 R 1-15:12:37 2 c-13-[223-224]

6015 nes2.8 mp2\_24-ciA\_def2-qzvp bdnguye2 R 1-15:01:31 2 c-17-[13-14]

6058 nes2.8 mp2\_29A\_def2-qzvp bdnguye2 R 1-00:28:31 2 c-17-[23,25]

6079 nes2.8 mp2\_9A\_def2-qzvp bdnguye2 R 14:43:29 4 c-17-[5-8]

6100 ilg2.3 mp2\_19A\_def2-qzvp bdnguye2 R 4:03:09 1 c-13-37

6116 ilg2.3 mp2-1\_ghosts-25\_cc-pVTZ bdnguye2 R 2:39:22 1 c-14-37

6118 nes2.8 mp2\_27A\_def2-qzvp bdnguye2 R 2:34:55 4 c-17-[4,9-11]

6119 nes2.8 mp2\_25A\_def2-qzvp bdnguye2 R 2:33:13 4 c-17-[12,18,22,26]

6128 nes2.8 mp2\_29-ciA\_def2-qzvp bdnguye2 R 1:25:12 4 c-12-[11-14]

6133 nes2.8 mp2\_21A\_def2-qzvp bdnguye2 R 8:53 6 c-12-[17,21-22,253],c-13-[14-15]

6134 nes2.8 mp2\_24A\_def2-qzvp bdnguye2 R 3:33 6 c-3-37,c-13-[16,18],c-17-[27-29]

6140 ilg2.3 mp2\_25AB\_def2-qzvp bdnguye2 R 11:21 1 c-13-32

6141 nes2.8 mp2-2\_ghosts-27\_cc-pVTZ bdnguye2 R 7:13 4 c-17-[5-8]

6143 has2.5 mp2-monomer1-24\_cc-pVTZ bdnguye2 R 4:02 1 c-19-292

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

5701919 mf\_s-b2.6 gks-pbe-1\_cc-pVQZ bdnguye2 R 30-05:23:04 1 c-16-12

5803860 mf\_i-b2.8 mp2-1\_ghosts-8\_cc-pVTZ bdnguye2 R 4:06:52 1 c-9-411

5803863 mf\_i-b2.8 mp2\_10AB\_cc-pVTZ bdnguye2 R 4:05:02 1 c-9-413

5803872 mf\_i-b2.8 mp2-1\_ghosts-12\_cc-pVTZ bdnguye2 R 2:01:35 1 c-9-374

5803875 mf\_i-b2.8 mp2-monomer1-20\_cc-pVTZ bdnguye2 R 1:45:39 1 c-9-373

5803878 mf\_i-b2.8 mp2-1\_ghosts-13\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

5803880 mf\_i-b2.8 mp2-monomer1-13\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5803882 mf\_i-b2.8 mp2\_13A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5803885 mf\_i-b2.8 mp2\_24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5804012 mf\_i-b2.8 mp2-1\_ghosts-19\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5804013 mf\_i-b2.8 mp2-monomer1-19\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5804014 mf\_i-b2.8 mp2\_27A\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

5804015 mf\_i-b2.8 mp2-2\_ghosts-24\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

5804016 mf\_i-b2.8 mp2-1\_ghosts-24\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

**03/13/18:**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

5701919 mf\_s-b2.6 gks-pbe-1\_cc-pVQZ bdnguye2 R 42-05:10:27 1 c-16-12

x5854727 mf\_i-b2.8 mp2\_23-ciAB\_cc-pVTZ bdnguye2 R 1:24:16 5 c-9-[334,372-374,411]

5854882 mf\_i-b2.8 mp2\_10AB\_cc-pVTZ bdnguye2 PD 0:00 5 (Priority)

x5854899 mf\_i-b2.8 mp2\_19AB\_cc-pVQZ bdnguye2 PD 0:00 5 (Resources)

x5854979 mf\_i-b2.8 mp2-monomer1-19\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x5854980 mf\_i-b2.8 mp2-1\_ghosts-19\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

+5855007 mf\_i-b2.8 mp2-1\_ghosts-20\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x5855039 mf\_i-b2.8 mp2\_24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x5855040 mf\_i-b2.8 mp2\_25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x5855041 mf\_i-b2.8 mp2\_27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x5855042 mf\_i-b2.8 mp2\_28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

~~5855043 mf\_i-b2.8 mp2\_29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)~~

