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XTLGRF 200
DESCRP A0131
REMARK 1x1-clean-{100}-step
FIXATOMS 18 29
CRYSTX 2.79100 9.25650 56.48410 90.00000 90.00000 98.67070
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HETATM 1 Pt 1.80467 2.59432 14.99149 Pt 0 0 0.00000
HETATM 2 Pt 0.07056 0.47837 15.59298 Pt 0 0 0.00000
HETATM 3 Pt 1.09640 7.20255 16.19482 Pt 0 0 0.00000
HETATM 4 Pt 2.12355 4.67519 16.80284 Pt 0 0 0.00000
HETATM 5 Pt 0.39064 2.56825 17.40929 Pt 0 0 0.00000
HETATM 6 Pt 1.41747 9.30073 18.00629 Pt 0 0 0.00000
HETATM 7 Pt 2.44425 6.77632 18.60820 Pt 0 0 0.00000
HETATM 8 Pt 0.71217 4.67176 19.21252 Pt 0 0 0.00000
HETATM 9 Pt 1.73903 2.14602 19.81554 Pt 0 0 0.00000
HETATM 10 Pt 2.76589 8.87785 20.41518 Pt 0 0 0.00000
HETATM 11 Pt 1.03334 6.77372 21.01733 Pt 0 0 0.00000
HETATM 12 Pt 2.06010 4.24875 21.62041 Pt 0 0 0.00000
HETATM 13 Pt 0.32781 2.14410 22.22268 Pt 0 0 0.00000
HETATM 14 Pt 1.35477 8.87594 22.82370 Pt 0 0 0.00000
HETATM 15 Pt 2.38113 6.35099 23.42577 Pt 0 0 0.00000
HETATM 16 Pt 0.64852 4.24697 24.02827 Pt 0 0 0.00000
HETATM 17 Pt 1.67498 1.72189 24.63050 Pt 0 0 0.00000
HETATM 18 Pt 2.70220 8.45346 25.23200 Pt 0 0 0.00000
HETATM 19 Pt 0.96929 6.34961 25.83377 Pt 0 0 0.00000
HETATM 20 Pt 1.99540 3.82486 26.43605 Pt 0 0 0.00000
HETATM 21 Pt 0.26257 1.72123 27.03866 Pt 0 0 0.00000
HETATM 22 Pt 1.29010 8.45236 27.63998 Pt 0 0 0.00000
HETATM 23 Pt 2.31589 5.92817 28.24189 Pt 0 0 0.00000
HETATM 24 Pt 0.58349 3.82410 28.84396 Pt 0 0 0.00000
HETATM 25 Pt 1.60927 1.29978 29.44624 Pt 0 0 0.00000
HETATM 26 Pt 2.63596 8.03124 30.04748 Pt 0 0 0.00000
HETATM 27 Pt 0.90424 5.92711 30.64967 Pt 0 0 0.00000
HETATM 28 Pt 1.93042 3.40237 31.25206 Pt 0 0 0.00000
HETATM 29 Pt 0.19807 1.29868 31.85393 Pt 0 0 0.00000
HETATM 30 Pt 1.22446 8.03002 32.45538 Pt 0 0 0.00000
HETATM 31 Pt 2.25096 5.50489 33.05811 Pt 0 0 0.00000
HETATM 32 Pt 0.51816 3.40109 33.66043 Pt 0 0 0.00000
HETATM 33 Pt 1.54461 0.87595 34.26150 Pt 0 0 0.00000
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HETATM 36 Pt 1.86475 2.97833 36.06897 Pt 0 0 0.00000
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HETATM 40 Pt 0.45216 2.97562 38.47787 Pt 0 0 0.00000
HETATM 41 Pt 1.47877 0.45126 39.07537 Pt 0 0 0.00000
HETATM 42 Pt 2.50505 7.17999 39.68121 Pt 0 0 0.00000
HETATM 43 Pt 0.77159 5.07323 40.28921 Pt 0 0 0.00000
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HETATM 45 Pt 0.06286 0.42453 41.49339 Pt 0 0 0.00000
UNIT ENERGY kcal
ENERGY -5848.049294
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XTLGRF 200
DESCRP A0187
REMARK 2x1-clean-{100}-step
FIXATOMS 35 58
CRYSTX 5.58200 9.25650 56.48410 90.00000 90.00000 98.67070
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 1.82061 2.80470 14.99148 Pt 0 0 0.00000
HETATM 2 Pt 4.57972 2.38394 14.99149 Pt 0 0 0.00000

