

```

XTLGRF 200
DESCRP A0162
REMARK 1x1-clean-{111}-step
FIXATOMS      15      25
CRYSTX      2.79100      8.37290      55.65550      90.00000      90.00000      90.00000
FORMAT ATOM      (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
HETATM      1 Pt      2.09325      1.72050      14.99747      Pt      0 0      0.00000
HETATM      2 Pt      0.69775      4.06539      15.64967      Pt      0 0      0.00000
HETATM      3 Pt      2.09325      6.40695      16.30307      Pt      0 0      0.00000
HETATM      4 Pt      0.69775      0.35161      16.98669      Pt      0 0      0.00000
HETATM      5 Pt      2.09325      2.67768      17.63112      Pt      0 0      0.00000
HETATM      6 Pt      0.69775      5.00545      18.28247      Pt      0 0      0.00000
HETATM      7 Pt      2.09325      7.32583      18.95030      Pt      0 0      0.00000
HETATM      8 Pt      0.69775      1.28171      19.60854      Pt      0 0      0.00000
HETATM      9 Pt      2.09325      3.60833      20.26045      Pt      0 0      0.00000
HETATM     10 Pt      0.69775      5.93102      20.92093      Pt      0 0      0.00000
HETATM     11 Pt      2.09325      8.25656      21.58025      Pt      0 0      0.00000
HETATM     12 Pt      0.69775      2.21094      22.23633      Pt      0 0      0.00000
HETATM     13 Pt      2.09325      4.53546      22.89434      Pt      0 0      0.00000
HETATM     14 Pt      0.69775      6.86093      23.55274      Pt      0 0      0.00000
HETATM     15 Pt      2.09325      0.81426      24.21017      Pt      0 0      0.00000
HETATM     16 Pt      0.69775      3.13987      24.86804      Pt      0 0      0.00000
HETATM     17 Pt      2.09325      5.46555      25.52588      Pt      0 0      0.00000
HETATM     18 Pt      0.69775      7.79133      26.18378      Pt      0 0      0.00000
HETATM     19 Pt      2.09325      1.74428      26.84148      Pt      0 0      0.00000
HETATM     20 Pt      0.69775      4.07015      27.49902      Pt      0 0      0.00000
HETATM     21 Pt      2.09325      6.39597      28.15648      Pt      0 0      0.00000
HETATM     22 Pt      0.69775      0.34894      28.81402      Pt      0 0      0.00000
HETATM     23 Pt      2.09325      2.67479      29.47172      Pt      0 0      0.00000
HETATM     24 Pt      0.69775      5.00057      30.12962      Pt      0 0      0.00000
HETATM     25 Pt      2.09325      7.32625      30.78746      Pt      0 0      0.00000
HETATM     26 Pt      0.69775      1.27904      31.44538      Pt      0 0      0.00000
HETATM     27 Pt      2.09325      3.60520      32.10276      Pt      0 0      0.00000
