**Legend:** \* some error; + job resubmitted

**12/12/17:**

Gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

4928010 mf\_ilg2.3 pbe-20AB\_cc-pVQZ bdnguye2 R 18-01:35:43 1 c-16-18

4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 16-00:15:52 1 c-16-33

5081397 mf\_i-b2.8 tpss-26-ciAB\_cc-pVTZ bdnguye2 R 2-21:14:23 1 c-9-372

5087328 mf\_i-b2.8 pbe-14AB\_cc-pVQZ bdnguye2 R 1-05:39:37 1 c-9-373

5106172 mf\_nes2.8 tpss-14AB\_cc-pVQZ bdnguye2 R 15:17 1 c-5-9

5106177 mf\_ilg2.3 15\_monomer1\_jobbsse bdnguye2 PD 0:00 1 (Resources)

5106178 mf\_ilg2.3 15\_1ghosts\_jobbsse bdnguye2 PD 0:00 1 (Resources)

5106180 mf\_ilg2.3 15\_ghost2\_jobbsse bdnguye2 PD 0:00 1 (Resources)

5106374 mf\_i-b2.8 1\_ghosts-tpss-13\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

5106523 mf\_nes2.8 tpss-11A\_cc-pvtz bdnguye2 R 12:43 1 c-5-41

5106589 mf\_nes2.8 tpss-11A\_cc-pvqz bdnguye2 PD 0:00 1 (Priority)

5106607 mf\_s-b2.6 tpss-12AB\_cc-pVQZ bdnguye2 R 2:37 1 c-16-12

5106608 mf\_s-b2.6 tpss-12AB\_cc-pVTZ bdnguye2 R 0:30 1 c-16-12

Gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

3034 ilg2.3 1\_ghosts-tpss-20\_cc-pVQZ bdnguye2 R 14-00:37:06 1 c-14-42

3035 ilg2.3 tpss-8AB\_cc-pVQZ bdnguye2 R 14-00:36:31 1 c-15-18

3046 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 13-22:05:23 1 c-13-32

3117 ilg2.3 tpss-24AB\_cc-pVQZ bdnguye2 R 10-22:45:11 1 c-14-37

3149 ilg2.3 1\_ghosts-tpss-24-ci\_cc-pVQZ bdnguye2 R 8-00:34:57 1 c-13-38

3168 brd2.4 gks-pbe-1A\_cc-pVQZ bdnguye2 R 7-22:39:05 1 c-19-413

3237 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 4-06:09:25 1 c-15-24

3274 nes2.8 np800-pbe-1\_cc-pVTZ bdnguye2 R 3-22:19:27 1 c-12-12

3296 ilg2.3 tpss-15AB\_cc-pVTZ bdnguye2 R 5:19:57 1 c-15-25

3297 ilg2.3 tpss-19AB\_cc-pVQZ bdnguye2 R 5:05:13 1 c-13-33

3300 nes2.8 tpss-24-ciA\_cc-pvqz bdnguye2 R 4:41:19 1 c-13-224

3306 nes2.8 tpss-30-ciAB\_cc-pVQZ bdnguye2 R 3:57:12 1 c-13-222

3307 nes2.8 tpss-11AB\_cc-pVQZ bdnguye2 R 3:37:48 1 c-13-221

3309 nes2.8 tpss-30-ciAB\_cc-pVTZ bdnguye2 R 1:56:30 1 c-12-251

**12/13/17:**

Jobs that moved to lustre and run on gp2:

5108537 bdnguye2 mf\_nes2. tpss-24-ciB-cc-pVQZ -- 1 8 -- 96:00 Q 00:00

--

5108538 bdnguye2 mf\_nes2. tpss-25-ciA\_cc-pVTZ -- 1 8 -- 196:0 Q 00:00

--

5108540 bdnguye2 mf\_ilg2. tpss-25-ciA\_cc-pVQZ -- 1 10 -- 196:0 Q 00:00

--

5108544 bdnguye2 mf\_ilg2. tpss-25-ciAB\_cc-pVTZ -- 1 10 -- 196:0 Q 00:00

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x4928010 mf\_ilg2.3 pbe-20AB\_cc-pVQZ bdnguye2 R 19-01:13:45 1 c-16-18

4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 16-23:53:54 1 c-16-33

x5081397 mf\_i-b2.8 tpss-26-ciAB\_cc-pVTZ bdnguye2 R 3-20:52:25 1 c-9-372

5087328 mf\_i-b2.8 pbe-14AB\_cc-pVQZ bdnguye2 R 2-05:17:39 1 c-9-373

5106374 mf\_i-b2.8 1\_ghosts-tpss-13\_cc-pVQZ bdnguye2 R 21:23:33 1 c-9-371

x5106652 mf\_nes2.8 tpss-25-ciAB\_cc-pVQZ bdnguye2 R 21:35:49 1 c-8-251

x5106655 mf\_ilg2.3 tpss-26-ciAB\_cc-pVQZ bdnguye2 R 21:30:14 1 c-15-42

x5108471 mf\_nes2.8 tpss-27-ciAB\_cc-pVQZ bdnguye2 R 5:56:37 1 c-8-31

x5108525 mf\_nes2.8 1\_ghosts-tpss-27-ciAB\_cc-pVQZ bdnguye2 R 5:30 1 c-5-18

x5108533 mf\_s-b2.6 1\_ghosts-tpss-24\_cc-pVQZ bdnguye2 R 4:55:32 1 c-16-12

x5108545 mf\_ilg2.3 tpss-26-ciAB\_cc-pVTZ bdnguye2 R 2:39:26 1 c-15-33

Gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3034 ilg2.3 1\_ghosts-tpss-20\_cc-pVQZ bdnguye2 R 15-00:12:00 1 c-14-42

3035 ilg2.3 tpss-8AB\_cc-pVQZ bdnguye2 R 15-00:11:25 1 c-15-18

x3046 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 14-21:40:17 1 c-13-32

3117 ilg2.3 tpss-24AB\_cc-pVQZ bdnguye2 R 11-22:20:05 1 c-14-37

x3149 ilg2.3 1\_ghosts-tpss-24-ci\_cc-pVQZ bdnguye2 R 9-00:09:51 1 c-13-38

x3168 brd2.4 gks-pbe-1A\_cc-pVQZ bdnguye2 R 8-22:13:59 1 c-19-413

3237 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 5-05:44:19 1 c-15-24

x3274 nes2.8 np800-pbe-1\_cc-pVTZ bdnguye2 R 4-21:54:21 1 c-12-12

3297 ilg2.3 tpss-19AB\_cc-pVQZ bdnguye2 R 1-04:40:07 1 c-13-33

x3307 nes2.8 tpss-11AB\_cc-pVQZ bdnguye2 R 1-03:12:42 1 c-13-221

x3317 nes2.8 tpss-23-ciAB\_cc-pVTZ bdnguye2 R 5:47:24 1 c-12-251

x3319 m2090 tpss-25-ciAB\_cc-pVQZ bdnguye2 R 5:25:22 1 c-3-41

x3320 nes2.8 monomer1-tpss-25-ci\_cc-pVTZ bdnguye2 R 5:23:23 1 c-12-252

x3321 nes2.8 tpss-24-ciA\_cc-pVQZ bdnguye2 R 5:22:07 1 c-12-253

x3323 nes2.8 tpss-25-ciA\_cc-pVTZ bdnguye2 R 3:51:35 1 c-13-223

x3324 nes2.8 tpss-25-ciAB\_cc-pVTZ bdnguye2 R 3:47:27 1 c-13-224

x3325 has2.5 tpss-25-ciA\_cc-pVQZ bdnguye2 R 1:56:39 1 c-19-294

\*3326 ilg2.3 tpss-15AB\_cc-pVQZ bdnguye2 R 3:39:26 1 c-15-25

x3327 has2.5 tpss-30-ciAB\_cc-pVQZ bdnguye2 R 3:36:40 1 c-19-292

**12/18/17:**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 22-04:47:39 1 c-16-33

5087328 mf\_i-b2.8 pbe-14AB\_cc-pVQZ bdnguye2 R 7-10:11:24 1 c-9-373

5106374 mf\_i-b2.8 1\_ghosts-tpss-13\_cc-pVQZ bdnguye2 R 6-02:17:18 1 c-9-371

5119887 mf\_s-b2.6 tpss-24-ciAB\_cc-pVTZ bdnguye2 R 20:54:47 1 c-16-12

x5120731 mf\_i-b2.8 tpss-24-ciAB\_cc-pVQZ bdnguye2 R 45:43 1 c-9-374

x5120732 mf\_i-b2.8 monomer1-tpss-26-ciAB\_cc-pVQZ bdnguye2 R 43:33 1 c-9-374

x5120740 mf\_ilg2.3 monomer2\_jobbsse bdnguye2 R 31:39 1 c-16-28

x5120744 mf\_ilg2.3 comp3a\_ghost2\_jobbsse bdnguye2 PD 0:00 1 (Priority)

x5120746 mf\_ilg2.3 comp3a\_1ghosts\_jobbsse bdnguye2 PD 0:00 1 (Priority)

x5120770 mf\_i-b2.8 1\_ghosts-tpss-16AB\_cc-pVQZ bdnguye2 R 1:21 1 c-9-372

x5120771 mf\_i-b2.8 2\_ghosts-tpss-16AB\_cc-pVQZ bdnguye2 R 1:21 1 c-9-411

x5120772 mf\_i-b2.8 monomer1-tpss-16AB\_cc-pVQZ bdnguye2 R 1:21 1 c-9-412

x5120773 mf\_i-b2.8 monomer2-tpss-16AB\_cc-pVQZ bdnguye2 R 1:21 1 c-9-413

x5120776 mf\_i-b2.8 1\_ghosts-16AB\_cc-pvtz bdnguye2 R 0:03 1 c-9-413

x5120777 mf\_i-b2.8 2\_ghosts-16AB\_cc-pvtz bdnguye2 R 0:03 1 c-9-414

x5120778 mf\_i-b2.8 monomer1-tpss-16AB\_cc-pvtz bdnguye2 R 0:03 1 c-9-414

x5120779 mf\_nes2.8 monomer2-tpss-16AB\_cc-pvtz bdnguye2 PD 0:00 1 (Resources)