~~5855223 mf\_i-b2.8 mp2-1\_ghosts-7\_cc-pVQZ bdnguye2 PD 0:00 5 (None)~~

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x6849 ilg2.3 mp2-monomer1-20\_cc-pVQZ bdnguye2 R 3:28:42 7 c-14-[38,41-42],c-15-[18-19,24-25]

x6909 brd2.4 mp2\_26AB\_cc-pVTZ bdnguye2 R 3:02:48 1 c-19-411

x6926 brd2.4 mp2-2\_ghosts-25\_cc-pVQZ bdnguye2 R 1:22:11 1 c-19-412

x6930 brd2.4 mp2\_26-ciAB\_cc-pVTZ bdnguye2 R 48:42 1 c-19-413

6934 has2.5 mp2-2\_ghosts-24\_cc-pVQZ bdnguye2 R 36:02 1 c-19-293

x6936 nes2.8 mp2-2\_ghosts-25\_cc-pVQZ bdnguye2 R 31:35 5 c-13-[11-15]

x6937 nes2.8 mp2-1\_ghosts-25\_cc-pVQZ bdnguye2 R 28:27 4 c-13-[16-18,221]

x6942 ilg2.3 mp2-2\_ghosts-27\_cc-pVQZ bdnguye2 R 19:21 5 c-13-[32-33,37-38,42]

x6943 nes2.8 mp2-1\_ghosts-27\_cc-pVQZ bdnguye2 R 17:14 4 c-17-[10-13]

x6944 nes2.8 mp2-1\_ghosts-28\_cc-pVQZ bdnguye2 R 15:42 4 c-17-[14,16-18]

x6945 ilg2.3 mp2-2\_ghosts-28\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x6946 ilg2.3 mp2\_27-ciA\_cc-pVQZ bdnguye2 PD 0:00 5 (Resources)

x6947 ilg2.3 mp2-1\_ghosts-26-ci\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x6948 ilg2.3 mp2-monomer1-26-ci\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

x6949 ilg2.3 mp2-2\_ghosts-7\_cc-pVQZ bdnguye2 PD 0:00 5 (Priority)

**03/13/2018: continuation**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

6934 has2.5 mp2-2\_ghosts-24\_cc-pVQZ bdnguye2 R 10:45:53 1 c-19-291

6966 brd2.4 mp2-1\_ghosts-24\_cc-pVQZ bdnguye2 R 6:32:45 1 c-19-412

Need freeze x6982 nes2.8 mp2-1\_ghosts-26\_cc-pVTZ bdnguye2 R 2:36:40 6 c-13-[12-17]

6983 nes2.8 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 2:34:38 4 c-13-[18,221-223]

x6987 ilg2.3 mp2\_27-ciA\_cc-pVQZ bdnguye2 R 2:15:56 1 c-13-38

-6993 ilg2.3 mp2-monomer1-26-ci\_cc-pVQZ bdnguye2 R 1:25:12 4 c-14-[41-42],c-15-[18-19]

x6999 brd2.4 mp2\_29-ciAB\_cc-pVQZ bdnguye2 R 39:10 1 c-19-413

x7000 brd2.4 mp2\_26-ciAB\_cc-pVTZ bdnguye2 R 24:05 1 c-19-414

7007 m-c2.2 mp2-2\_ghosts-7\_cc-pVQZ bdnguye2 R 0:52 1 c-9-29

x7005 ilg2.3 mp2-1\_ghosts-25\_cc-pVQZ bdnguye2 R 1:58 1 c-15-24

x7006 brd2.4 mp2-monomer1-19\_cc-pVQZ bdnguye2 R 7:43 1 c-19-411

x7008 brd2.4 mp2-1\_ghosts-7\_cc-pVQZ bdnguye2 R 2:13 1 c-19-413

x7009 nes2.8 mp2-1\_ghosts-26\_cc-pVTZ bdnguye2 R 0:01 6 c-13-[12-17]

+7010 brd2.4 mp2-1\_ghosts-8\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

+7011 brd2.4 mp2-2\_ghosts-8\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+7012 brd2.4 mp2-2\_ghosts-10\_cc-pVQZ bdnguye2 R 9:08 1 c-19-411

+7013 has2.5 mp2-1\_ghosts-10\_cc-pVQZ bdnguye2 PD 0:00 2 (Resources)

+7014 ilg2.3 mp2-1\_ghosts-20\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x7015 brd2.4 mp2-2\_ghosts-25\_cc-pVQZ bdnguye2 R 7:32 1 c-19-414

+7022 brd2.4 mp2-monomer1-19\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