HETATM     28 Pt      0.69775      5.93067      32.76116      Pt      0 0      0.00000
HETATM     29 Pt      2.09325      8.25519      33.41918      Pt      0 0      0.00000
HETATM     30 Pt      0.69775      2.20956      34.07525      Pt      0 0      0.00000
HETATM     31 Pt      2.09325      4.53511      34.73456      Pt      0 0      0.00000
HETATM     32 Pt      0.69775      6.85779      35.39506      Pt      0 0      0.00000
HETATM     33 Pt      2.09325      0.81152      36.04696      Pt      0 0      0.00000
HETATM     34 Pt      0.69775      3.14030      36.70520      Pt      0 0      0.00000
HETATM     35 Pt      2.09325      5.46068      37.37303      Pt      0 0      0.00000
HETATM     36 Pt      0.69775      7.78845      38.02438      Pt      0 0      0.00000
HETATM     37 Pt      2.09325      1.74162      38.66881      Pt      0 0      0.00000
HETATM     38 Pt      0.69775      4.05918      39.35243      Pt      0 0      0.00000
HETATM     39 Pt      2.09325      6.40074      40.00583      Pt      0 0      0.00000
HETATM     40 Pt      0.69775      0.37273      40.65803      Pt      0 0      0.00000
UNIT ENERGY      kcal
ENERGY      -5193.615102
END

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XTLGRF 200
DESCRP A0208
REMARK 2x1-clean-{111}-step
FIXATOMS      29      50
CRYSTX      5.58200      8.37290      55.65550      90.00000      90.00000      90.00000
FORMAT ATOM      (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)
HETATM      1 Pt      2.09325      1.72050      14.99747      Pt      0 0      0.00000
HETATM      2 Pt      4.88425      1.72050      14.99747      Pt      0 0      0.00000
HETATM      3 Pt      0.69775      4.06539      15.64967      Pt      0 0      0.00000
HETATM      4 Pt      3.48875      4.06539      15.64967      Pt      0 0      0.00000
HETATM      5 Pt      2.09325      6.40695      16.30307      Pt      0 0      0.00000
HETATM      6 Pt      4.88425      6.40695      16.30307      Pt      0 0      0.00000
HETATM      7 Pt      0.69775      0.35161      16.98669      Pt      0 0      0.00000

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HETATM	8	Pt	3.48875	0.35161	16.98669	Pt	0	0	0.00000
HETATM	9	Pt	2.09325	2.67768	17.63112	Pt	0	0	0.00000
HETATM	10	Pt	4.88425	2.67768	17.63112	Pt	0	0	0.00000
HETATM	11	Pt	0.69775	5.00545	18.28247	Pt	0	0	0.00000
HETATM	12	Pt	3.48875	5.00545	18.28247	Pt	0	0	0.00000
HETATM	13	Pt	2.09325	7.32583	18.95030	Pt	0	0	0.00000
HETATM	14	Pt	4.88425	7.32583	18.95030	Pt	0	0	0.00000
HETATM	15	Pt	0.69775	1.28171	19.60854	Pt	0	0	0.00000
HETATM	16	Pt	3.48875	1.28171	19.60854	Pt	0	0	0.00000