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

3035 ilg2.3 tpss-8AB\_cc-pVQZ bdnguye2 R 20-05:07:57 1 c-15-18

3117 ilg2.3 tpss-24AB\_cc-pVQZ bdnguye2 R 17-03:16:37 1 c-14-37

3237 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 10-10:40:51 1 c-15-24

3297 ilg2.3 tpss-19AB\_cc-pVQZ bdnguye2 R 6-09:36:39 1 c-13-33

3348 nes2.8 tpss-26-ciAB\_cc-pVTZ bdnguye2 R 4-09:26:07 1 c-13-221

x3368 nes2.8 tpss-27-ciAB\_cc-pVTZ bdnguye2 R 3-08:26:32 1 c-13-223

\*3378 has2.5 1\_ghosts-tpss-19\_cc-pVQZ bdnguye2 R 57:43 1 c-19-292

x3379 nes2.8 1\_ghosts-tpss-15\_cc-pVTZ bdnguye2 R 39:22 1 c-12-252

x3380 nes2.8 2\_ghosts-tpss-15\_cc-pVTZ bdnguye2 R 38:42 1 c-13-9

x3381 has2.5 np200\_tpss-16AB\_cc-pVTZ bdnguye2 R 1:03 1 c-19-293

x3382 nes2.8 tpss-15A\_cc-pVTZ bdnguye2 R 0:27 1 c-13-222

x3383 nes2.8 tpss-16B\_cc-pwCVTZ bdnguye2 R 0:01 1 c-5-10

\* Compute 19-1\_ghosts molecule with mf\_s-b2.6

**12/19/17:**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 23-03:05:30 1 c-16-33

x5087328 mf\_i-b2.8 pbe-14AB\_cc-pVQZ bdnguye2 R 8-08:29:15 1 c-9-373

x5106374 mf\_i-b2.8 1\_ghosts-tpss-13\_cc-pVQZ bdnguye2 R 7-00:35:09 1 c-9-371

x5119887 mf\_s-b2.6 tpss-24-ciAB\_cc-pVTZ bdnguye2 R 1-19:12:38 1 c-16-12

x5132458 mf\_nes2.8 1\_ghosts-tpss-5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132459 mf\_nes2.8 2\_ghosts-tpss-5AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132476 mf\_nes2.8 1\_ghosts-tpss-6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132477 mf\_nes2.8 2\_ghosts-tpss-6AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132492 mf\_nes2.8 1\_ghosts-tpss-7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132493 mf\_nes2.8 2\_ghosts-tpss-7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132504 mf\_nes2.8 monomer2-pbe-12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132529 mf\_nes2.8 2\_ghosts-tpss-29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132534 mf\_nes2.8 1\_ghosts-tpss-29AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132540 mf\_nes2.8 1\_ghosts-tpss-30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132559 mf\_nes2.8 2\_ghosts-tpss-30AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132613 mf\_nes2.8 1\_ghosts-tpss-8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132614 mf\_nes2.8 2\_ghosts-tpss-8AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132615 mf\_nes2.8 1\_ghosts-tpss-11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132616 mf\_nes2.8 2\_ghosts-tpss-11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132617 mf\_nes2.8 1\_ghosts-tpss-12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132618 mf\_nes2.8 2\_ghosts-tpss-12AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132619 mf\_nes2.8 1\_ghosts-tpss-13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132620 mf\_nes2.8 2\_ghosts-tpss-13AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132621 mf\_nes2.8 1\_ghosts-tpss-14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132622 mf\_nes2.8 2\_ghosts-tpss-14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132623 mf\_nes2.8 1\_ghosts-tpss-19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132624 mf\_nes2.8 2\_ghosts-tpss-19AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132625 mf\_nes2.8 1\_ghosts-tpss-20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132626 mf\_nes2.8 2\_ghosts-tpss-20AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132627 mf\_nes2.8 1\_ghosts-tpss-22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5132628 mf\_nes2.8 2\_ghosts-tpss-22AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132629 mf\_nes2.8 1\_ghosts-tpss-23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132630 mf\_nes2.8 2\_ghosts-tpss-23AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132631 mf\_nes2.8 1\_ghosts-tpss-24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132632 mf\_nes2.8 2\_ghosts-tpss-24AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132633 mf\_nes2.8 1\_ghosts-tpss-25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132634 mf\_nes2.8 2\_ghosts-tpss-25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132635 mf\_nes2.8 1\_ghosts-tpss-26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+5132636 mf\_nes2.8 2\_ghosts-tpss-26AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5134403 mf\_nes2.8 monomer2-tpss-8AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3035 ilg2.3 tpss-8AB\_cc-pVQZ bdnguye2 R 21-03:24:05 1 c-15-18

3117 ilg2.3 tpss-24AB\_cc-pVQZ bdnguye2 R 18-01:32:45 1 c-14-37

x3297 ilg2.3 tpss-19AB\_cc-pVQZ bdnguye2 R 7-07:52:47 1 c-13-33

x3348 nes2.8 tpss-26-ciAB\_cc-pVTZ bdnguye2 R 5-07:42:15 1 c-13-221

x3391 nes2.8 monomer1-tpss-26-ci\_cc-pVQZ bdnguye2 R 6:45:04 1 c-12-252

x3443 nes2.8 1\_ghosts-tpss-15\_cc-pVQZ bdnguye2 R 54:10 1 c-13-10

x3444 nes2.8 2\_ghosts-tpss-15\_cc-pVQZ bdnguye2 R 53:56 1 c-13-11

\*3445 ilg2.3 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 53:10 1 c-15-24

\*3447 nes2.8 1\_ghosts-tpss-16\_cc-pVQZ bdnguye2 R 52:33 1 c-13-15

\*3448 has2.5 tpss-12AB\_cc-pVQ+dZ bdnguye2 R 51:13 1 c-19-294

+3449 has2.5 tpss-24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

+3450 brd2.4 gks-pbe-1\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

+3451 brd2.4 gks-pbe-1AB\_def2-qzvp bdnguye2 PD 0:00 1 (Resources)

+3452 nes2.8 monomer1-pbe-24AB\_cc-pVQZ bdnguye2 R 35:17 1 c-13-224

x3453 nes2.8 monomer1-pbe-5\_cc-pVQZ bdnguye2 R 0:08 1 c-13-9

x3454 nes2.8 monomer2-pbe\_5\_cc-pVTZ bdnguye2 R 0:08 1 c-13-13

x3455 nes2.8 monomer1-pbe\_6\_cc-pVQZ bdnguye2 R 0:08 1 c-13-14

x3456 nes2.8 monomer2-pbe\_6\_cc-pVTZ bdnguye2 R 0:08 1 c-13-16

x3457 nes2.8 monomer1-pbe-7\_cc-pVQZ bdnguye2 R 0:08 1 c-13-17

x3458 nes2.8 monomer2-pbe\_7\_cc-pVTZ bdnguye2 R 0:08 1 c-13-18

x3459 nes2.8 monomer1-pbe-8\_cc-pVQZ bdnguye2 R 0:08 1 c-13-222

x3460 nes2.8 monomer2-pbe-8\_cc-pVQZ bdnguye2 R 0:05 1 c-13-223

3461 ilg2.3 monomer1-pbe-19\_cc-pVQZ bdnguye2 R 0:05 1 c-15-25

x3462 ilg2.3 monomer2-pbe-19\_cc-pVQZ bdnguye2 R 0:05 1 c-15-25

+3463 ilg2.3 monomer1-pbe-20\_cc-pVQZ bdnguye2 R 0:05 1 c-13-32

x3464 ilg2.3 monomer2-pbe-20\_cc-pVQZ bdnguye2 R 0:05 1 c-13-32

x3465 ilg2.3 monomer1-pbe-22\_cc-pVQZ bdnguye2 R 0:05 1 c-13-38

x3466 ilg2.3 monomer2-pbe-22\_cc-pVQZ bdnguye2 R 0:05 1 c-13-38

x3467 ilg2.3 monomer1-pbe-23\_cc-pVQZ bdnguye2 R 0:05 1 c-13-42

x3468 ilg2.3 monomer2-pbe-23\_cc-pVQZ bdnguye2 R 0:05 1 c-13-42

+3469 nes2.8,il monomer1-pbe-25\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x3470 nes2.8,il monomer2-pbe-25\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

+3471 nes2.8,il monomer1-pbe-26\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x3472 nes2.8,il monomer2-pbe-26\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x3473 nes2.8,il monomer1-pbe-29\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x3474 nes2.8,il monomer2-pbe-29\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

3475 nes2.8,il monomer1-pbe-30\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x3476 nes2.8,il monomer2-pbe-30\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

**12/26/17:**

gplogin 1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 29-21:51:42 1 c-16-33

x5274897 mf\_s-b2.6 (cl\_cc-pVQ+TZ tpss-24-ciAB\_cc-pVTZ bdnguye2 R 1:47:01 1 c-16-12

x5274966 mf\_ilg2.3 1\_ghosts-tpss-11AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-33

x5274967 mf\_ilg2.3 2\_ghosts-tpss-11AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-33

x5274968 mf\_ilg2.3 1\_ghosts-tpss-12AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-34

x5274969 mf\_ilg2.3 2\_ghosts-tpss-12AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-34

x5274970 mf\_ilg2.3 1\_ghosts-tpss-13AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-37

x5274971 mf\_ilg2.3 2\_ghosts-tpss-13AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-37

x5274972 mf\_ilg2.3 1\_ghosts-tpss-19AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-38

x5274973 mf\_ilg2.3 2\_ghosts-tpss-19AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-38

x5274974 mf\_ilg2.3 1\_ghosts-tpss-20AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-41

x5274975 mf\_ilg2.3 2\_ghosts-tpss-20AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-15-41

x5274976 mf\_ilg2.3 1\_ghosts-tpss-23AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-18

x5274977 mf\_ilg2.3 2\_ghosts-tpss-23AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-18

x5274978 mf\_ilg2.3 1\_ghosts-tpss-24AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-19

x5274979 mf\_ilg2.3 2\_ghosts-tpss-24AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-19

x5274980 mf\_ilg2.3 1\_ghosts-tpss-25AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-28