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HETATM	6	Pt	3.87144	6.99217	16.19482	Pt	0	0	0.00000
HETATM	7	Pt	2.13949	4.88557	16.80283	Pt	0	0	0.00000
HETATM	8	Pt	4.89859	4.46481	16.80283	Pt	0	0	0.00000
HETATM	9	Pt	0.40658	2.77864	17.40929	Pt	0	0	0.00000
HETATM	10	Pt	3.16568	2.35788	17.40929	Pt	0	0	0.00000
HETATM	11	Pt	1.43341	9.51111	18.00629	Pt	0	0	0.00000
HETATM	12	Pt	4.19251	9.09035	18.00629	Pt	0	0	0.00000
HETATM	13	Pt	2.46019	6.98670	18.60820	Pt	0	0	0.00000
HETATM	14	Pt	5.21929	6.56594	18.60820	Pt	0	0	0.00000
HETATM	15	Pt	0.72811	4.88215	19.21252	Pt	0	0	0.00000
HETATM	16	Pt	3.48722	4.46139	19.21252	Pt	0	0	0.00000
HETATM	17	Pt	1.75497	2.35641	19.81554	Pt	0	0	0.00000
HETATM	18	Pt	4.51407	1.93565	19.81554	Pt	0	0	0.00000
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HETATM	20	Pt	5.54093	8.66748	20.41517	Pt	0	0	0.00000
HETATM	21	Pt	1.04929	6.98411	21.01733	Pt	0	0	0.00000
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HETATM	23	Pt	2.07605	4.45914	21.62041	Pt	0	0	0.00000
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HETATM	26	Pt	3.10286	1.93373	22.22268	Pt	0	0	0.00000
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HETATM	28	Pt	4.12982	8.66557	22.82370	Pt	0	0	0.00000
HETATM	29	Pt	2.39708	6.56138	23.42576	Pt	0	0	0.00000
HETATM	30	Pt	5.15619	6.14062	23.42577	Pt	0	0	0.00000
HETATM	31	Pt	0.66447	4.45736	24.02828	Pt	0	0	0.00000
HETATM	32	Pt	3.42357	4.03660	24.02828	Pt	0	0	0.00000
HETATM	33	Pt	1.69093	1.93228	24.63050	Pt	0	0	0.00000
HETATM	34	Pt	4.45002	1.51152	24.63050	Pt	0	0	0.00000
HETATM	35	Pt	2.71815	8.66384	25.23200	Pt	0	0	0.00000
HETATM	36	Pt	5.47725	8.24309	25.23200	Pt	0	0	0.00000
HETATM	37	Pt	0.98523	6.55999	25.83377	Pt	0	0	0.00000
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HETATM	39	Pt	2.01135	4.03525	26.43606	Pt	0	0	0.00000
HETATM	40	Pt	4.77045	3.61449	26.43606	Pt	0	0	0.00000
HETATM	41	Pt	0.27852	1.93161	27.03867	Pt	0	0	0.00000
HETATM	42	Pt	3.03762	1.51086	27.03867	Pt	0	0	0.00000
HETATM	43	Pt	1.30605	8.66274	27.63998	Pt	0	0	0.00000
HETATM	44	Pt	4.06515	8.24198	27.63998	Pt	0	0	0.00000
HETATM	45	Pt	2.33183	6.13855	28.24190	Pt	0	0	0.00000
HETATM	46	Pt	5.09093	5.71779	28.24190	Pt	0	0	0.00000
HETATM	47	Pt	0.59943	4.03448	28.84396	Pt	0	0	0.00000
HETATM	48	Pt	3.35853	3.61372	28.84396	Pt	0	0	0.00000
HETATM	49	Pt	1.62521	1.51016	29.44624	Pt	0	0	0.00000
HETATM	50	Pt	4.38431	1.08940	29.44624	Pt	0	0	0.00000
HETATM	51	Pt	2.65189	8.24161	30.04747	Pt	0	0	0.00000
HETATM	52	Pt	5.41100	7.82085	30.04747	Pt	0	0	0.00000
HETATM	53	Pt	0.92018	6.13748	30.64967	Pt	0	0	0.00000
HETATM	54	Pt	3.67928	5.71672	30.64967	Pt	0	0	0.00000
HETATM	55	Pt	1.94637	3.61274	31.25206	Pt	0	0	0.00000
HETATM	56	Pt	4.70547	3.19198	31.25206	Pt	0	0	0.00000
HETATM	57	Pt	0.21401	1.50905	31.85393	Pt	0	0	0.00000
HETATM	58	Pt	2.97311	1.08830	31.85393	Pt	0	0	0.00000
HETATM	59	Pt	1.24040	8.24039	32.45538	Pt	0	0	0.00000
HETATM	60	Pt	3.99950	7.81964	32.45538	Pt	0	0	0.00000
HETATM	61	Pt	2.26691	5.71526	33.05811	Pt	0	0	0.00000
HETATM	62	Pt	5.02601	5.29450	33.05811	Pt	0	0	0.00000
HETATM	63	Pt	0.53410	3.61147	33.66043	Pt	0	0	0.00000
HETATM	64	Pt	3.29321	3.19071	33.66043	Pt	0	0	0.00000
HETATM	65	Pt	1.56055	1.08633	34.26150	Pt	0	0	0.00000