HETATM	17	Pt	2.09325	3.60833	20.26045	Pt	0	0	0.00000
HETATM	18	Pt	4.88425	3.60833	20.26045	Pt	0	0	0.00000
HETATM	19	Pt	0.69775	5.93102	20.92093	Pt	0	0	0.00000
HETATM	20	Pt	3.48875	5.93102	20.92093	Pt	0	0	0.00000
HETATM	21	Pt	2.09325	8.25656	21.58025	Pt	0	0	0.00000
HETATM	22	Pt	4.88425	8.25656	21.58025	Pt	0	0	0.00000
HETATM	23	Pt	0.69775	2.21094	22.23633	Pt	0	0	0.00000
HETATM	24	Pt	3.48875	2.21094	22.23633	Pt	0	0	0.00000
HETATM	25	Pt	2.09325	4.53546	22.89434	Pt	0	0	0.00000
HETATM	26	Pt	4.88425	4.53546	22.89434	Pt	0	0	0.00000
HETATM	27	Pt	0.69775	6.86093	23.55274	Pt	0	0	0.00000
HETATM	28	Pt	3.48875	6.86093	23.55274	Pt	0	0	0.00000
HETATM	29	Pt	2.09325	0.81426	24.21017	Pt	0	0	0.00000
HETATM	30	Pt	4.88425	0.81426	24.21017	Pt	0	0	0.00000
HETATM	31	Pt	0.69775	3.13987	24.86804	Pt	0	0	0.00000
HETATM	32	Pt	3.48875	3.13987	24.86804	Pt	0	0	0.00000
HETATM	33	Pt	2.09325	5.46555	25.52588	Pt	0	0	0.00000
HETATM	34	Pt	4.88425	5.46555	25.52588	Pt	0	0	0.00000
HETATM	35	Pt	0.69775	7.79133	26.18378	Pt	0	0	0.00000
HETATM	36	Pt	3.48875	7.79133	26.18378	Pt	0	0	0.00000
HETATM	37	Pt	2.09325	1.74428	26.84148	Pt	0	0	0.00000
HETATM	38	Pt	4.88425	1.74428	26.84148	Pt	0	0	0.00000
HETATM	39	Pt	0.69775	4.07015	27.49902	Pt	0	0	0.00000
HETATM	40	Pt	3.48875	4.07015	27.49902	Pt	0	0	0.00000
HETATM	41	Pt	2.09325	6.39597	28.15648	Pt	0	0	0.00000
HETATM	42	Pt	4.88425	6.39597	28.15648	Pt	0	0	0.00000
HETATM	43	Pt	0.69775	0.34894	28.81402	Pt	0	0	0.00000
HETATM	44	Pt	3.48875	0.34894	28.81402	Pt	0	0	0.00000
HETATM	45	Pt	2.09325	2.67479	29.47172	Pt	0	0	0.00000
HETATM	46	Pt	4.88425	2.67479	29.47172	Pt	0	0	0.00000
HETATM	47	Pt	0.69775	5.00057	30.12962	Pt	0	0	0.00000
HETATM	48	Pt	3.48875	5.00057	30.12962	Pt	0	0	0.00000
HETATM	49	Pt	2.09325	7.32625	30.78746	Pt	0	0	0.00000
HETATM	50	Pt	4.88425	7.32625	30.78746	Pt	0	0	0.00000
HETATM	51	Pt	0.69775	1.27904	31.44539	Pt	0	0	0.00000
HETATM	52	Pt	3.48875	1.27904	31.44539	Pt	0	0	0.00000
HETATM	53	Pt	2.09325	3.60520	32.10276	Pt	0	0	0.00000
HETATM	54	Pt	4.88425	3.60520	32.10276	Pt	0	0	0.00000
HETATM	55	Pt	0.69775	5.93067	32.76116	Pt	0	0	0.00000
HETATM	56	Pt	3.48875	5.93067	32.76116	Pt	0	0	0.00000
HETATM	57	Pt	2.09325	8.25519	33.41917	Pt	0	0	0.00000
HETATM	58	Pt	4.88425	8.25519	33.41917	Pt	0	0	0.00000
HETATM	59	Pt	0.69775	2.20956	34.07525	Pt	0	0	0.00000
HETATM	60	Pt	3.48875	2.20956	34.07525	Pt	0	0	0.00000
HETATM	61	Pt	2.09325	4.53511	34.73456	Pt	0	0	0.00000
HETATM	62	Pt	4.88425	4.53511	34.73456	Pt	0	0	0.00000
HETATM	63	Pt	0.69775	6.85779	35.39506	Pt	0	0	0.00000
HETATM	64	Pt	3.48875	6.85779	35.39506	Pt	0	0	0.00000
HETATM	65	Pt	2.09325	0.81152	36.04696	Pt	0	0	0.00000
HETATM	66	Pt	4.88425	0.81152	36.04696	Pt	0	0	0.00000