+7023 brd2.4 mp2-1\_ghosts-8\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+7025 brd2.4 mp2-2\_ghosts-8\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+7026 brd2.4 mp2\_26-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x7027 m-c1.9 mp2-monomer1-24-ci\_cc-pVQZ bdnguye2 R 1:07 4 c-9-[15,17,19,21]

+7028 m-c1.9 mp2-monomer1-25-ci\_cc-pVQZ bdnguye2 R 0:20 5 c-9-[23,25,27,35,39]

**03/14/2018: MP2 Calculations allocate memory**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

6934 has2.5 mp2-2\_ghosts-24\_cc-pVQZ bdnguye2 R 21:10:21 1 c-19-291

6966 brd2.4 mp2-1\_ghosts-24\_cc-pVQZ bdnguye2 R 16:57:13 1 c-19-412

x6983 nes2.8 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 12:59:06 4 c-13-[18,221-223]

x7007 m-c2.2 mp2-2\_ghosts-7\_cc-pVQZ bdnguye2 R 10:10:09 1 c-9-29

7013 has2.5 mp2-1\_ghosts-10\_cc-pVQZ bdnguye2 PD 0:00 2 (Resources)

x7031 brd2.4 mp2-2\_ghosts-10\_cc-pVQZ bdnguye2 R 9:32 1 c-19-413

+7032 brd2.4 mp2-monomer1-19\_cc-pVQZ bdnguye2 R 3:38 1 c-19-411

7035 ilg2.3 mp2-1\_ghosts-26-ci\_cc-pVQZ bdnguye2 R 19:27 1 c-13-38

x7036 ilg2.3 mp2-monomer1-25-ci\_cc-pVQZ bdnguye2 R 14:24 1 c-15-18

7037 ilg2.3 mp2\_26-ciAB\_cc-pVTZ bdnguye2 R 14:23 2 c-14-42,c-15-19

7038 ilg2.3 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 8:47 1 c-14-41

7039 ilg2.3 mp2-monomer1-27-ci\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

+7040 ilg2.3 mp2-1\_ghosts-20\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

**03/15/2018: MP2 Calculations**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

6934 has2.5 mp2-2\_ghosts-24\_cc-pVQZ bdnguye2 R 1-15:18:48 1 c-19-291

6966 brd2.4 mp2-1\_ghosts-24\_cc-pVQZ bdnguye2 R 1-11:05:40 1 c-19-412

x7035 ilg2.3 mp2-1\_ghosts-26-ci\_cc-pVQZ bdnguye2 R 18:27:54 1 c-13-38

+7038 ilg2.3 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 18:17:14 1 c-14-41

x7039 ilg2.3 mp2-monomer1-27-ci\_cc-pVQZ bdnguye2 R 9:53:08 1 c-14-37

+7116 ilg2.3 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 1:28:18 1 c-15-18

x7119 brd2.4 mp2\_10AB\_cc-pVTZ bdnguye2 R 1:07:06 1 c-19-413

+7121 has2.5 mp2-1\_ghosts-20\_cc-pVQZ bdnguye2 R 1:01:05 1 c-19-294

7122 m-c2.2 mp2-monomer1-24-ci\_cc-pVQZ bdnguye2 R 58:27 1 c-9-29

7124 has2.5 mp2-1\_ghosts-10\_cc-pVQZ bdnguye2 R 27:06 2 c-19-[292-293]

+7127 brd2.4 mp2-1\_ghosts-14\_cc-pVQZ bdnguye2 R 8:58 1 c-19-414

+7128 brd2.4 mp2\_14AB\_cc-pVTZ bdnguye2 R 4:24 1 c-19-411

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

5701919 mf\_s-b2.6 gks-pbe-1\_cc-pVQZ bdnguye2 R 44-06:39:45 1 c-16-12

x5868870 mf\_i-b2.8 mp2-1\_ghosts-8\_cc-pVQZ bdnguye2 R 1:02:31 1 c-9-413

x5868937 mf\_i-b2.8 mp2-2\_ghosts-24-ci\_cc-pVQZ bdnguye2 R 44:44 1 c-9-374

x5869001 mf\_i-b2.8 mp2-monomer1-26-ci\_cc-pVQZ bdnguye2 R 41:39 1 c-9-373

x5869011 mf\_i-b2.8 mp2-2\_ghosts-8\_cc-pVQZ bdnguye2 R 37:34 1 c-9-411

x5869058 mf\_ilg2.3 mp2-1\_ghosts-24-ci\_cc-pVQZ bdnguye2 R 26:27 4 c-15-[34,41-42],c-16-18