HETATM	66	Pt	4.31966	0.66557	34.26150	Pt	0	0	0.00000
HETATM	67	Pt	2.58713	7.81784	34.86333	Pt	0	0	0.00000
HETATM	68	Pt	5.34622	7.39708	34.86333	Pt	0	0	0.00000
HETATM	69	Pt	0.85420	5.71340	35.46674	Pt	0	0	0.00000
HETATM	70	Pt	3.61330	5.29264	35.46674	Pt	0	0	0.00000
HETATM	71	Pt	1.88070	3.18871	36.06897	Pt	0	0	0.00000
HETATM	72	Pt	4.63981	2.76795	36.06897	Pt	0	0	0.00000
HETATM	73	Pt	0.14809	1.08432	36.66876	Pt	0	0	0.00000
HETATM	74	Pt	2.90720	0.66356	36.66877	Pt	0	0	0.00000
HETATM	75	Pt	1.17467	7.81547	37.27150	Pt	0	0	0.00000
HETATM	76	Pt	3.93377	7.39472	37.27150	Pt	0	0	0.00000
HETATM	77	Pt	2.20054	5.28980	37.87563	Pt	0	0	0.00000
HETATM	78	Pt	4.95965	4.86904	37.87563	Pt	0	0	0.00000
HETATM	79	Pt	0.46813	3.18600	38.47787	Pt	0	0	0.00000
HETATM	80	Pt	3.22723	2.76524	38.47787	Pt	0	0	0.00000
HETATM	81	Pt	1.49474	0.66164	39.07537	Pt	0	0	0.00000
HETATM	82	Pt	4.25384	0.24088	39.07537	Pt	0	0	0.00000
HETATM	83	Pt	2.52101	7.39037	39.68121	Pt	0	0	0.00000
HETATM	84	Pt	5.28011	6.96961	39.68122	Pt	0	0	0.00000
HETATM	85	Pt	0.78755	5.28360	40.28921	Pt	0	0	0.00000
HETATM	86	Pt	3.54666	4.86285	40.28921	Pt	0	0	0.00000
HETATM	87	Pt	1.81319	2.75115	40.89144	Pt	0	0	0.00000
HETATM	88	Pt	4.57230	2.33039	40.89144	Pt	0	0	0.00000
HETATM	89	Pt	0.07884	0.63491	41.49340	Pt	0	0	0.00000
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UNIT ENERGY kcal
ENERGY -11696.098575
END