HETATM	67	Pt	0.69775	3.14030	36.70520	Pt	0	0	0.00000
HETATM	68	Pt	3.48875	3.14030	36.70520	Pt	0	0	0.00000
HETATM	69	Pt	2.09325	5.46068	37.37303	Pt	0	0	0.00000
HETATM	70	Pt	4.88425	5.46068	37.37303	Pt	0	0	0.00000

HETATM	71	Pt	0.69775	7.78845	38.02438	Pt	0	0	0.00000
HETATM	72	Pt	3.48875	7.78845	38.02438	Pt	0	0	0.00000
HETATM	73	Pt	2.09325	1.74162	38.66881	Pt	0	0	0.00000
HETATM	74	Pt	4.88425	1.74162	38.66881	Pt	0	0	0.00000
HETATM	75	Pt	0.69775	4.05918	39.35243	Pt	0	0	0.00000
HETATM	76	Pt	3.48875	4.05918	39.35243	Pt	0	0	0.00000
HETATM	77	Pt	2.09325	6.40074	40.00583	Pt	0	0	0.00000
HETATM	78	Pt	4.88425	6.40074	40.00583	Pt	0	0	0.00000
HETATM	79	Pt	0.69775	0.37273	40.65803	Pt	0	0	0.00000
HETATM	80	Pt	3.48875	0.37273	40.65803	Pt	0	0	0.00000
UNIT ENERGY kcal									
ENERGY -10387.230187									
END									

XTLGRF 200
DESCRP A0218
REMARK 2x1-fcc-{111}-step
FIXATOMS 29 50
CRYSTX 5.58200 8.37290 55.65550 90.00000 90.00000 90.00000
FORMAT ATOM (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)

HETATM	1	Pt	2.10611	1.69341	14.89542	Pt	0	0	0.00000
HETATM	2	Pt	4.86854	1.69341	14.89542	Pt	0	0	0.00000
HETATM	3	Pt	0.69633	4.05517	15.68307	Pt	0	0	0.00000
HETATM	4	Pt	3.48733	4.02975	15.57085	Pt	0	0	0.00000
HETATM	5	Pt	2.08580	6.40671	16.29345	Pt	0	0	0.00000
HETATM	6	Pt	4.88885	6.40671	16.29345	Pt	0	0	0.00000
HETATM	7	Pt	0.69633	0.32751	17.03642	Pt	0	0	0.00000
HETATM	8	Pt	3.48733	0.34609	16.95511	Pt	0	0	0.00000
HETATM	9	Pt	2.09538	2.66322	17.60699	Pt	0	0	0.00000
HETATM	10	Pt	4.87927	2.66322	17.60699	Pt	0	0	0.00000
HETATM	11	Pt	0.69633	4.99882	18.28696	Pt	0	0	0.00000
HETATM	12	Pt	3.48733	4.99692	18.29355	Pt	0	0	0.00000
HETATM	13	Pt	2.09734	7.31516	18.95455	Pt	0	0	0.00000
HETATM	14	Pt	4.87731	7.31516	18.95455	Pt	0	0	0.00000
HETATM	15	Pt	0.69633	1.27991	19.61375	Pt	0	0	0.00000
HETATM	16	Pt	3.48733	1.27407	19.59424	Pt	0	0	0.00000
HETATM	17	Pt	2.09194	3.59896	20.25651	Pt	0	0	0.00000
HETATM	18	Pt	4.88272	3.59896	20.25651	Pt	0	0	0.00000
HETATM	19	Pt	0.69633	5.92359	20.92260	Pt	0	0	0.00000
HETATM	20	Pt	3.48733	5.92238	20.92637	Pt	0	0	0.00000
HETATM	21	Pt	2.09266	8.25238	21.57918	Pt	0	0	0.00000
HETATM	22	Pt	4.88200	8.25238	21.57918	Pt	0	0	0.00000
HETATM	23	Pt	0.69633	2.20690	22.23763	Pt	0	0	0.00000
HETATM	24	Pt	3.48733	2.20543	22.23238	Pt	0	0	0.00000
HETATM	25	Pt	2.09178	4.53003	22.89466	Pt	0	0	0.00000
HETATM	26	Pt	4.88288	4.53003	22.89466	Pt	0	0	0.00000
HETATM	27	Pt	0.69633	6.85743	23.55246	Pt	0	0	0.00000
HETATM	28	Pt	3.48733	6.85748	23.55360	Pt	0	0	0.00000
HETATM	29	Pt	2.09183	0.81168	24.21050	Pt	0	0	0.00000
HETATM	30	Pt	4.88283	0.81168	24.21050	Pt	0	0	0.00000