x5274981 mf\_ilg2.3 2\_ghosts-tpss-25AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-28

x5274982 mf\_ilg2.3 1\_ghosts-tpss-26AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-29

x5274983 mf\_ilg2.3 2\_ghosts-tpss-26AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-29

x5274984 mf\_ilg2.3 1\_ghosts-tpss-8AB\_cc-pVQZ bdnguye2 R 1:17:55 1 c-16-32

x5274985 mf\_ilg2.3 2\_ghosts-tpss-8AB\_cc-pVQZ bdnguye2 R 1:17:52 1 c-16-32

x5274986 mf\_ilg2.3 1\_ghosts-tpss-14AB\_cc-pVQZ bdnguye2 R 1:16:46 1 c-16-37

x5274987 mf\_ilg2.3 2\_ghosts-tpss-14AB\_cc-pVQZ bdnguye2 R 1:16:31 1 c-16-37

x5275053 mf\_nes2.8 monomer1-pbe-16\_cc-pVQZ bdnguye2 R 1:00:53 1 c-5-24

x5275057 mf\_nes2.8 pbe-16AB\_cc-pVTZ bdnguye2 R 55:05 1 c-5-26

\*5275122 mf\_i-b2.8 pbe-16AB\_cc-pVQZ bdnguye2 R 53:00 1 c-9-332

+5275124 mf\_nes2.8 pbe-16AB\_def2-qzvp bdnguye2 R 51:08 1 c-8-253

x5275256 mf\_ilg2.3 1\_ghosts-tpss-16\_cc-pVQZ bdnguye2 R 12:10 1 c-16-41

x5275257 mf\_ilg2.3 2\_ghosts-tpss-16\_cc-pVQZ bdnguye2 R 5:31 1 c-16-42

\* incorrect npoints 16AB+cc-pVQZ

gplogin 2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3117 ilg2.3 tpss-24AB\_cc-pVQZ bdnguye2 R 24-20:18:56 1 c-14-37

x3461 ilg2.3 monomer1-pbe-19\_cc-pVQZ bdnguye2 R 6-18:46:16 1 c-15-25

3596 has2.5 monomer1-pbe-20\_cc-pVQZ bdnguye2 R 4-02:20:31 1 c-19-293

x3600 nes2.8 monomer1-pbe-24\_cc-pVQZ bdnguye2 R 4-02:14:54 1 c-13-221

x3706 ilg2.3 monomer1-pbe-12\_cc-pVQZ bdnguye2 R 1:05:06 1 c-13-33

+3707 ilg2.3 monomer2-pbe-11\_cc-pVQZ bdnguye2 R 1:03:10 1 c-13-32

x3708 ilg2.3 monomer1-pbe-11\_cc-pVQZ bdnguye2 R 1:02:56 1 c-13-37

x3711 nes2.8 1\_ghosts-pbe-16\_cc-pVQZ bdnguye2 R 29:51 1 c-12-252

x3712 nes2.8 1\_ghosts-pbe-16\_cc-pVQZ bdnguye2 R 29:46 1 c-13-9

x3714 nes2.8 1\_ghosts-pbe-5\_cc-pVQZ bdnguye2 R 0:04 1 c-13-10

x3715 nes2.8 2\_ghosts-pbe-5\_cc-pVQZ bdnguye2 R 0:04 1 c-13-13

x3716 nes2.8 1\_ghosts-pbe\_6\_cc-pVQZ bdnguye2 R 0:04 1 c-13-14

x3717 nes2.8 2\_ghosts-pbe\_6\_cc-pVQZ bdnguye2 R 0:04 1 c-13-15

+3718 nes2.8 1\_ghosts-pbe-7\_cc-pVQZ bdnguye2 R 0:04 1 c-13-16

+3719 nes2.8 2\_ghosts-pbe-7\_cc-pVQZ bdnguye2 R 0:04 1 c-13-18

x3720 nes2.8 1\_ghosts-pbe-22\_cc-pVQZ bdnguye2 R 0:04 1 c-13-223

+3721 ilg2.3 2\_ghosts-pbe-22\_cc-pVQZ bdnguye2 R 0:04 1 c-13-32

3722 ilg2.3 1\_ghosts-pbe-29\_cc-pVQZ bdnguye2 R 0:04 1 c-13-33

x3723 ilg2.3 2\_ghosts-pbe-29\_cc-pVQZ bdnguye2 R 0:04 1 c-13-37

x3724 ilg2.3 1\_ghosts-pbe-30\_cc-pVQZ bdnguye2 R 0:04 1 c-13-38

x3725 ilg2.3 2\_ghosts-pbe-30\_cc-pVQZ bdnguye2 R 0:04 1 c-13-38

**12/27/17: Calculation Check-up**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3775 has2.5 2\_ghosts-pbe-7\_cc-pVQZ bdnguye2 R 17:49 1 c-19-291

x3776 has2.5 1\_ghosts-pbe-7\_cc-pVQZ bdnguye2 R 16:40 1 c-19-292

x3778 brd2.4 2\_ghosts-pbe-22\_cc-pVQZ bdnguye2 R 14:19 1 c-19-411

+3780 nes2.8 pbe-16AB\_cc-pVQZ bdnguye2 R 6:26 1 c-12-252

x3781 nes2.8 monomer2-pbe-14\_cc-pVQZ bdnguye2 R 2:00 1 c-13-9

+3782 brd2.4 monomer1-pbe-14\_cc-pVQZ bdnguye2 R 1:09 1 c-19-412

x3783 nes2.8 monomer2-pbe-12AB\_cc-pVQZ bdnguye2 R 0:00 1 c-13-18

+3785 brd2.4 monomer1-pbe-13\_cc-pVQZ bdnguye2 R 4:31 1 c-19-413

x3786 ilg2.3 monomer1-tpss-25\_cc-pVQZ bdnguye2 R 0:01 1 c-13-42

x3787 nes2.8 tpss-24A\_def2-qzvp bdnguye2 R 0:01 1 c-13-16

**12/28/17: Calculations of 2\_ghosts molecules**

gplogin2:

\*3818 brd2.4 monomer1-pbe-14\_cc-pVQZ bdnguye2 R 6:59 1 c-19-411

3819 ilg2.3 monomer2-pbe-12\_cc-pVQZ bdnguye2 R 5:54 1 c-13-32

\*3820 brd2.4 monomer1-pbe-13\_cc-pVQZ bdnguye2 R 5:02 1 c-19-412

3823 ilg2.3 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 7:21 1 c-13-37

x+\*\*3824 ilg2.3 2\_ghosts-pbe-19\_cc-pVQZ bdnguye2 R 7:21 1 c-14-37

x+\*\*3825 ilg2.3 2\_ghosts-pbe-20\_cc-pVQZ bdnguye2 R 7:21 1 c-14-41

x3826 ilg2.3 2\_ghosts-pbe-23\_cc-pVQZ bdnguye2 R 7:21 1 c-14-42

3827 ilg2.3 2\_ghosts-pbe-24\_cc-pVQZ bdnguye2 R 7:21 1 c-15-18

x\*\*3828 ilg2.3 2\_ghosts-pbe-25\_cc-pVQZ bdnguye2 R 7:21 1 c-15-19

+\*\*3829 ilg2.3 2\_ghosts-pbe-26\_cc-pVQZ bdnguye2 R 7:21 1 c-15-24

+\*\*3830 brd2.4 1\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 5:18 1 c-19-413

\*\*3832 brd2.4 1\_ghosts-pbe-26\_cc-pVQZ bdnguye2 R 4:07 1 c-19-414

\* need larger memory

\*\* missing frozen core flags

**1/3/18: S30L cc-pV(T+d)Z and cc-pV(Q+d)Z basis sets running**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x4949929 mf\_ilg2.3 pbe-13AB\_cc-pVQZ bdnguye2 R 36-20:48:51 1 c-16-33

x5495010 mf\_nes2.8 tpss-24-ciB-cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5495011 mf\_s-b2.6 tpss-13AB\_cc-pVQZ bdnguye2 R 22:14:10 1 c-16-12

x5502954 mf\_i-b2.8 1\_ghosts-pbe-19\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x5502988 mf\_i-b2.8 tpss-11AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5503099 mf\_i-b2.8 tpss-11A\_cc-pvqz bdnguye2 R 12:54 1 c-9-334

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3596 has2.5 monomer1-pbe-20\_cc-pVQZ bdnguye2 R 11-01:19:59 1 c-19-293

x3819 ilg2.3 monomer2-pbe-12\_cc-pVQZ bdnguye2 R 5-01:12:59 1 c-13-32

\*3823 ilg2.3 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 5-00:20:04 1 c-13-37

x+3827 ilg2.3 2\_ghosts-pbe-24\_cc-pVQZ bdnguye2 R 5-00:20:04 1 c-15-18

+4013 ilg2.3 1\_ghosts-pbe-25\_cc-pVQZ bdnguye2 R 2-12:53:34 1 c-15-24

x4301 ilg2.3 2\_ghosts-pbe-26\_cc-pVQZ bdnguye2 R 22:32:33 1 c-13-38

x4305 ilg2.3 monomer1-tpss-25\_cc-pVQZ bdnguye2 R 21:50:05 1 c-13-42

x4307 has2.5 tpss-11AB\_cc-pVTZ bdnguye2 R 2:23:17 1 c-19-292

x4308 nes2.8 tpss-11A\_cc-pVTZ bdnguye2 R 2:20:15 1 c-12-252

x+4310 brd2.4 tpss-12AB\_cc-pVQ+dZ bdnguye2 R 2:06:48 1 c-19-412

x4312 nes2.8 1\_ghosts-11AB\_cc-pvtz bdnguye2 R 1:54:30 1 c-13-18

x4313 nes2.8 monomer1-tpss-11AB\_cc-pVQZ bdnguye2 R 1:50:18 1 c-13-16

x4314 nes2.8 1\_ghosts-tpss-11AB\_cc-pVQZ bdnguye2 R 1:41:45 1 c-13-15

x4317 nes2.8 1\_ghosts-tpss-12AB\_cc-pVTZ bdnguye2 R 1:26:17 1 c-13-13

x4318 nes2.8 monomer2-tpss-12AB\_cc-pVQZ bdnguye2 R 1:22:00 1 c-13-10

x4319 nes2.8 1\_ghosts-tpss-12AB\_cc-pVQZ bdnguye2 R 1:17:30 1 c-13-9

x4320 nes2.8 tpss-26-ciA\_cc-pvtz bdnguye2 R 55:36 1 c-12-21

~~4321 ilg2.3 tpss-27-ciAB\_cc-pVTZ bdnguye2 CG 0:20 1 c-13-32~~

x4322 ilg2.3 tpss-27-ciAB\_cc-pVTZ bdnguye2 R 50:36 1 c-13-33

x4327 nes2.8 tpss-28-ciAB\_cc-pVQZ bdnguye2 R 10:45 1 c-13-223

x4328 nes2.8 tpss-24-ciB-cc-pVQZ bdnguye2 R 0:38 1 c-13-14

\* not frozen core calculation but rather all electron

**1/3/18: Updated computations cc-pV(T+d)Z & cc-pV(Q+d)Z**

gplogin1:

x5508768 mf\_i-b2.8 tpss-11A\_cc-pVQZ bdnguye2 R 32:49 1 c-9-332

x5508875 mf\_i-b2.8 tpss-19AB\_cc-pVQZ bdnguye2 R 5:02 1 c-9-333

x5508885 mf\_i-b2.8 tpss-12AB\_cc-pVQZ bdnguye2 R 1:30 1 c-9-372

x5508886 mf\_i-b2.8 1\_ghosts-tpss-12\_cc-pVQZ bdnguye2 R 0:16 1 c-9-374

+5508892 mf\_i-b2.8 monomer1-tpss-14\_cc-pVQZ bdnguye2 R 7:43 1 c-9-412  
 x5508896 mf\_i-b2.8 1\_ghosts-tpss-14\_cc-pVQZ bdnguye2 R 6:35 1 c-9-413  
 x5508903 mf\_ilg2.3 tpss-14AB\_cc-pVQZ bdnguye2 R 3:08 1 c-15-33

x5508928 mf\_i-b2.8 1\_ghosts-pbe-24\_cc-pVQZ bdnguye2 R 3:03:21 1 c-9-412

gplogin2:

+4329 brd2.4 1\_ghosts-pbe-26\_cc-pVQZ bdnguye2 R 12:13 1 c-19-411

x\*4330 brd2.4 tpss-12AB\_cc-pVQ+dZ bdnguye2 R 10:37 1 c-19-412

x4331 has2.5 1\_ghosts-tpss-11\_cc-pVTZ bdnguye2 R 8:50 1 c-19-291

x4332 nes2.8 monomer1-tpss-11\_cc-pVTZ bdnguye2 R 7:31 1 c-12-252

x4333 nes2.8 monomer1-tpss-11\_cc-pVTZ bdnguye2 R 6:15 1 c-13-10

x4334 nes2.8 1\_ghosts-tpss-12\_cc-pVTZ bdnguye2 R 5:01 1 c-13-13

x4335 nes2.8 monomer1-tpss-12\_cc-pVTZ bdnguye2 R 3:29 1 c-13-14

x4336 nes2.8 monomer1-tpss-12\_cc-pVTZ bdnguye2 R 1:53 1 c-13-16

x4337 nes2.8 tpss-26-ciA\_cc-pVTZ bdnguye2 R 0:17 1 c-13-18

x4338 nes2.8 tpss-28-ciAB\_cc-pVQZ bdnguye2 R 4:17 1 c-13-223

x4339 ilg2.3 2\_ghosts-pbe-24\_cc-pVQZ bdnguye2 R 0:06 1 c-13-42

x\*4340 has2.5 pbe-8AB\_cc-pVQZ bdnguye2 R 1:42 1 c-19-292

\*4341 brd2.4 1\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 0:01 1 c-19-413

x4342 brd2.4 monomer2-pbe-11\_cc-pVQZ bdnguye2 R 0:01 1 c-19-414

\* Failed due to not large enough memory available

**1/4/17: Additional calculations**

gplogin1:

x5517000 mf\_nes2.8 tpss-comp7AB\_cc-pVTZ bdnguye2 R 10:29 1 c-3-341

x5517015 mf\_nes2.8 tpss-comp7AB\_cc-pVQZ bdnguye2 R 7:47 1 c-3-342

\*5517022 mf\_nes2.8 tpss\_12B-cc-pVTZ bdnguye2 R 6:13 1 c-3-343

\*5517023 mf\_nes2.8 tpss\_12B-cc-pVQZ bdnguye2 R 5:09 1 c-3-344

\* Calculation crashed -> potentially the nodes reset

**1/10/18: Resubmission of large complexes and begin computation of PBE CI-ghost molecules**

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x3823 ilg2.3 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 12-23:27:10 1 c-13-37

4305 ilg2.3 monomer1-tpss-25\_cc-pVQZ bdnguye2 R 7-13:09:24 1 c-13-38

\*4359 brd2.4 tpss-14AB\_cc-pVQZ bdnguye2 R 25:06 1 c-19-411

x4360 nes2.8 monomer2-tpss-23-ci\_cc-pVTZ bdnguye2 R 27:14 1 c-13-9

x4361 nes2.8 monomer2-tpss-24-ci\_cc-pVTZ bdnguye2 R 27:14 1 c-13-10

x4362 nes2.8 monomer2-tpss-25-ci\_cc-pVTZ bdnguye2 R 27:14 1 c-13-11

x4363 nes2.8 monomer2-tpss-26-ci\_cc-pVTZ bdnguye2 R 27:14 1 c-13-13

x4368 nes2.8 monomer1-tpss-23-ci\_cc-pVTZ bdnguye2 R 4:02 1 c-13-14

x4369 nes2.8 monomer1-tpss-24-ci\_cc-pVTZ bdnguye2 R 4:02 1 c-13-15

x4370 nes2.8 monomer1-tpss-25-ci\_cc-pVTZ bdnguye2 R 4:02 1 c-13-16

+4371 nes2.8 monomer1-tpss-27-ci\_cc-pVTZ bdnguye2 R 4:02 1 c-13-17

x4372 nes2.8 monomer1-tpss-28-ci\_cc-pVTZ bdnguye2 R 4:02 1 c-13-18

x4373 nes2.8 monomer1-tpss-29-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

x4374 nes2.8 monomer1-tpss-30-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x4375 nes2.8 monomer2-tpss-27-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x4376 nes2.8 monomer2-tpss-28-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x4377 nes2.8 monomer2-tpss-29-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x4378 nes2.8 monomer2-tpss-30-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

\* Out of memory and will submit onto mf\_i-b2.8

gplogin1:  
 JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x5508896 mf\_i-b2.8 1\_ghosts-tpss-14\_cc-pVQZ bdnguye2 R 6-22:16:05 1 c-9-413

x5531227 mf\_i-b2.8 tpss-12AB\_cc-pVQ+dZ bdnguye2 R 4-10:14:07 1 c-9-371

x5540702 mf\_s-b2.6 pbe-8AB\_cc-pVQZ bdnguye2 R 1-10:02:18 1 c-16-12

x5540703 mf\_i-b2.8 1\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 1-09:59:24 1 c-9-333

x5544414 mf\_ilg2.3 tpss-comp7AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x5544415 mf\_ilg2.3 tpss-comp7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546085 mf\_i-b2.8 1\_ghosts-pbe-20\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546093 mf\_ilg2.3 1\_ghosts-tpss-25AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546145 mf\_ilg2.3 pbe-26-ci\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

5546274 mf\_i-b2.8 tpss-14AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546942 mf\_nes2.8 2\_ghosts-pbe-23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546943 mf\_nes2.8 2\_ghosts-pbe-24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546944 mf\_nes2.8 2\_ghosts-pbe-25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546945 mf\_nes2.8 2\_ghosts-pbe-26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546946 mf\_nes2.8 2\_ghosts-pbe-27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546947 mf\_nes2.8 2\_ghosts-pbe-28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546948 mf\_nes2.8 2\_ghosts-pbe-29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546949 mf\_nes2.8 2\_ghosts-pbe-30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546961 mf\_nes2.8 1\_ghosts-pbe-23-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546962 mf\_ilg2.3 1\_ghosts-pbe-24-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546963 mf\_nes2.8 1\_ghosts-pbe-25-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546964 mf\_nes2.8 1\_ghosts-pbe-26-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546965 mf\_nes2.8 1\_ghosts-pbe-27-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546966 mf\_nes2.8 1\_ghosts-pbe-28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546967 mf\_ilg2.3 1\_ghosts-pbe-29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5546968 mf\_ilg2.3 1\_ghosts-pbe-30-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

**1/12/18: 1\_ghosts and 2\_ghosts molecule of the counterions compounds**

gplogin1:

x5555523 mf\_i-b2.8 tpss-comp7AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5555588 mf\_ilg2.3 1\_ghosts-pbe-28-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5556954 mf\_i-b2.8 1\_ghosts-tpss-11\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

gplogin2:

x4387 ilg2.3 2\_ghosts-tpss23-ci\_cc-pVTZ bdnguye2 R 9:52 1 c-13-37

x4388 ilg2.3 2\_ghosts-tpss25-ci\_cc-pVTZ bdnguye2 R 9:52 1 c-13-37

x4389 ilg2.3 2\_ghosts-tpss26-ci\_cc-pVTZ bdnguye2 R 9:52 1 c-13-38

x4390 ilg2.3 2\_ghosts-tpss27-ci\_cc-pVTZ bdnguye2 R 9:49 1 c-13-38

x4391 ilg2.3 2\_ghosts-tpss28-ci\_cc-pVTZ bdnguye2 R 9:49 1 c-14-37

x4392 ilg2.3 2\_ghosts-tpss29-ci\_cc-pVTZ bdnguye2 R 9:49 1 c-14-37

x4393 ilg2.3 2\_ghosts-tpss30-ci\_cc-pVTZ bdnguye2 R 9:49 1 c-14-41

x4394 ilg2.3 1\_ghosts-pbe-23-ci\_cc-pVTZ bdnguye2 R 0:07 1 c-14-41

+\*4395 ilg2.3 1\_ghosts-pbe-24-ci\_cc-pVTZ bdnguye2 R 0:07 1 c-14-42

+\*4396 ilg2.3 1\_ghosts-pbe-27-ci\_cc-pVTZ bdnguye2 R 0:07 1 c-14-42

+\*4397 ilg2.3 1\_ghosts-pbe-29-ci\_cc-pVTZ bdnguye2 R 0:04 1 c-15-18

+\*4398 ilg2.3 1\_ghosts-pbe-30-ci\_cc-pVTZ bdnguye2 R 0:04 1 c-15-18

+\*4408 has2.5 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 6:40 1 c-19-291