x5869142 mf\_i-b2.8 mp2-1\_ghosts-11\_cc-pVQZ bdnguye2 R 15:18 1 c-9-412

x5869146 mf\_ilg2.3 mp2-monomer1-13\_cc-pVQZ bdnguye2 R 12:11 1 c-16-37

x5869202 mf\_ilg2.3 mp2-2\_ghosts-13\_cc-pVQZ bdnguye2 R 6:28 1 c-16-38

5869206 mf\_ilg2.3 mp2-1\_ghosts-13\_cc-pVQZ bdnguye2 R 5:19 1 c-16-41

5869217 mf\_i-b2.8 mp2\_13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

**03/16/2018: Home Stretch MP2 Calculations**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

5701919 mf\_s-b2.6 gks-pbe-1\_cc-pVQZ bdnguye2 R 45-14:43:16 1 c-16-12

5869217 mf\_i-b2.8 mp2\_13AB\_cc-pVTZ bdnguye2 R 1-06:10:36 1 c-9-331

x5910135 mf\_i-b2.8 mp2-2\_ghosts-11\_cc-pVQZ bdnguye2 R 11:55:32 1 c-9-411

5910231 mf\_i-b2.8 mp2-1\_ghosts-13\_cc-pVQZ bdnguye2 R 11:42:25 1 c-9-372

5910630 mf\_i-b2.8 mp2\_28AB\_cc-pVTZ bdnguye2 R 10:27:27 1 c-9-412

5914109 mf\_ilg2.3 mp2-2\_ghosts-12\_cc-pVQZ bdnguye2 R 23:57 3 c-16-[32,37-38]

5914118 mf\_ilg2.3 mp2\_11AB\_cc-pVQZ bdnguye2 R 19:37 2 c-16-[41-42]

x5914211 mf\_i-b2.8 mp2-monomer1-14\_cc-pVQZ bdnguye2 R 12:29 2 c-9-[334,371]

x5914218 mf\_i-b2.8 mp2-2\_ghosts-24\_cc-pVQZ bdnguye2 R 7:46 1 c-9-413

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x7122 m-c2.2 mp2-monomer1-24-ci\_cc-pVQZ bdnguye2 R 1-09:06:10 1 c-9-29

+7133 ilg2.3 mp2-1\_ghosts-14\_cc-pVQZ bdnguye2 R 1-00:36:38 2 c-14-[37,41]

7134 brd2.4 mp2\_14AB\_cc-pVTZ bdnguye2 R 1-00:35:44 1 c-19-414

x7143 ilg2.3 mp2-monomer1-19\_cc-pVQZ bdnguye2 R 22:43:21 1 c-15-19

7147 ilg2.3 mp2-monomer1-13\_cc-pVQZ bdnguye2 R 21:45:14 1 c-14-42

x7224 has2.5 mp2-1\_ghosts-20\_cc-pVQZ bdnguye2 R 11:57:02 2 c-19-[291,294]

x7240 brd2.4 mp2-1\_ghosts-10\_cc-pVQZ bdnguye2 R 46:22 1 c-19-412

7245 has2.5 mp2-1\_ghosts-12\_cc-pVQZ bdnguye2 R 40:28 2 c-19-[292-293]

+7303 brd2.4 mp2\_12AB\_cc-pVQZ bdnguye2 R 23:33 1 c-19-411

x7306 ilg2.3 mp2-1\_ghosts-24-ci\_cc-pVQZ bdnguye2 R 1:42 2 c-13-38,c-15-18

**03/18/2018: last few calcs**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x7147 ilg2.3 mp2-monomer1-13\_cc-pVQZ bdnguye2 R 2-12:53:49 1 c-14-42