HETATM	31	Pt	0.69633	3.13729	24.86837	Pt	0	0	0.00000
HETATM	32	Pt	3.48733	3.13729	24.86837	Pt	0	0	0.00000
HETATM	33	Pt	2.09183	5.46297	25.52621	Pt	0	0	0.00000
HETATM	34	Pt	4.88283	5.46297	25.52621	Pt	0	0	0.00000
HETATM	35	Pt	0.69633	7.78875	26.18411	Pt	0	0	0.00000
HETATM	36	Pt	3.48733	7.78875	26.18411	Pt	0	0	0.00000
HETATM	37	Pt	2.09183	1.74170	26.84181	Pt	0	0	0.00000
HETATM	38	Pt	4.88283	1.74170	26.84181	Pt	0	0	0.00000
HETATM	39	Pt	0.69633	4.06757	27.49935	Pt	0	0	0.00000
HETATM	40	Pt	3.48733	4.06757	27.49935	Pt	0	0	0.00000
HETATM	41	Pt	2.09183	6.39339	28.15681	Pt	0	0	0.00000
HETATM	42	Pt	4.88283	6.39339	28.15681	Pt	0	0	0.00000
HETATM	43	Pt	0.69633	0.34636	28.81435	Pt	0	0	0.00000

HETATM	44	Pt	3.48733	0.34636	28.81435	Pt	0	0	0.00000
HETATM	45	Pt	2.09183	2.67221	29.47205	Pt	0	0	0.00000
HETATM	46	Pt	4.88283	2.67221	29.47205	Pt	0	0	0.00000
HETATM	47	Pt	0.69633	4.99799	30.12995	Pt	0	0	0.00000
HETATM	48	Pt	3.48733	4.99799	30.12995	Pt	0	0	0.00000
HETATM	49	Pt	2.09183	7.32367	30.78779	Pt	0	0	0.00000
HETATM	50	Pt	4.88283	7.32367	30.78779	Pt	0	0	0.00000
HETATM	51	Pt	0.69671	1.27315	31.44683	Pt	0	0	0.00000
HETATM	52	Pt	3.48718	1.27316	31.44681	Pt	0	0	0.00000
HETATM	53	Pt	2.09199	3.59820	32.10257	Pt	0	0	0.00000
HETATM	54	Pt	4.88299	3.59810	32.10361	Pt	0	0	0.00000
HETATM	55	Pt	0.69641	5.92382	32.76126	Pt	0	0	0.00000
HETATM	56	Pt	3.48749	5.92381	32.76135	Pt	0	0	0.00000
HETATM	57	Pt	2.09192	8.24588	33.42475	Pt	0	0	0.00000
HETATM	58	Pt	4.88290	8.24451	33.41928	Pt	0	0	0.00000
HETATM	59	Pt	0.69720	2.19775	34.07719	Pt	0	0	0.00000
HETATM	60	Pt	3.48653	2.19779	34.07715	Pt	0	0	0.00000
HETATM	61	Pt	2.09181	4.52657	34.72975	Pt	0	0	0.00000
HETATM	62	Pt	4.88279	4.52523	34.73333	Pt	0	0	0.00000
HETATM	63	Pt	0.69635	6.84740	35.40065	Pt	0	0	0.00000
HETATM	64	Pt	3.48702	6.84739	35.40089	Pt	0	0	0.00000
HETATM	65	Pt	2.09174	0.79841	36.06208	Pt	0	0	0.00000
HETATM	66	Pt	4.88263	0.79263	36.04226	Pt	0	0	0.00000
HETATM	67	Pt	0.70179	3.13001	36.70108	Pt	0	0	0.00000
HETATM	68	Pt	3.48185	3.13017	36.70098	Pt	0	0	0.00000
HETATM	69	Pt	2.09172	5.44667	37.36453	Pt	0	0	0.00000
HETATM	70	Pt	4.88276	5.44447	37.37059	Pt	0	0	0.00000
HETATM	71	Pt	0.69984	7.77929	38.04984	Pt	0	0	0.00000
HETATM	72	Pt	3.48375	7.77921	38.05046	Pt	0	0	0.00000
HETATM	73	Pt	2.09245	1.72396	38.69933	Pt	0	0	0.00000
HETATM	74	Pt	4.88288	1.74273	38.61803	Pt	0	0	0.00000
HETATM	75	Pt	0.69039	4.03462	39.36405	Pt	0	0	0.00000
HETATM	76	Pt	3.49355	4.03499	39.36397	Pt	0	0	0.00000
HETATM	77	Pt	2.09147	6.41245	40.08919	Pt	0	0	0.00000
HETATM	78	Pt	4.88279	6.38664	39.97514	Pt	0	0	0.00000
HETATM	79	Pt	0.71161	0.37886	40.75811	Pt	0	0	0.00000
