

Below: is the input and relevant part of the output of the BeH2 PES scan.  
The "guess=always" forces a default initial guess at each geometry, rather than reading orbitals from the previous geometry as the guess at the next geometry.

```
%chk=beh2_scan.chk  
%mem=6MW  
%nproc=1  
# cas(2,2)/3-21g scan guess=always
```

BeH2 scan

```
0 1  
X  
be      X      R1  
h1      x      R2   be 90.  
h2      x      R2   be 90. h1 180.
```

```
r1 3.51    7  -0.5  
r2 0.4     40.2
```

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Summary of the potential surface scan:

N	r1	r2	SCF
1	3.5100	0.4000	-15.62344
2	3.0100	0.4000	-15.62117
3	2.5100	0.4000	-15.61367
4	2.0100	0.4000	-15.59276
5	1.5100	0.4000	-15.54703
6	1.0100	0.4000	-15.42336
7	0.5100	0.4000	-14.63092
8	0.0100	0.4000	-12.64872
9	3.5100	0.6000	-15.55535
10	3.0100	0.6000	-15.55290
11	2.5100	0.6000	-15.54496
12	2.0100	0.6000	-15.52347
13	1.5100	0.6000	-15.51156
14	1.0100	0.6000	-15.48215
15	0.5100	0.6000	-15.17666
16	0.0100	0.6000	-14.54831
17	3.5100	0.8000	-15.46048
18	3.0100	0.8000	-15.52241
19	2.5100	0.8000	-15.51395
20	2.0100	0.8000	-15.45613
21	1.5100	0.8000	-15.51354
22	1.0100	0.8000	-15.56274
23	0.5100	0.8000	-15.46846
24	0.0100	0.8000	-15.27801

25	3.5100	1.0000	-15.39575
26	3.0100	1.0000	-15.49411
27	2.5100	1.0000	-15.48716
28	2.0100	1.0000	-15.44812
29	1.5100	1.0000	-15.50106
30	1.0100	1.0000	-15.59683
31	0.5100	1.0000	-15.61040
32	0.0100	1.0000	-15.56591
33	3.5100	1.2000	-15.48474
34	3.0100	1.2000	-15.48306
35	2.5100	1.2000	-15.47815
36	2.0100	1.2000	-15.43225
37	1.5100	1.2000	-15.50203
38	1.0100	1.2000	-15.60211
39	0.5100	1.2000	-15.65860
40	0.0100	1.2000	-15.66552

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Input for optimizations while driving "scanning" a coordinate.

```
%chk=beh2_scan.chk
%mem=6MW
%nproc=1
# cas(2,2)/3-21g opt=z-matrix
```

BeH2 scan

```
0 1
X
be          X          R1
h1          x          R2   be   90.
h2          x          R2   be   90. h1 180.

r1  3.01  s  6   -0.5
r2  0.4
```