+7378 has2.5 mp2-1\_ghosts-14\_cc-pVQZ bdnguye2 R 19:07 1 c-19-293

x7380 has2.5 mp2\_14AB\_cc-pVTZ bdnguye2 R 13:32 1 c-19-294

7383 ilg2.3 mp2\_12AB\_cc-pVQZ bdnguye2 R 11:49 1 c-15-19

7384 ilg2.3 mp2-1\_ghosts-24-ci\_cc-pVQZ bdnguye2 R 8:52 1 c-15-18

Gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

-5701919 mf\_s-b2.6 gks-pbe-1\_cc-pVQZ bdnguye2 R 47-05:57:35 1 c-16-12

x5869217 mf\_i-b2.8 mp2\_13AB\_cc-pVTZ bdnguye2 R 2-21:24:55 1 c-9-331

x5910231 mf\_i-b2.8 mp2-1\_ghosts-13\_cc-pVQZ bdnguye2 R 2-02:56:44 1 c-9-372

x5918298 mf\_i-b2.8 mp2-monomer1-14\_cc-pVQZ bdnguye2 R 1-01:45:12 1 c-9-373

x5927867 mf\_i-b2.8 mp2-1\_ghosts-12\_cc-pVQZ bdnguye2 R 8:44 1 c-9-413

x5927897 mf\_i-b2.8 mp2-1\_ghosts-24\_cc-pVQZ bdnguye2 R 4:29 1 c-9-332

**03/29/18: Closer check in with calculations and recomputing**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x6007684 mf\_ilg2.3 mp2\_12AB\_cc-pVQZ bdnguye2 R 5:39:16 1 c-16-41

6008599 mf\_nes2.8 mp2-1\_ghosts-9\_cc-pVTZ bdnguye2 CG 7:18 1 c-6-27

6008601 mf\_nes2.8 mp2-2\_ghosts-9\_cc-pVTZ bdnguye2 CG 5:53 1 c-7-14

+6009362 mf\_ilg2.3 mp2\_13AB\_cc-pVTZ bdnguye2 R 18:41 1 c-16-37

+6009363 c6145 mp2-1\_ghosts-26\_cc-pVTZ bdnguye2 R 15:31 1 c-12-29

x6009369 mf\_ilg2.3 mp2\_29AB\_cc-pVTZ bdnguye2 R 1:17 1 c-16-29

x6009374 c6145 mp2-1\_ghosts-26\_cc-pVQZ bdnguye2 R 0:30 1 c-12-30

x6009377 c6145 mp2-2\_ghosts-23\_cc-pVQZ bdnguye2 R 0:01 1 c-12-33

+6009400 c6145 mp2\_28AB\_cc-pVTZ bdnguye2 R 0:41 1 c-12-34

+6009407 c6145 mp2\_27AB\_cc-pVTZ bdnguye2 R 0:01 1 c-12-37

6009816 c6145 mp2\_27A\_cc-pVTZ bdnguye2 R 47:46 1 c-12-29

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

7892 has2.5 mp2\_13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

+7977 nes2.8 mp2-1\_ghosts-26\_cc-pVTZ bdnguye2 R 1:46:12 6 c-17-[9,13,23-26]

x7987 ilg2.3 mp2-supermol-30\_cc-pVQZ bdnguye2 R 38:00 1 c-13-38

**04/01/18: Calcuations Redo**

gplogin1:

+6016759 c6145 mp2\_13AB\_cc-pVTZ bdnguye2 R 0:00 2 c-12-42,c-13-27

+6016760 mf\_ilg2.3 mp2\_28AB\_cc-pVTZ bdnguye2 R 0:12 1 c-16-37

6016762 mf\_ilg2.3 mp2\_27AB\_cc-pVTZ bdnguye2 R 7:15 1 c-16-37

6016769 c6145 mp2\_13AB\_cc-pVTZ bdnguye2 R 0:07 1 c-12-42

gplogin2:

8063 ilg2.3 mp2-1\_ghosts-26\_cc-pVTZ bdnguye2 R 25:46 1 c-13-32

8064 ilg2.3 mp2\_27A\_cc-pVTZ bdnguye2 R 0:02 1 c-13-38

8065 ilg2.3 mp2\_28AB\_cc-pVTZ bdnguye2 R 0:01 1 c-14-42

**04/06/18: Redo MP2 Calcs**

gologin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

6008601 mf\_nes2.8 mp2-2\_ghosts-9\_cc-pVTZ bdnguye2 CG 5:53 1 c-7-14

6021945 mf\_ilg2.3 mp2-monomer1-13AB\_cc-pVTZ bdnguye2 R 16:36:55 1 c-15-38

6021946 mf\_ilg2.3 mp2-monomer1-14AB\_cc-pVTZ bdnguye2 R 16:36:55 1 c-15-41

6022178 mf\_s-b2.6 mp2\_3AB\_cc-pVQZ bdnguye2 R 11:02:29 1 c-16-12

6022179 mf\_s-b2.6 mp2\_4AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

6022180 mf\_s-b2.6 mp2\_5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022181 mf\_s-b2.6 mp2\_6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022182 mf\_s-b2.6 mp2\_7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022183 mf\_s-b2.6 mp2\_8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022184 mf\_s-b2.6 mp2\_9AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022185 mf\_s-b2.6 mp2\_10AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022186 mf\_s-b2.6 mp2\_11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022187 mf\_s-b2.6 mp2\_12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022188 mf\_s-b2.6 mp2\_13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022189 mf\_s-b2.6 mp2\_14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022190 mf\_s-b2.6 mp2\_15AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022191 mf\_s-b2.6 mp2\_16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022192 mf\_s-b2.6 mp2\_17AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022193 mf\_s-b2.6 mp2\_18AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022194 mf\_s-b2.6 mp2\_19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022195 mf\_s-b2.6 mp2\_20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022196 mf\_s-b2.6 mp2\_21AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022197 mf\_s-b2.6 mp2\_22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022198 mf\_s-b2.6 mp2\_23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022199 mf\_s-b2.6 mp2\_24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022200 mf\_s-b2.6 mp2\_25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022201 mf\_s-b2.6 mp2\_26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022258 mf\_s-b2.6 mp2\_28AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022261 mf\_s-b2.6 mp2\_29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022262 mf\_s-b2.6 mp2\_30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022264 mf\_s-b2.6 mp2\_23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022265 mf\_s-b2.6 mp2\_24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022267 mf\_s-b2.6 mp2\_25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022269 mf\_s-b2.6 mp2\_26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022271 mf\_s-b2.6 mp2\_27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022272 mf\_s-b2.6 mp2\_28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022273 mf\_s-b2.6 mp2\_29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6022274 mf\_s-b2.6 mp2\_30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

6023482 mf\_ilg2.3 mp2-2\_ghosts-24AB\_cc-pVTZ bdnguye2 R 15:22:22 1 c-16-32

6028280 mf\_ilg2.3 mp2-2\_ghosts-24-ciAB\_cc-pVTZ bdnguye2 R 2:21:11 1 c-16-29

6028281 mf\_ilg2.3 mp2-2\_ghosts-25-ciAB\_cc-pVTZ bdnguye2 R 2:21:11 1 c-16-37

6028282 mf\_ilg2.3 mp2-2\_ghosts-26-ciAB\_cc-pVTZ bdnguye2 R 2:21:11 1 c-16-41

6028916 mf\_ilg2.3 mp2-2\_ghosts-24AB\_cc-pVTZ bdnguye2 R 1:01:51 1 c-16-18

6028917 mf\_ilg2.3 mp2-2\_ghosts-25AB\_cc-pVTZ bdnguye2 R 40:44 1 c-15-33

6028918 mf\_ilg2.3 mp2-2\_ghosts-26AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6028919 mf\_ilg2.3 mp2-2\_ghosts-27AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6028920 mf\_ilg2.3 mp2-2\_ghosts-28AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6028921 mf\_ilg2.3 mp2-2\_ghosts-29AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6028922 mf\_ilg2.3 mp2-2\_ghosts-30AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6028990 mf\_i-b2.8 mp2-2\_ghosts-4AB\_cc-pVTZ bdnguye2 R 43:13 1 c-9-413

6029001 mf\_i-b2.8 mp2-2\_ghosts-19AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

6029002 mf\_i-b2.8 mp2-2\_ghosts-20AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029003 mf\_i-b2.8 mp2-2\_ghosts-21AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029555 mf\_i-b2.8 mp2-2\_ghosts-1AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029556 mf\_i-b2.8 mp2-2\_ghosts-2AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029557 mf\_i-b2.8 mp2-2\_ghosts-3AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029558 mf\_i-b2.8 mp2-2\_ghosts-4AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029559 mf\_i-b2.8 mp2-2\_ghosts-5AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029560 mf\_i-b2.8 mp2-2\_ghosts-6AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029561 mf\_i-b2.8 mp2-2\_ghosts-7AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029562 mf\_i-b2.8 mp2-2\_ghosts-8AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029563 mf\_i-b2.8 mp2-2\_ghosts-9AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029564 mf\_i-b2.8 mp2-2\_ghosts-10AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029565 mf\_i-b2.8 mp2-2\_ghosts-11AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029566 mf\_i-b2.8 mp2-2\_ghosts-12AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029567 mf\_i-b2.8 mp2-2\_ghosts-13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029568 mf\_i-b2.8 mp2-2\_ghosts-14AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029569 mf\_i-b2.8 mp2-2\_ghosts-15AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029570 mf\_i-b2.8 mp2-2\_ghosts-16AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029571 mf\_i-b2.8 mp2-2\_ghosts-17AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029572 mf\_i-b2.8 mp2-2\_ghosts-18AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029573 mf\_i-b2.8 mp2-2\_ghosts-19AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029574 mf\_i-b2.8 mp2-2\_ghosts-20AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029575 mf\_i-b2.8 mp2-2\_ghosts-21AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029576 mf\_i-b2.8 mp2-2\_ghosts-22AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029577 mf\_i-b2.8 mp2-2\_ghosts-23AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029578 mf\_i-b2.8 mp2-2\_ghosts-24AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029579 mf\_i-b2.8 mp2-2\_ghosts-25AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029580 mf\_i-b2.8 mp2-2\_ghosts-26AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029581 mf\_i-b2.8 mp2-2\_ghosts-27AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029582 mf\_i-b2.8 mp2-2\_ghosts-28AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029583 mf\_i-b2.8 mp2-2\_ghosts-29AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029584 mf\_i-b2.8 mp2-2\_ghosts-30AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029585 mf\_i-b2.8 mp2-2\_ghosts-23-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029586 mf\_i-b2.8 mp2-2\_ghosts-24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029587 mf\_i-b2.8 mp2-2\_ghosts-25-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029588 mf\_i-b2.8 mp2-2\_ghosts-26-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029589 mf\_i-b2.8 mp2-2\_ghosts-27-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029590 mf\_i-b2.8 mp2-2\_ghosts-28-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029591 mf\_i-b2.8 mp2-2\_ghosts-29-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029592 mf\_i-b2.8 mp2-2\_ghosts-30-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029890 mf\_ilg2.3 mp2\_1A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-38