XTLGRF 200
DESCRP A0195
REMARK 2x1-bridge-{100}-step
FIXATOMS 35 58
CRYSTX 5.58200 9.25650 56.48410 90.00000 90.00000 98.67070
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HETATM	2	Pt	4.52596	2.47790	14.89022	Pt	0	0	0.00000
HETATM	3	Pt	0.08814	0.70789	15.56101	Pt	0	0	0.00000
HETATM	4	Pt	2.84457	0.26909	15.61445	Pt	0	0	0.00000
HETATM	5	Pt	1.10824	7.41891	16.18951	Pt	0	0	0.00000
HETATM	6	Pt	3.87259	6.99646	16.18942	Pt	0	0	0.00000
HETATM	7	Pt	2.13500	4.88532	16.79010	Pt	0	0	0.00000
HETATM	8	Pt	4.89656	4.46367	16.79232	Pt	0	0	0.00000
HETATM	9	Pt	0.40423	2.77700	17.45168	Pt	0	0	0.00000
HETATM	10	Pt	3.16403	2.36338	17.38131	Pt	0	0	0.00000
HETATM	11	Pt	1.42867	9.51187	18.00574	Pt	0	0	0.00000
HETATM	12	Pt	4.19195	9.09051	18.00550	Pt	0	0	0.00000
HETATM	13	Pt	2.45741	6.98739	18.60176	Pt	0	0	0.00000
HETATM	14	Pt	5.21594	6.56561	18.60455	Pt	0	0	0.00000
HETATM	15	Pt	0.72584	4.88771	19.21261	Pt	0	0	0.00000
HETATM	16	Pt	3.48317	4.45987	19.20317	Pt	0	0	0.00000
HETATM	17	Pt	1.75720	2.35658	19.81935	Pt	0	0	0.00000
HETATM	18	Pt	4.50546	1.93768	19.81909	Pt	0	0	0.00000
HETATM	19	Pt	2.77842	9.08703	20.41451	Pt	0	0	0.00000
HETATM	20	Pt	5.53775	8.66939	20.41415	Pt	0	0	0.00000
HETATM	21	Pt	1.04636	6.98631	21.01555	Pt	0	0	0.00000
HETATM	22	Pt	3.80508	6.56314	21.01320	Pt	0	0	0.00000
HETATM	23	Pt	2.07375	4.46049	21.61866	Pt	0	0	0.00000
HETATM	24	Pt	4.83144	4.04000	21.61840	Pt	0	0	0.00000
HETATM	25	Pt	0.34097	2.35618	22.22299	Pt	0	0	0.00000
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HETATM	27	Pt	1.36821	9.08776	22.82355	Pt	0	0	0.00000
HETATM	28	Pt	4.12756	8.66621	22.82294	Pt	0	0	0.00000