x4409 has2.5 1\_ghosts-pbe-25\_cc-pVQZ bdnguye2 R 3:30 1 c-19-292

x4410 has2.5 2\_ghosts-pbe-24-ci\_cc-pVTZ bdnguye2 R 0:01 1 c-19-293

\* Need to be computed on separate nodes, use #SBATCH exclusive

**1/17/18: Checkup calculations**

gplogin1:

x5562967 mf\_i-b2.8 1\_ghosts-pbe-26-ci\_cc-pVQZ bdnguye2 R 2-07:41:07 1 c-9-333

\*5562972 mf\_i-b2.8 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 2-07:11:58 1 c-9-412

x5562973 mf\_i-b2.8 1\_ghosts-tpss-19\_cc-pVQZ bdnguye2 R 2-07:07:40 1 c-9-413

x5562976 mf\_s-b2.6 pbe-12AB\_cc-pVQZ bdnguye2 R 2-06:51:52 1 c-16-12

x5563933 mf\_i-b2.8 1\_ghosts-pbe-30-ci\_cc-pVTZ bdnguye2 R 14:54 1 c-9-373

x5563934 mf\_i-b2.8 2\_ghosts-pbe-14\_cc-pVQZ bdnguye2 R 6:54 1 c-9-411

5563936 mf\_i-b2.8 1\_ghosts-pbe-14\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

5563937 mf\_i-b2.8 monomer1-pbe-13\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

5563938 mf\_i-b2.8 1\_ghosts-pbe-13\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5563939 mf\_i-b2.8 2\_ghosts-pbe-13\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5571231 mf\_i-b2.8 pbe-16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x5571233 mf\_i-b2.8 pbe-16AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x5571238 mf\_i-b2.8 monomer1-tpss-27-ci\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

\*5571241 mf\_i-b2.8 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x5571243 mf\_i-b2.8 1\_ghosts-pbe-27-ci\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

x5571252 mf\_nes2.8 monomer2-tpss-11AB\_cc-pvtz bdnguye2 PD 0:00 1 (Resources)

\* Computed the 1\_ghost molecule of complex 8

gplogin2:

x4440 nes2.8 monomer1-tpss-26-ci\_cc-pVTZ bdnguye2 R 2-07:17:57 1 c-13-10

4444 ilg2.3 1\_ghosts-pbe-29-ci\_cc-pVTZ bdnguye2 R 2-06:59:52 1 c-13-32

\*\*4467 has2.5 1\_ghosts-pbe-11\_cc-pVQZ bdnguye2 R 2:20 1 c-19-292

x4468 has2.5 2\_ghosts-pbe-12\_cc-pVQZ bdnguye2 R 1:28 1 c-19-294

x4470 m2090 1\_ghosts-pbe-24-ci\_cc-pVTZ bdnguye2 R 0:52 1 c-3-41

x\*4490 has2.5 monomer1-tpss-27-ci\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

x4498 nes2.8 pbe\_15A\_cc-pVQZ bdnguye2 R 1:12:33 1 c-13-18

x4501 nes2.8 pbe\_15A\_cc-pVTZ bdnguye2 R 21:53 1 c-17-4

x4502 ilg2.3 pbe-16AB\_cc-pVTZ bdnguye2 R 16:29 1 c-15-25

x4503 ilg2.3 pbe-16AB\_cc-pVTZ bdnguye2 R 13:34 1 c-15-25

\*\* weird energies in the excel sheet but, found that monomer2 of complex 11 did not have frozen core approximation

**1/24/18: Final Round of Calculations**

gplogin1:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x5607945 mf\_nes2.8 monomer2-pbe-11\_cc-pVTZ bdnguye2 R 0:01 1 c-7-18

5607959 mf\_s-b2.6 monomer1-pbe-14\_cc-pVQZ bdnguye2 R 0:14 1 c-16-12

x5608199 mf\_nes2.8 2\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 0:02 1 c-7-20

x5608217 mf\_nes2.8 monomer1-pbe-16AB\_cc-pVTZ bdnguye2 R 0:01 1 c-7-21

x5608280 mf\_nes2.8 1\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 0:10 1 c-7-20

x5608311 mf\_nes2.8 2\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 0:22 1 c-7-21

x5608313 mf\_nes2.8 ecp28\_2\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 0:01 1 c-5-37

x5608321 mf\_nes2.8 monomer1-tpss-16AB\_cc-pVTZ bdnguye2 R 0:01 1 c-5-39

x5608363 mf\_nes2.8 2\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 0:02 1 c-5-40

x5608509 mf\_nes2.8 monomer1-pbe-16AB\_cc-pVTZ bdnguye2 R 0:02 1 c-5-42

x5608544 mf\_nes2.8 monomer1-pbe-15AB\_cc-pVTZ bdnguye2 R 2:06 1 c-6-29

x5608571 mf\_nes2.8 1\_ghosts-pbe-15AB\_cc-pVTZ bdnguye2 R 0:01 1 c-8-21

x5608721 mf\_nes2.8 monomer1-pbe-15AB\_cc-pVQZ bdnguye2 PD 0:00 1 (None)

x5608752 mf\_nes2.8 1\_ghosts-pbe-15AB\_cc-pVQZ bdnguye2 R 0:01 1 c-6-29

x5608813 mf\_nes2.8 pbe-15AB\_cc-pVTZ bdnguye2 R 0:01 1 c-8-251

x5608849 mf\_nes2.8 pbe-15AB\_cc-pVQZ bdnguye2 R 0:02 1 c-5-13

x5608916 mf\_nes2.8 tpss-16AB\_cc-pVTZ bdnguye2 PD 0:00 1 (None)

x5608928 mf\_nes2.8 tpss-15A\_cc-pVQZ bdnguye2 R 0:01 1 c-5-42

x5608929 mf\_nes2.8 monomer1-tpss-16\_cc-pVTZ bdnguye2 R 1:43 1 c-7-20

x5608932 mf\_nes2.8 monomer1-tpss-16AB\_cc-pvtz bdnguye2 R 0:06 1 c-8-251

x5608934 mf\_ilg2.3 1\_ghosts-tpss-16\_cc-pVTZ bdnguye2 R 6:43 1 c-15-33

x5608938 mf\_nes2.8 1\_ghosts-16AB\_cc-pvtz bdnguye2 R 5:05 1 c-7-21

x5608985 mf\_nes2.8 2\_ghosts-16AB\_cc-pvtz bdnguye2 R 0:04 1 c-5-37

x5609056 mf\_nes2.8 1\_ghosts-tpss-16AB\_cc-pVQZ bdnguye2 R 3:46 1 c-8-251

x5609059 mf\_nes2.8 monomer1-tpss-16AB\_cc-pVQZ bdnguye2 R 3:24 1 c-5-39

x5609114 mf\_nes2.8 2\_ghosts-tpss-16AB\_cc-pVQZ bdnguye2 R 0:01 1 c-5-18

x5609163 mf\_nes2.8 tpss-16AB\_cc-pVQZ bdnguye2 R 0:32 1 c-5-20

x5611378 mf\_nes2.8 pbe\_15AB\_cc-pVTZ bdnguye2 R 32:22 1 c-7-20

\*5611381 mf\_nes2.8 pbe\_15AB\_cc-pVQZ bdnguye2 R 30:56 1 c-7-21

x5611412 mf\_nes2.8 monomer1-tpss-16\_cc-pVTZ bdnguye2 R 20:27 1 c-7-13

x5611451 mf\_nes2.8 1\_ghosts-tpss-16\_cc-pVTZ bdnguye2 R 17:20 1 c-5-37

x5611453 mf\_ilg2.3 2\_ghosts-tpss-16\_cc-pVTZ bdnguye2 R 16:45 1 c-16-38

x5611462 mf\_nes2.8 1\_ghosts-tpss-16\_cc-pVQZ bdnguye2 R 15:19 1 c-5-39

x5611468 mf\_nes2.8 monomer1-tpss-16\_cc-pVQZ bdnguye2 R 14:20 1 c-5-40

x5611478 mf\_nes2.8 2\_ghosts-tpss-16\_cc-pVQZ bdnguye2 R 13:20 1 c-5-42

x5611603 mf\_nes2.8 1\_ghosts-pbe-16AB\_cc-pVTZ bdnguye2 R 4:31 1 c-7-14

x5611618 mf\_nes2.8 monomer1-pbe-16\_cc-pVQZ bdnguye2 R 0:51 1 c-6-29

x5611624 mf\_nes2.8 monomer1-tpss-15AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

x5611636 mf\_nes2.8 1\_ghosts-tpss-15AB\_cc-pVTZ bdnguye2 R 1:20 1 c-5-18

x5611638 mf\_i-b2.8 monomer1-tpss-15AB\_cc-pVQZ bdnguye2 R 0:41 1 c-9-332

x5611644 mf\_nes2.8 1\_ghosts-tpss-15AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

x5611721 mf\_i-b2.8 29-ciA\_cc-pvqz bdnguye2 R 2:35 1 c-9-413

x5611728 mf\_nes2.8 pbe-29-ciB\_cc-pVQZ bdnguye2 R 1:18 1 c-5-20

x5611733 mf\_nes2.8 pbe-29-ciAB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

gplogin2:

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

x4444 ilg2.3 1\_ghosts-pbe-29-ci\_cc-pVTZ bdnguye2 R 8-22:21:12 1 c-13-32

x4512 has2.5 1\_ghosts-pbe-12\_cc-pVQZ bdnguye2 R 1-22:55:18 1 c-19-292

x4519 has2.5 2\_ghosts-pbe-8\_cc-pVQZ bdnguye2 R 1-22:50:13 1 c-19-294

x4582 brd2.4 pbe\_15A\_cc-pVQZ bdnguye2 R 0:01 1 c-19-411

x4583 ilg2.3 1\_ghosts-pbe-16\_cc-pVQZ bdnguye2 R 0:00 1 c-13-33

x4586 has2.5 tpss-16AB\_cc-pVTZ bdnguye2 R 15:31 1 c-19-293

x4587 nes2.8 tpss-15A\_cc-pVQZ bdnguye2 R 11:48 1 c-12-251

x4588 nes2.8 tpss-16AB\_cc-pVQZ bdnguye2 R 1:44 1 c-12-252

x4589 nes2.8 1\_ghosts-pbe-16\_cc-pVQZ bdnguye2 R 2:50 1 c-12-253

**1/29/18: Observation of complex 15 & 16**

- Computing with the correct basis sets with the corresponding ecp basis and jkbas

**02/17/19: Jobs submitted for rirpa(HF), riaxk cc-pVQZ and edit mp2\_monomer2 energy**

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

481520 ilg2.3 pbe-cbhAB\_cc-pVQZ bdnguye2 R 8-21:31:12 1 c-12-38

489676 brd2.4 rirpa\_9AB\_cc-pVTZ bdnguye2 R 1:07:59 1 c-14-10

489677 nes2.8 rirpa\_9B\_cc-pVQZ bdnguye2 R 1:01:40 1 c-6-212

489678 nes2.8 rirpa\_9A\_cc-pVQZ bdnguye2 R 58:40 1 c-3-341

~~489681 ilg2.3 mp2-monomer2-9AB\_cc-pVQZ bdnguye2 R 31:50 1 c-12-37~~

**02/19/19: Continuation from two days ago**

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

481520 ilg2.3 pbe-cbhAB\_cc-pVQZ bdnguye2 R 9-22:32:29 1 c-12-38

489678 nes2.8 rirpa\_9A\_cc-pVQZ bdnguye2 R 1-01:59:57 1 c-3-341

~~490841 brd2.4 mp2\_15A\_cc-pV5Z bdnguye2 R 34:46 1 c-19-412~~

~~490847 ilg2.3 mp2-monomer2-15\_cc-pVQZ bdnguye2 R 15:29 1 c-12-37~~

~~490849 ilg2.3 mp2-monomer1-15\_cc-pV5Z bdnguye2 R 7:51 1 c-12-37~~

\*490853 ilg2.3 mp2-2\_ghosts-15\_cc-pV5Z bdnguye2 R 1:51 1 c-12-37

\*490854 nes2.8,il mp2-1\_ghosts-15\_cc-pV5Z bdnguye2 PD 0:00 1 (None)

~~490861 m2090 pbe-15AB\_cc-pV5Z bdnguye2 R 0:52 1 c-3-41~~

~~490858 sib2.9 pbe\_15A\_cc-pV5Z bdnguye2 R 0:08 1 c-9-334~~

~~490862 nes2.8,il pbe\_15B\_cc-pV5Z bdnguye2 PD 0:00 1 (None)~~

**02/20/19: Submission for L7 test set printing out the largest eigenvalue at each freq**

495514 sib2.9 pbe\_15AB\_cc-pV5Z bdnguye2 R 3:06:54 1 c-9-334

~~495541 brd2.4 mp2-monomer1-15\_cc-pV5Z bdnguye2 R 2:57:53 1 c-19-412~~

~~496021 brd2.4 pbe-c3aAB\_cc-pVTZ bdnguye2 R 12:55 1 c-19-411~~

~~496050 ilg2.3 pbe-c3gcAB\_cc-pVTZ bdnguye2 R 6:12 1 c-15-25~~

~~496057 has2.5 pbe-gcgcAB\_cc-pVTZ bdnguye2 R 4:12 1 c-19-291~~

~~496059 sib2.9 pbe-cbhAB\_cc-pVTZ bdnguye2 R 3:12 1 c-9-373~~

~~496064 has2.5 pbe-gggAB\_cc-pVTZ bdnguye2 R 1:43 1 c-19-291~~

~~496168 has2.5,br pbe-pheAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

**02/22/2019: RIRPA and MP2 submission for complex 15**

499429 ilg2.3 mp2-2\_ghosts-15\_cc-pV5Z bdnguye2 R 23:05 1 c-13-38

499430 ilg2.3 mp2-1\_ghosts-15\_cc-pV5Z bdnguye2 R 22:05 1 c-14-38

499431 ilg2.3 mp2-monomer1-15\_cc-pV5Z bdnguye2 R 17:33 1 c-15-25

499437 ilg2.3 pbe\_15AB\_cc-pV5Z bdnguye2 R 0:31 1 c-15-33

**RPA with HF reference orbitals**

499472 nes2.8 mp2\_1B\_cc-pVTZ bdnguye2 R 2:01 1 c-6-212

499474 ilg2.3 mp2\_3B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-34

499475 ilg2.3 mp2\_4B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-34

499476 ilg2.3 mp2\_5B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-34

499477 ilg2.3 mp2\_6B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-34

499479 ilg2.3 mp2\_8B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-38

499480 ilg2.3 mp2\_10B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-38

499481 ilg2.3 mp2\_11B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-38

499482 ilg2.3 mp2\_12B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-41

499483 ilg2.3 mp2\_13B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-41

499484 ilg2.3 mp2\_14B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-41

499485 ilg2.3 mp2\_15B\_cc-pVTZ bdnguye2 R 2:01 1 c-15-41

499486 ilg2.3 mp2\_16B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-18

499487 ilg2.3 mp2\_17B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-18

499488 ilg2.3 mp2\_18B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-18

499489 ilg2.3 mp2\_19B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-18

499490 ilg2.3 mp2\_20B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-19

499491 ilg2.3 mp2\_21B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-19

499492 ilg2.3 mp2\_22B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-19

499493 ilg2.3 mp2\_23B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-19

499494 ilg2.3 mp2\_24B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-23

499495 ilg2.3 mp2\_25B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-23

499496 ilg2.3 mp2\_26B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-23

499497 ilg2.3 mp2\_27B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-23

499498 ilg2.3 mp2\_28B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-28

499500 ilg2.3 mp2\_30B\_cc-pVTZ bdnguye2 R 2:01 1 c-16-28

499501 ilg2.3 mp2\_23-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-28

499502 ilg2.3 mp2\_24-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-32

499503 ilg2.3 mp2\_25-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-32

499504 ilg2.3 mp2\_26-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-32

499505 ilg2.3 mp2\_27-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-33

499506 ilg2.3 mp2\_28-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-33

499508 ilg2.3 mp2\_30-ciB\_cc-pVTZ bdnguye2 R 2:01 1 c-16-37

499512 nes2.8,si rirpa\_9A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499555 nes2.8,si rirpa\_1A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499556 nes2.8,si rirpa\_3A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499557 nes2.8,si rirpa\_5A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499558 nes2.8,si rirpa\_7A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499559 nes2.8,si rirpa\_8A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499560 nes2.8,si rirpa\_10A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499561 nes2.8,si rirpa\_12A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499562 nes2.8,si rirpa\_14A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499563 nes2.8,si rirpa\_15A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499564 nes2.8,si rirpa\_18A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499565 nes2.8,si rirpa\_19A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499566 nes2.8,si rirpa\_20A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499567 nes2.8,si rirpa\_21A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499568 nes2.8,si rirpa\_22A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499569 nes2.8,si rirpa\_23A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499570 nes2.8,si rirpa\_24A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499571 nes2.8,si rirpa\_25A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499572 nes2.8,si rirpa\_27A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499573 nes2.8,si rirpa\_29A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499574 nes2.8,si rirpa\_23-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499575 nes2.8,si rirpa\_24-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499576 nes2.8,si rirpa\_25-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499577 nes2.8,si rirpa\_28-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499578 nes2.8,si rirpa\_29-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

499585 bdnguye2 brd2.4 rirpa\_1AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:27

c-14-10/16

499586 bdnguye2 brd2.4 rirpa\_2AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:27

c-14-10/16

499588 bdnguye2 has2.5 rirpa\_4AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:27

c-19-291/16

499589 bdnguye2 has2.5 rirpa\_5AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:27

c-19-291/16

499590 bdnguye2 ilg2.3 rirpa\_6AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:26

c-15-34/16

499592 bdnguye2 brd2.4 rirpa\_8AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:24

c-14-12/16

499593 bdnguye2 ilg2.3 rirpa\_10AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:26

c-16-37/16

499594 bdnguye2 ilg2.3 rirpa\_11AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:26

c-16-37/16

499595 bdnguye2 ilg2.3 rirpa\_12AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:24

c-16-19/16

499596 bdnguye2 ilg2.3 rirpa\_13AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:02

c-15-25/16

499597 bdnguye2 ilg2.3 rirpa\_14AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:02

c-15-25/16

499600 bdnguye2 ilg2.3 rirpa\_17AB\_cc-pVTZ -- 1 16 -- 100:0 R 00:02

c-15-25/16

499601 bdnguye2 nes2.8,i rirpa\_18AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499602 bdnguye2 nes2.8,i rirpa\_19AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499603 bdnguye2 nes2.8,i rirpa\_20AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499604 bdnguye2 nes2.8,i rirpa\_21AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499605 bdnguye2 nes2.8,i rirpa\_22AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499606 bdnguye2 nes2.8,i rirpa\_23AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499607 bdnguye2 nes2.8,i rirpa\_24AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

--

499608 bdnguye2 nes2.8,i rirpa\_25AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499609 bdnguye2 nes2.8,i rirpa\_26AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499610 bdnguye2 nes2.8,i rirpa\_27AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499611 bdnguye2 nes2.8,i rirpa\_28AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499612 bdnguye2 nes2.8,i rirpa\_29AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499613 bdnguye2 nes2.8,i rirpa\_30AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499614 bdnguye2 nes2.8,i rirpa\_23-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499615 bdnguye2 nes2.8,i rirpa\_24-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499616 bdnguye2 nes2.8,i rirpa\_25-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499617 bdnguye2 nes2.8,i rirpa\_26-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499618 bdnguye2 nes2.8,i rirpa\_27-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499619 bdnguye2 nes2.8,i rirpa\_28-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499620 bdnguye2 nes2.8,i rirpa\_29-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499621 bdnguye2 nes2.8,i rirpa\_30-ciAB\_cc-pVT -- 1 8 -- 100:0 Q 00:00