6029891 mf\_ilg2.3 mp2\_3A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-38

6029892 mf\_ilg2.3 mp2\_5A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-38

6029893 mf\_ilg2.3 mp2\_7A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-41

6029894 mf\_ilg2.3 mp2\_8A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-41

6029895 mf\_ilg2.3 mp2\_10A\_cc-pVTZ bdnguye2 R 2:45 1 c-15-41

6029896 mf\_ilg2.3 mp2\_11A\_cc-pVTZ bdnguye2 R 2:45 1 c-16-32

6029897 mf\_ilg2.3 mp2\_14A\_cc-pVTZ bdnguye2 R 2:45 1 c-16-32

6029898 mf\_ilg2.3 mp2\_15A\_cc-pVTZ bdnguye2 R 2:45 1 c-16-32

6029899 mf\_ilg2.3 mp2\_18A\_cc-pVTZ bdnguye2 R 2:45 1 c-16-42

6029900 mf\_ilg2.3 mp2\_19A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029901 mf\_ilg2.3 mp2\_21A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029902 mf\_ilg2.3 mp2\_22A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029903 mf\_ilg2.3 mp2\_23A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029904 mf\_ilg2.3 mp2\_24A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029905 mf\_ilg2.3 mp2\_25A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029906 mf\_ilg2.3 mp2\_27A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029907 mf\_ilg2.3 mp2\_29A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029908 mf\_ilg2.3 mp2\_23-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029909 mf\_ilg2.3 mp2\_24-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029910 mf\_ilg2.3 mp2\_25-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029911 mf\_ilg2.3 mp2\_27-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

6029912 mf\_ilg2.3 mp2\_29-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

8216 ilg2.3 mp2\_7AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-37

8217 ilg2.3 mp2\_8AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-37

8218 ilg2.3 mp2\_9AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-37

8219 ilg2.3 mp2\_10AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-37

8220 ilg2.3 mp2\_11AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-38

8221 ilg2.3 mp2\_12AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-13-38

8228 ilg2.3 mp2\_19AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-14-37

8229 ilg2.3 mp2\_20AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-14-37

8230 ilg2.3 mp2\_21AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-14-37

8233 ilg2.3 mp2\_24AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-14-38

8234 ilg2.3 mp2\_25AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-14-38

8236 ilg2.3 mp2\_27AB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-15-18

8241 ilg2.3 mp2\_24-ciAB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-15-19

8242 ilg2.3 mp2\_25-ciAB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-15-19

8243 ilg2.3 mp2\_26-ciAB\_cc-pVTZ bdnguye2 R 18:01:05 1 c-15-19

8262 ilg2.3 mp2-2\_ghosts-11AB\_cc-pVTZ bdnguye2 R 4:03:42 1 c-15-25

8263 ilg2.3 mp2-2\_ghosts-12AB\_cc-pVTZ bdnguye2 R 3:02:58 1 c-13-33

8264 ilg2.3 mp2-2\_ghosts-13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

8265 ilg2.3 mp2-2\_ghosts-14AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