HETATM	29	Pt	2.39528	6.56364	23.42458	Pt	0	0	0.00000
HETATM	30	Pt	5.15413	6.14282	23.42460	Pt	0	0	0.00000
HETATM	31	Pt	0.66284	4.46044	24.02736	Pt	0	0	0.00000
HETATM	32	Pt	3.42203	4.03963	24.02783	Pt	0	0	0.00000
HETATM	33	Pt	1.69002	1.93637	24.63087	Pt	0	0	0.00000
HETATM	34	Pt	4.44945	1.51533	24.63074	Pt	0	0	0.00000
HETATM	35	Pt	2.71901	8.66951	25.23200	Pt	0	0	0.00000
HETATM	36	Pt	5.47811	8.24876	25.23200	Pt	0	0	0.00000
HETATM	37	Pt	0.98609	6.56566	25.83377	Pt	0	0	0.00000
HETATM	38	Pt	3.74519	6.14491	25.83376	Pt	0	0	0.00000
HETATM	39	Pt	2.01221	4.04092	26.43606	Pt	0	0	0.00000
HETATM	40	Pt	4.77131	3.62016	26.43606	Pt	0	0	0.00000
HETATM	41	Pt	0.27938	1.93728	27.03867	Pt	0	0	0.00000
HETATM	42	Pt	3.03848	1.51653	27.03867	Pt	0	0	0.00000
HETATM	43	Pt	1.30691	8.66841	27.63998	Pt	0	0	0.00000
HETATM	44	Pt	4.06601	8.24765	27.63998	Pt	0	0	0.00000
HETATM	45	Pt	2.33269	6.14422	28.24190	Pt	0	0	0.00000
HETATM	46	Pt	5.09179	5.72346	28.24190	Pt	0	0	0.00000
HETATM	47	Pt	0.60029	4.04015	28.84396	Pt	0	0	0.00000
HETATM	48	Pt	3.35939	3.61939	28.84396	Pt	0	0	0.00000
HETATM	49	Pt	1.62607	1.51583	29.44624	Pt	0	0	0.00000
HETATM	50	Pt	4.38517	1.09507	29.44624	Pt	0	0	0.00000
HETATM	51	Pt	2.65275	8.24728	30.04747	Pt	0	0	0.00000
HETATM	52	Pt	5.41186	7.82652	30.04747	Pt	0	0	0.00000
HETATM	53	Pt	0.92104	6.14315	30.64967	Pt	0	0	0.00000
HETATM	54	Pt	3.68014	5.72239	30.64967	Pt	0	0	0.00000
HETATM	55	Pt	1.94723	3.61841	31.25206	Pt	0	0	0.00000
HETATM	56	Pt	4.70633	3.19765	31.25206	Pt	0	0	0.00000
HETATM	57	Pt	0.21487	1.51472	31.85393	Pt	0	0	0.00000
HETATM	58	Pt	2.97397	1.09397	31.85393	Pt	0	0	0.00000
HETATM	59	Pt	1.24229	8.24735	32.45641	Pt	0	0	0.00000
HETATM	60	Pt	4.00145	7.82663	32.45685	Pt	0	0	0.00000
HETATM	61	Pt	2.26950	5.72358	33.05956	Pt	0	0	0.00000
HETATM	62	Pt	5.02885	5.30289	33.05953	Pt	0	0	0.00000
HETATM	63	Pt	0.53722	3.62090	33.66127	Pt	0	0	0.00000
HETATM	64	Pt	3.29657	3.19942	33.66073	Pt	0	0	0.00000
HETATM	65	Pt	1.56409	1.09645	34.25937	Pt	0	0	0.00000
HETATM	66	Pt	4.32320	0.67466	34.26165	Pt	0	0	0.00000
HETATM	67	Pt	2.59029	7.82705	34.86582	Pt	0	0	0.00000
HETATM	68	Pt	5.35080	7.40604	34.86606	Pt	0	0	0.00000
HETATM	69	Pt	0.85907	5.72452	35.47111	Pt	0	0	0.00000
HETATM	70	Pt	3.61779	5.30138	35.46880	Pt	0	0	0.00000
HETATM	71	Pt	1.88574	3.20078	36.06997	Pt	0	0	0.00000
HETATM	72	Pt	4.64463	2.77691	36.07035	Pt	0	0	0.00000
HETATM	73	Pt	0.15849	1.09377	36.66564	Pt	0	0	0.00000
HETATM	74	Pt	2.90677	0.67486	36.66538	Pt	0	0	0.00000
HETATM	75	Pt	1.18064	7.82818	37.28139	Pt	0	0	0.00000
HETATM	76	Pt	3.93801	7.40035	37.27196	Pt	0	0	0.00000
HETATM	77	Pt	2.20641	5.30068	37.88270	Pt	0	0	0.00000
HETATM	78	Pt	4.96609	4.88098	37.87997	Pt	0	0	0.00000
HETATM	79	Pt	0.47192	3.19763	38.47919	Pt	0	0	0.00000
HETATM	80	Pt	3.23518	2.77626	38.47895	Pt	0	0	0.00000
HETATM	81	Pt	1.49981	0.66827	39.10350	Pt	0	0	0.00000
HETATM	82	Pt	4.25963	0.25465	39.03312	Pt	0	0	0.00000
HETATM	83	Pt	2.52869	7.40278	39.69440	Pt	0	0	0.00000
HETATM	84	Pt	5.28533	6.98302	39.69239	Pt	0	0	0.00000
HETATM	85	Pt	0.79109	5.29170	40.29518	Pt	0	0	0.00000
HETATM	86	Pt	3.55541	4.86926	40.29510	Pt	0	0	0.00000
HETATM	87	Pt	1.81915	2.76249	40.87046	Pt	0	0	0.00000
HETATM	88	Pt	4.57560	2.32381	40.92382	Pt	0	0	0.00000
HETATM	89	Pt	0.13826	0.55353	41.59490	Pt	0	0	0.00000
HETATM	90	Pt	2.75868	0.15452	41.59751	Pt	0	0	0.00000
HETATM	91	O	1.39775	0.03189	42.82258	O	0	0	0.00000