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499622 bdnguye2 ilg2.3 rirpa\_15A\_cc-pVTZ -- 1 16 -- 72:00 R 00:02

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499623 bdnguye2 nes2.8,i rirpa\_3AB\_cc-pVTZ -- 1 8 -- 100:0 Q 00:00

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499624 bdnguye2 nes2.8,i mp2\_7B\_cc-pVTZ -- 1 8 -- 48:00 Q 00:00

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499625 bdnguye2 nes2.8,i mp2\_22B\_cc-pVTZ -- 1 8 -- 48:00 Q 00:00

**02/23/19: Submission of CP for S30L with RPA(HF)**

500366 ilg2.3 rirpa\_28AB\_cc-pVTZ bdnguye2 R 3:27:39 1 c-14-42

500367 ilg2.3 rirpa\_26-ciAB\_cc-pVTZ bdnguye2 R 14:23:54 1 c-15-25

500370 nes2.8 rirpa\_2AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500371 nes2.8 rirpa\_3AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500372 nes2.8 rirpa\_4AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500373 nes2.8 rirpa\_5AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500374 nes2.8 rirpa\_6AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500375 nes2.8 rirpa\_7AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500376 nes2.8 rirpa\_8AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500377 nes2.8 rirpa\_9AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500378 nes2.8 rirpa\_10AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500379 nes2.8 rirpa\_11AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500380 nes2.8 rirpa\_12AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500381 nes2.8 rirpa\_13AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500382 nes2.8 rirpa\_14AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500383 nes2.8 rirpa\_15AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500384 nes2.8 rirpa\_16AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500385 nes2.8 rirpa\_17AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500386 nes2.8 rirpa\_18AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500387 nes2.8 rirpa\_19AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500388 nes2.8 rirpa\_20AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500389 nes2.8 rirpa\_21AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500390 nes2.8 rirpa\_22AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500391 nes2.8 rirpa\_23AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500392 nes2.8 rirpa\_24AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500393 nes2.8 rirpa\_25AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500394 nes2.8 rirpa\_26AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500395 nes2.8 rirpa\_27AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500396 nes2.8 rirpa\_28AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500397 nes2.8 rirpa\_29AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500398 nes2.8 rirpa\_30AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500399 nes2.8 rirpa\_23-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500400 nes2.8 rirpa\_24-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500401 nes2.8 rirpa\_25-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500402 nes2.8 rirpa\_26-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500403 nes2.8 rirpa\_27-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500404 nes2.8 rirpa\_28-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500405 nes2.8 rirpa\_29-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500406 nes2.8 rirpa\_30-ciAB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500407 ilg2.3 rirpa\_19AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500408 ilg2.3 rirpa\_22AB\_cc-pVTZ bdnguye2 R 12:57:46 1 c-16-18

500514 ilg2.3 rirpa\_20A\_cc-pVTZ bdnguye2 R 6:19 1 c-13-38

500515 ilg2.3,br rirpa\_21A\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

500516 ilg2.3,br rirpa\_24A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500518 ilg2.3,br rirpa\_24-ciA\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500519 ilg2.3 rirpa\_4AB\_cc-pVTZ bdnguye2 R 53:25 1 c-16-37

500520 brd2.4 rirpa\_30AB\_cc-pVTZ bdnguye2 R 53:25 1 c-19-413

500523 ilg2.3,br rirpa\_27-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500524 ilg2.3,br rirpa\_27AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500525 ilg2.3,br rirpa\_24AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500527 ilg2.3,br rirpa\_25AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500528 ilg2.3,br rirpa\_18AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500529 ilg2.3,br rirpa\_15AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500530 ilg2.3,br rirpa\_16AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500531 ilg2.3,br rirpa\_8AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500533 ilg2.3,br rirpa\_24-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500534 ilg2.3,br rirpa\_25-ciAB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

~~500536 ilg2.3,br rirpa\_1AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500537 ilg2.3,br rirpa\_2AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500538 ilg2.3,br rirpa\_3AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500539 ilg2.3,br rirpa\_4AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500540 ilg2.3,br rirpa\_5AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500541 ilg2.3,br rirpa\_6AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500542 ilg2.3,br rirpa\_7AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500543 ilg2.3,br rirpa\_8AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500544 ilg2.3,br rirpa\_9AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500545 ilg2.3,br rirpa\_10AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500546 ilg2.3,br rirpa\_11AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500547 ilg2.3,br rirpa\_12AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500548 ilg2.3,br rirpa\_13AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500549 ilg2.3,br rirpa\_14AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500550 ilg2.3,br rirpa\_15AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500551 ilg2.3,br rirpa\_16AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500552 ilg2.3,br rirpa\_17AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500553 ilg2.3,br rirpa\_18AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500554 ilg2.3,br rirpa\_19AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500555 ilg2.3,br rirpa\_20AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500556 ilg2.3,br rirpa\_21AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500557 ilg2.3,br rirpa\_22AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500558 ilg2.3,br rirpa\_23AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500559 ilg2.3,br rirpa\_24AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500560 ilg2.3,br rirpa\_25AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500561 ilg2.3,br rirpa\_26AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500562 ilg2.3,br rirpa\_27AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500563 ilg2.3,br rirpa\_28AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500564 ilg2.3,br rirpa\_29AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500565 ilg2.3,br rirpa\_30AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500566 ilg2.3,br rirpa\_23-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500567 ilg2.3,br rirpa\_24-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500568 ilg2.3,br rirpa\_25-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500569 ilg2.3,br rirpa\_26-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500570 ilg2.3,br rirpa\_27-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500571 ilg2.3,br rirpa\_28-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500572 ilg2.3,br rirpa\_29-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500573 ilg2.3,br rirpa\_30-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500575 nes2.8 rirpa\_1AB\_monomer2\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500578 ilg2.3,br rirpa\_1AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500579 ilg2.3,br rirpa\_1AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500580 ilg2.3,br rirpa\_2AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500581 ilg2.3,br rirpa\_2AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500582 ilg2.3,br rirpa\_3AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500583 ilg2.3,br rirpa\_3AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500584 ilg2.3,br rirpa\_4AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500585 ilg2.3,br rirpa\_4AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500586 ilg2.3,br rirpa\_5AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500587 ilg2.3,br rirpa\_5AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500588 ilg2.3,br rirpa\_6AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500589 ilg2.3,br rirpa\_6AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500590 ilg2.3,br rirpa\_7AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500591 ilg2.3,br rirpa\_7AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500592 ilg2.3,br rirpa\_8AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500593 ilg2.3,br rirpa\_8AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500594 ilg2.3,br rirpa\_9AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500595 ilg2.3,br rirpa\_9AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500596 ilg2.3,br rirpa\_10AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500597 ilg2.3,br rirpa\_10AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500598 ilg2.3,br rirpa\_11AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500599 ilg2.3,br rirpa\_11AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500600 ilg2.3,br rirpa\_12AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500601 ilg2.3,br rirpa\_12AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500602 ilg2.3,br rirpa\_13AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500603 ilg2.3,br rirpa\_13AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500604 ilg2.3,br rirpa\_14AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500605 ilg2.3,br rirpa\_14AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500606 ilg2.3,br rirpa\_15AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500607 ilg2.3,br rirpa\_15AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500608 ilg2.3,br rirpa\_16AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500609 ilg2.3,br rirpa\_16AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500610 ilg2.3,br rirpa\_17AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500611 ilg2.3,br rirpa\_17AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500612 ilg2.3,br rirpa\_18AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500613 ilg2.3,br rirpa\_18AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500614 ilg2.3,br rirpa\_19AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500615 ilg2.3,br rirpa\_19AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500616 ilg2.3,br rirpa\_20AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500617 ilg2.3,br rirpa\_20AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500618 ilg2.3,br rirpa\_21AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500619 ilg2.3,br rirpa\_21AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500620 ilg2.3,br rirpa\_22AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500621 ilg2.3,br rirpa\_22AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500622 ilg2.3,br rirpa\_23AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500623 ilg2.3,br rirpa\_23AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500624 ilg2.3,br rirpa\_24AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500625 ilg2.3,br rirpa\_24AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500626 ilg2.3,br rirpa\_25AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500627 ilg2.3,br rirpa\_25AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500628 ilg2.3,br rirpa\_26AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500629 ilg2.3,br rirpa\_26AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500630 ilg2.3,br rirpa\_27AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500631 ilg2.3,br rirpa\_27AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500632 ilg2.3,br rirpa\_28AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500633 ilg2.3,br rirpa\_28AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500634 ilg2.3,br rirpa\_29AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500635 ilg2.3,br rirpa\_29AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500636 ilg2.3,br rirpa\_30AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500637 ilg2.3,br rirpa\_30AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500638 ilg2.3,br rirpa\_23-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500639 ilg2.3,br rirpa\_23-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500640 ilg2.3,br rirpa\_24-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500641 ilg2.3,br rirpa\_24-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500642 ilg2.3,br rirpa\_25-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500643 ilg2.3,br rirpa\_25-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500644 ilg2.3,br rirpa\_26-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500645 ilg2.3,br rirpa\_26-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500646 ilg2.3,br rirpa\_27-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500647 ilg2.3,br rirpa\_27-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500648 ilg2.3,br rirpa\_28-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500649 ilg2.3,br rirpa\_28-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500650 ilg2.3,br rirpa\_29-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500651 ilg2.3,br rirpa\_29-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500652 ilg2.3,br rirpa\_30-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)~~

~~500653 ilg2.3,br rirpa\_30-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority~~)

**02/24/19: Resubmission due to the jobs in the queue being deleted**

500809 ilg2.3 rirpa\_11AB\_monomer1\_cc-pVTZ bdnguye2 R 20:35 1 c-15-25

500810 ilg2.3,br rirpa\_12AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

500811 ilg2.3,br rirpa\_13AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500812 ilg2.3,br rirpa\_14AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500813 ilg2.3,br rirpa\_15AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500814 ilg2.3,br rirpa\_16AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500815 ilg2.3,br rirpa\_17AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500816 ilg2.3,br rirpa\_18AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500817 ilg2.3,br rirpa\_19AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500818 ilg2.3,br rirpa\_20AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500820 m2090 rirpa\_21AB\_monomer1\_cc-pVTZ bdnguye2 R 18:38 1 c-3-41