8312 has2.5 mp2-2\_ghosts-17AB\_cc-pVTZ bdnguye2 R 19:35 1 c-19-294

8313 has2.5 mp2-2\_ghosts-18AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

8315 nes2.8 mp2-1\_ghosts-15\_cc-pVQZ bdnguye2 PD 0:00 2 (Priority)

8316 nes2.8 mp2-monomer1-15\_cc-pVQZ bdnguye2 PD 0:00 4 (Priority)

8318 ilg2.3 mp2-monomer1-1AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8319 ilg2.3 mp2-monomer1-2AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8320 ilg2.3 mp2-monomer1-3AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8321 ilg2.3 mp2-monomer1-4AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8322 ilg2.3 mp2-monomer1-5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8323 ilg2.3 mp2-monomer1-6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8324 ilg2.3 mp2-monomer1-7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8325 ilg2.3 mp2-monomer1-8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8326 ilg2.3 mp2-monomer1-9AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8327 ilg2.3 mp2-monomer1-10AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8328 ilg2.3 mp2-monomer1-11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8329 ilg2.3 mp2-monomer1-12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8330 ilg2.3 mp2-monomer1-13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8331 ilg2.3 mp2-monomer1-14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8332 ilg2.3 mp2-monomer1-16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8333 ilg2.3 mp2-monomer1-17AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8334 ilg2.3 mp2-monomer1-18AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8335 ilg2.3 mp2-monomer1-19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8336 ilg2.3 mp2-monomer1-20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8337 ilg2.3 mp2-monomer1-21AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8338 ilg2.3 mp2-monomer1-22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8339 ilg2.3 mp2-monomer1-23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8340 ilg2.3 mp2-monomer1-24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8341 ilg2.3 mp2-monomer1-25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8342 ilg2.3 mp2-monomer1-26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8343 ilg2.3 mp2-monomer1-27AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8344 ilg2.3 mp2-monomer1-28AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8345 ilg2.3 mp2-monomer1-29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8346 ilg2.3 mp2-monomer1-30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8347 ilg2.3 mp2-monomer1-23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8348 ilg2.3 mp2-monomer1-24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8349 ilg2.3 mp2-monomer1-25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8350 ilg2.3 mp2-monomer1-26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8351 ilg2.3 mp2-monomer1-27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8352 ilg2.3 mp2-monomer1-28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8353 ilg2.3 mp2-monomer1-29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8354 ilg2.3 mp2-monomer1-30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8355 has2.5 mp2-1\_ghosts-1AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8356 has2.5 mp2-1\_ghosts-2AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8357 has2.5 mp2-1\_ghosts-3AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8358 has2.5 mp2-1\_ghosts-4AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8359 has2.5 mp2-1\_ghosts-5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8360 has2.5 mp2-1\_ghosts-6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8361 has2.5 mp2-1\_ghosts-7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8362 has2.5 mp2-1\_ghosts-8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8363 has2.5 mp2-1\_ghosts-9AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8364 has2.5 mp2-1\_ghosts-10AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8365 has2.5 mp2-1\_ghosts-11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8366 has2.5 mp2-1\_ghosts-12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8367 has2.5 mp2-1\_ghosts-13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8368 has2.5 mp2-1\_ghosts-14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8369 has2.5 mp2-1\_ghosts-16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8370 has2.5 mp2-1\_ghosts-17AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8371 has2.5 mp2-1\_ghosts-18AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8372 has2.5 mp2-1\_ghosts-19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8373 has2.5 mp2-1\_ghosts-20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8374 has2.5 mp2-1\_ghosts-21AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8375 has2.5 mp2-1\_ghosts-22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8376 has2.5 mp2-1\_ghosts-23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8377 has2.5 mp2-1\_ghosts-24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8378 has2.5 mp2-1\_ghosts-25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8379 has2.5 mp2-1\_ghosts-26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8380 has2.5 mp2-1\_ghosts-27AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8381 has2.5 mp2-1\_ghosts-28AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8382 has2.5 mp2-1\_ghosts-29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8383 has2.5 mp2-1\_ghosts-30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8384 has2.5 mp2-1\_ghosts-23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8385 has2.5 mp2-1\_ghosts-24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8386 has2.5 mp2-1\_ghosts-25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8387 has2.5 mp2-1\_ghosts-26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8388 has2.5 mp2-1\_ghosts-27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8389 has2.5 mp2-1\_ghosts-28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8390 has2.5 mp2-1\_ghosts-29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

8391 has2.5 mp2-1\_ghosts-30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)