HETATM	80	Pt	3.47332	0.37710	40.76070	Pt	0	0	0.00000
HETATM	81	O	2.09039	7.69174	41.59578	O	0	0	0.00000
HETATM	82	O	3.48733	2.75557	14.06093	O	0	0	0.00000

UNIT ENERGY kcal
ENERGY -10587.881656
END

XTLGRF 200
DESCRP A0159
REMARK 1x1-fcc-{111}-step
FIXATOMS 15 25
CRYSTX 2.79100 8.37290 55.65550 90.00000 90.00000 90.00000
FORMAT ATOM (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)

HETATM	1	Pt	2.08468	1.70041	14.75267	Pt	0	0	0.00000
HETATM	2	Pt	0.68919	4.01750	15.63458	Pt	0	0	0.00000
HETATM	3	Pt	2.08469	6.40570	16.27432	Pt	0	0	0.00000
HETATM	4	Pt	0.68919	0.33937	16.98493	Pt	0	0	0.00000
HETATM	5	Pt	2.08469	2.65629	17.60345	Pt	0	0	0.00000
HETATM	6	Pt	0.68920	5.00455	18.30464	Pt	0	0	0.00000
HETATM	7	Pt	2.08470	7.32127	18.94703	Pt	0	0	0.00000
HETATM	8	Pt	0.68920	1.27765	19.60163	Pt	0	0	0.00000
HETATM	9	Pt	2.08470	3.59800	20.25856	Pt	0	0	0.00000
HETATM	10	Pt	0.68920	5.92693	20.92515	Pt	0	0	0.00000
HETATM	11	Pt	2.08470	8.25425	21.57744	Pt	0	0	0.00000
HETATM	12	Pt	0.68921	2.20622	22.23558	Pt	0	0	0.00000
HETATM	13	Pt	2.08471	4.53083	22.89460	Pt	0	0	0.00000
HETATM	14	Pt	0.68921	6.85828	23.55281	Pt	0	0	0.00000

HETATM	15	Pt	2.08471	0.81144	24.21058	Pt	0	0	0.00000
HETATM	16	Pt	0.68921	3.13705	24.86845	Pt	0	0	0.00000
HETATM	17	Pt	2.08471	5.46273	25.52629	Pt	0	0	0.00000
HETATM	18	Pt	0.68921	7.78851	26.18419	Pt	0	0	0.00000
HETATM	19	Pt	2.08471	1.74146	26.84189	Pt	0	0	0.00000
HETATM	20	Pt	0.68921	4.06733	27.49943	Pt	0	0	0.00000
HETATM	21	Pt	2.08471	6.39315	28.15689	Pt	0	0	0.00000
HETATM	22	Pt	0.68921	0.34612	28.81443	Pt	0	0	0.00000
HETATM	23	Pt	2.08471	2.67197	29.47213	Pt	0	0	0.00000
HETATM	24	Pt	0.68921	4.99775	30.13003	Pt	0	0	0.00000
HETATM	25	Pt	2.08471	7.32343	30.78787	Pt	0	0	0.00000
HETATM	26	Pt	0.68921	1.27492	31.44707	Pt	0	0	0.00000
HETATM	27	Pt	2.08470	3.59976	32.10459	Pt	0	0	0.00000
HETATM	28	Pt	0.68920	5.92662	32.76243	Pt	0	0	0.00000
HETATM	29	Pt	2.08470	8.25046	33.42173	Pt	0	0	0.00000
HETATM	30	Pt	0.68920	2.20179	34.08051	Pt	0	0	0.00000
HETATM	31	Pt	2.08470	4.52803	34.73276	Pt	0	0	0.00000
HETATM	32	Pt	0.68919	6.85719	35.39886	Pt	0	0	0.00000
HETATM	33	Pt	2.08469	0.80394	36.05717	Pt	0	0	0.00000
HETATM	34	Pt	0.68919	3.13198	36.71232	Pt	0	0	0.00000
HETATM	35	Pt	2.08469	5.44906	37.35290	Pt	0	0	0.00000
HETATM	36	Pt	0.68919	7.79707	38.05513	Pt	0	0	0.00000
HETATM	37	Pt	2.08469	1.73959	38.67657	Pt	0	0	0.00000
HETATM	38	Pt	0.68919	4.04659	39.38427	Pt	0	0	0.00000
HETATM	39	Pt	2.08468	6.43251	40.02188	Pt	0	0	0.00000
HETATM	40	Pt	0.68918	0.37241	40.91085	Pt	0	0	0.00000
HETATM	41	O	2.08468	7.54172	41.63626	O	0	0	0.00000
HETATM	42	O	3.48019	2.90110	14.02306	O	0	0	0.00000

UNIT ENERGY kcal