500821 m2090 rirpa\_22AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500822 m2090 rirpa\_23AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500823 m2090 rirpa\_24AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500824 m2090 rirpa\_25AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500825 m2090 rirpa\_26AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500826 m2090 rirpa\_27AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500827 m2090 rirpa\_28AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500828 m2090 rirpa\_29AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500829 m2090 rirpa\_30AB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500830 m2090 rirpa\_23-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500831 m2090 rirpa\_24-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500832 m2090 rirpa\_25-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500833 m2090 rirpa\_26-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500834 m2090 rirpa\_27-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500835 m2090 rirpa\_28-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500836 m2090 rirpa\_29-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500837 m2090 rirpa\_30-ciAB\_monomer1\_cc-pVTZ bdnguye2 PD 0:00 1 (AssocMaxJobsLimit)

500838 ilg2.3,br rirpa\_7AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500839 ilg2.3,br rirpa\_8AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500840 ilg2.3,br rirpa\_21AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500841 ilg2.3,br rirpa\_10AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500842 ilg2.3,br rirpa\_11AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500843 ilg2.3,br rirpa\_12AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500844 ilg2.3,br rirpa\_13AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500845 ilg2.3,br rirpa\_14AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500850 ilg2.3,br rirpa\_17AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500852 ilg2.3,br rirpa\_19AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500854 ilg2.3,br rirpa\_1AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500855 ilg2.3,br rirpa\_1AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500856 ilg2.3,br rirpa\_2AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500857 ilg2.3,br rirpa\_2AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500858 ilg2.3,br rirpa\_3AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500859 ilg2.3,br rirpa\_3AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500860 ilg2.3,br rirpa\_4AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500861 ilg2.3,br rirpa\_4AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500862 ilg2.3,br rirpa\_5AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500863 ilg2.3,br rirpa\_5AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500864 ilg2.3,br rirpa\_6AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500865 ilg2.3,br rirpa\_6AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500866 ilg2.3,br rirpa\_7AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500867 ilg2.3,br rirpa\_7AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500868 ilg2.3,br rirpa\_8AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500869 ilg2.3,br rirpa\_8AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500870 ilg2.3,br rirpa\_9AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500871 ilg2.3,br rirpa\_9AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500872 ilg2.3,br rirpa\_10AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500873 ilg2.3,br rirpa\_10AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500874 ilg2.3,br rirpa\_11AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500875 ilg2.3,br rirpa\_11AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500876 ilg2.3,br rirpa\_12AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500877 ilg2.3,br rirpa\_12AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500878 ilg2.3,br rirpa\_13AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500879 ilg2.3,br rirpa\_13AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500880 ilg2.3,br rirpa\_14AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500881 ilg2.3,br rirpa\_14AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500882 ilg2.3,br rirpa\_15AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500883 ilg2.3,br rirpa\_15AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500884 ilg2.3,br rirpa\_16AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500885 ilg2.3,br rirpa\_16AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500886 ilg2.3,br rirpa\_17AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500887 ilg2.3,br rirpa\_17AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500888 ilg2.3,br rirpa\_18AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500889 ilg2.3,br rirpa\_18AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500890 ilg2.3,br rirpa\_19AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500891 ilg2.3,br rirpa\_19AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500892 ilg2.3,br rirpa\_20AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500893 ilg2.3,br rirpa\_20AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500894 ilg2.3,br rirpa\_21AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500895 ilg2.3,br rirpa\_21AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500896 ilg2.3,br rirpa\_22AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500897 ilg2.3,br rirpa\_22AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500898 ilg2.3,br rirpa\_23AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500899 ilg2.3,br rirpa\_23AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500900 ilg2.3,br rirpa\_24AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500901 ilg2.3,br rirpa\_24AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500902 ilg2.3,br rirpa\_25AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500903 ilg2.3,br rirpa\_25AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500904 ilg2.3,br rirpa\_26AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500905 ilg2.3,br rirpa\_26AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500906 ilg2.3,br rirpa\_27AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500907 ilg2.3,br rirpa\_27AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500908 ilg2.3,br rirpa\_28AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500909 ilg2.3,br rirpa\_28AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500910 ilg2.3,br rirpa\_29AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500911 ilg2.3,br rirpa\_29AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500912 ilg2.3,br rirpa\_30AB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500913 ilg2.3,br rirpa\_30AB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500914 ilg2.3,br rirpa\_23-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500915 ilg2.3,br rirpa\_23-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500916 ilg2.3,br rirpa\_24-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500917 ilg2.3,br rirpa\_24-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500918 ilg2.3,br rirpa\_25-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500919 ilg2.3,br rirpa\_25-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500920 ilg2.3,br rirpa\_26-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500921 ilg2.3,br rirpa\_26-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500922 ilg2.3,br rirpa\_27-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500923 ilg2.3,br rirpa\_27-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500924 ilg2.3,br rirpa\_28-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500925 ilg2.3,br rirpa\_28-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500926 ilg2.3,br rirpa\_29-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500927 ilg2.3,br rirpa\_29-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500928 ilg2.3,br rirpa\_30-ciAB\_2\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

500929 ilg2.3,br rirpa\_30-ciAB\_1\_ghosts\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

**03/03/19: Investigation of HF reference using triplet/singlet procedure and running mp4 calculations**

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

~~529358 brd2.4 mp4\_5B\_cc-pVTZ bdnguye2 R 4:38:11 1 c-14-10~~

529423 ilg2.3 rirpa\_24-ciAB\_cc-pVTZ bdnguye2 R 4:13:11 1 c-12-38

529756 brd2.4 mp2-2\_ghosts-18\_cc-pVTZ bdnguye2 R 2:55:11 1 c-19-412

530571 brd2.4 mp2-2\_ghosts-18\_cc-pVQZ bdnguye2 R 2:33:54 1 c-19-413

~~530705 brd2.4 mp2\_1A\_cc-pVTZ bdnguye2 R 1:59:13 1 c-14-12~~

~~530706 ilg2.3 mp2\_1AB\_cc-pVTZ bdnguye2 R 1:58:43 1 c-13-37~~

~~531141 ilg2.3 mp2\_3B\_cc-pVTZ bdnguye2 R 28:15 1 c-13-42~~

531222 brd2.4 mp2\_5A\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

531226 brd2.4 mp4\_5AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Resources)

~~531247 ilg2.3 mp2\_5B\_cc-pVTZ bdnguye2 R 8:33 1 c-14-38~~

~~531249 ilg2.3 mp2\_6B\_cc-pVTZ bdnguye2 R 7:33 1 c-15-24~~

~~531254 ilg2.3 mp2\_17B\_cc-pVTZ bdnguye2 R 6:11 1 c-15-25~~

**03/10/19: Submission of recomputing the SCF HF reference energies for MP2**

576025 ilg2.3 rirpa\_7AB\_cc-pVQZ bdnguye2 R 4:47:12 1 c-13-32

576026 brd2.4,si rirpa\_9AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Resources)

576029 ilg2.3 mp2\_3B\_cc-pVQZ bdnguye2 R 4:17:07 1 c-13-38

576031 ilg2.3 mp2\_5B\_cc-pVQZ bdnguye2 R 4:14:07 1 c-14-42

576037 ilg2.3 mp2-2-ghosts-3\_cc-pVTZ bdnguye2 R 3:38:02 1 c-15-33

576040 ilg2.3 mp2\_2-ghosts-4\_cc-pVTZ bdnguye2 R 3:35:02 1 c-15-38

576042 ilg2.3 mp2-2-ghosts-5\_cc-pVTZ bdnguye2 R 3:29:01 1 c-15-42

576045 ilg2.3 mp2-2-ghosts-6\_cc-pVTZ bdnguye2 R 3:26:01 1 c-16-23

576376 ilg2.3 mp2\_monomer2\_3\_cc-pVQZ bdnguye2 R 2:31:50 1 c-15-37

576377 ilg2.3 mp2\_2\_ghosts\_3\_cc-pVQZ bdnguye2 R 2:31:50 1 c-16-29

576379 ilg2.3 mp2\_2\_ghosts\_4\_cc-pVQZ bdnguye2 R 1:59:08 1 c-13-33

576381 ilg2.3 mp2\_2\_ghosts\_6\_cc-pVQZ bdnguye2 R 21:28 1 c-16-33

576383 ilg2.3 mp2-2\_ghosts-5\_cc-pVQZ bdnguye2 R 14:28 1 c-15-24

576384 m2090 mp2-monomer2-5\_cc-pVQZ bdnguye2 R 2:28:52 1 c-3-41

**03/13/19: Submission ricc2 energies correction**

584995 m-c2.2 mp2-2-ghosts-6\_cc-pVTZ bdnguye2 R 13:13:44 1 c-9-29

590066 ilg2.3 mp2-2\_ghosts-18AB\_cc-pVTZ bdnguye2 R 7:48 1 c-12-38

590070 ilg2.3 mp2-2\_ghosts-18AB\_cc-pVTZ bdnguye2 R 6:48 1 c-13-33

590075 brd2.4 mp2-monomer1-18AB\_cc-pVTZ bdnguye2 PD 0:00 1 (Priority)

590076 brd2.4 mp2-monomer1-18AB\_cc-pVQZ bdnguye2 PD 0:00 1 (Priority)

590082 ilg2.3 mp2-monomer2-3\_cc-pVTZ bdnguye2 R 1:48 1 c-15-41

590083 ilg2.3 mp2-2-ghosts-3\_cc-pVTZ bdnguye2 R 1:48 1 c-15-42

590085 ilg2.3 mp2\_2-ghosts-4\_cc-pVTZ bdnguye2 R 1:48 1 c-16-23

590086 ilg2.3 mp2-monomer2-5\_cc-pVTZ bdnguye2 R 1:48 1 c-16-28

590087 ilg2.3 mp2-2-ghosts-5\_cc-pVTZ bdnguye2 R 1:48 1 c-16-33

590094 ilg2.3 mp2-monomer2-6\_cc-pVTZ bdnguye2 PD 0:00 1 (None)