ENERGY -5379.172025
END

XTLGRF 200
DESCRP A0155
REMARK 1x1-fcc-top-{111}-step
FIXATOMS 15 25
CRYSTX 2.79100 8.37290 55.65550 90.00000 90.00000 90.00000
FORMAT ATOM (a6,1x,i5,1x,a5,1x,a3,1x,a1,1x,a5,3f10.5,1x,a5,i3,i2,1x,f8.5)

HETATM	1	Pt	2.07664	1.49047	14.39017	Pt	0	0	0.00000
HETATM	2	Pt	0.68114	3.86453	15.62440	Pt	0	0	0.00000
HETATM	3	Pt	2.07664	6.28717	16.23501	Pt	0	0	0.00000
HETATM	4	Pt	0.68113	0.39013	16.86084	Pt	0	0	0.00000
HETATM	5	Pt	2.07663	2.64857	17.66673	Pt	0	0	0.00000
HETATM	6	Pt	0.68112	4.98573	18.30769	Pt	0	0	0.00000
HETATM	7	Pt	2.07661	7.31963	18.89144	Pt	0	0	0.00000
HETATM	8	Pt	0.68109	1.26503	19.63494	Pt	0	0	0.00000
HETATM	9	Pt	2.07657	3.59726	20.27983	Pt	0	0	0.00000
HETATM	10	Pt	0.68105	5.93593	20.90888	Pt	0	0	0.00000
HETATM	11	Pt	2.07653	8.24373	21.57911	Pt	0	0	0.00000
HETATM	12	Pt	0.68099	2.20243	22.24758	Pt	0	0	0.00000
HETATM	13	Pt	2.07647	4.53644	22.89374	Pt	0	0	0.00000
HETATM	14	Pt	0.68094	6.85800	23.55354	Pt	0	0	0.00000
HETATM	15	Pt	2.07638	0.81195	24.21165	Pt	0	0	0.00000
HETATM	16	Pt	0.68088	3.13756	24.86952	Pt	0	0	0.00000
HETATM	17	Pt	2.07638	5.46324	25.52736	Pt	0	0	0.00000
HETATM	18	Pt	0.68088	7.78902	26.18526	Pt	0	0	0.00000
HETATM	19	Pt	2.07638	1.74197	26.84296	Pt	0	0	0.00000
HETATM	20	Pt	0.68088	4.06784	27.50050	Pt	0	0	0.00000
HETATM	21	Pt	2.07638	6.39366	28.15796	Pt	0	0	0.00000
HETATM	22	Pt	0.68088	0.34663	28.81550	Pt	0	0	0.00000
HETATM	23	Pt	2.07638	2.67248	29.47320	Pt	0	0	0.00000
HETATM	24	Pt	0.68088	4.99826	30.13110	Pt	0	0	0.00000
HETATM	25	Pt	2.07638	7.32394	30.78894	Pt	0	0	0.00000

HETATM	26	Pt	0.68098	1.27633	31.44526	Pt	0	0	0.00000
HETATM	27	Pt	2.07653	3.59753	32.10606	Pt	0	0	0.00000
HETATM	28	Pt	0.68106	5.91629	32.76497	Pt	0	0	0.00000
HETATM	29	Pt	2.07663	8.24815	33.41064	Pt	0	0	0.00000
HETATM	30	Pt	0.68117	2.20307	34.08090	Pt	0	0	0.00000
HETATM	31	Pt	2.07670	4.50884	34.75065	Pt	0	0	0.00000
HETATM	32	Pt	0.68123	6.84566	35.37937	Pt	0	0	0.00000
HETATM	33	Pt	2.07676	0.80228	36.02575	Pt	0	0	0.00000
HETATM	34	Pt	0.68128	3.11831	36.76890	Pt	0	0	0.00000
HETATM	35	Pt	2.07679	5.45149	37.35177	Pt	0	0	0.00000
HETATM	36	Pt	0.68130	7.78691	37.99451	Pt	0	0	0.00000
HETATM	37	Pt	2.07681	1.67077	38.80259	Pt	0	0	0.00000
HETATM	38	Pt	0.68131	4.14556	39.42448	Pt	0	0	0.00000
HETATM	39	Pt	2.07681	6.56660	40.03614	Pt	0	0	0.00000
HETATM	40	Pt	0.68130	0.56462	41.27311	Pt	0	0	0.00000
HETATM	41	O	2.07680	7.55783	41.76875	O	0	0	0.00000
HETATM	42	O	2.07681	10.31505	40.84137	O	0	0	0.00000
HETATM	43	O	3.47214	2.86988	13.89381	O	0	0	0.00000
HETATM	44	O	3.47213	0.11383	14.82299	O	0	0	0.00000
UNIT ENERGY kcal									
ENERGY -5538.434693									
END									