HETATM 92 O 3.26659 2.99873 13.66214 O 0 0 0.00000
UNIT ENERGY kcal
ENERGY -11877.433013
END

XTLGRF 200

DESCRP A0276

REMARK 2x1-fcc-bridge-{100}-step

FIXATOMS 35 58

CRYSTX 5.58200 9.25650 56.48410 90.00000 90.00000 98.67070

FORMAT ATOM (a6,lx,i5,lx,a5,lx,a3,lx,a1,lx,a5,3f10.5,lx,a5,i3,i2,lx,f8.5)

HETATM	1	Pt	2.01399	2.90409	14.63399	Pt	0	0	0.00000
HETATM	2	Pt	4.64672	2.62207	14.91625	Pt	0	0	0.00000
HETATM	3	Pt	0.14415	0.77491	15.47789	Pt	0	0	0.00000
HETATM	4	Pt	2.84223	0.31772	15.51891	Pt	0	0	0.00000
HETATM	5	Pt	1.12212	7.42085	16.21790	Pt	0	0	0.00000
HETATM	6	Pt	3.88410	6.99915	16.17410	Pt	0	0	0.00000
HETATM	7	Pt	2.13492	4.87582	16.78023	Pt	0	0	0.00000
HETATM	8	Pt	4.90708	4.50261	16.84478	Pt	0	0	0.00000
HETATM	9	Pt	0.42646	2.78429	17.43080	Pt	0	0	0.00000
HETATM	10	Pt	3.17940	2.37176	17.33628	Pt	0	0	0.00000
HETATM	11	Pt	1.44667	9.52306	17.98141	Pt	0	0	0.00000
HETATM	12	Pt	4.20436	9.09770	18.04972	Pt	0	0	0.00000
HETATM	13	Pt	2.47065	6.98825	18.60488	Pt	0	0	0.00000
HETATM	14	Pt	5.22915	6.58453	18.62317	Pt	0	0	0.00000
HETATM	15	Pt	0.73855	4.89534	19.22024	Pt	0	0	0.00000
HETATM	16	Pt	3.48745	4.46602	19.20832	Pt	0	0	0.00000
HETATM	17	Pt	1.77020	2.36253	19.80424	Pt	0	0	0.00000
HETATM	18	Pt	4.51706	1.95362	19.80995	Pt	0	0	0.00000
HETATM	19	Pt	2.78437	9.09669	20.41923	Pt	0	0	0.00000
HETATM	20	Pt	5.55457	8.68325	20.42231	Pt	0	0	0.00000
HETATM	21	Pt	1.05691	6.99585	21.02205	Pt	0	0	0.00000
HETATM	22	Pt	3.81415	6.57495	21.01816	Pt	0	0	0.00000
HETATM	23	Pt	2.08190	4.46936	21.62034	Pt	0	0	0.00000
HETATM	24	Pt	4.83902	4.05192	21.62024	Pt	0	0	0.00000
HETATM	25	Pt	0.34940	2.36923	22.21887	Pt	0	0	0.00000
HETATM	26	Pt	3.10753	1.94581	22.22061	Pt	0	0	0.00000
HETATM	27	Pt	1.37520	9.09923	22.82744	Pt	0	0	0.00000
HETATM	28	Pt	4.13430	8.67814	22.82457	Pt	0	0	0.00000
HETATM	29	Pt	2.40131	6.57312	23.42650	Pt	0	0	0.00000
HETATM	30	Pt	5.15969	6.15294	23.42649	Pt	0	0	0.00000
HETATM	31	Pt	0.66747	4.46948	24.02759	Pt	0	0	0.00000
HETATM	32	Pt	3.42676	4.04810	24.02804	Pt	0	0	0.00000
HETATM	33	Pt	1.69378	1.94459	24.62980	Pt	0	0	0.00000
HETATM	34	Pt	4.45307	1.52332	24.62938	Pt	0	0	0.00000
HETATM	35	Pt	2.71997	8.67491	25.23186	Pt	0	0	0.00000
HETATM	36	Pt	5.47907	8.25416	25.23186	Pt	0	0	0.00000
HETATM	37	Pt	0.98705	6.57106	25.83363	Pt	0	0	0.00000
HETATM	38	Pt	3.74615	6.15031	25.83362	Pt	0	0	0.00000
HETATM	39	Pt	2.01317	4.04632	26.43592	Pt	0	0	0.00000
HETATM	40	Pt	4.77227	3.62556	26.43592	Pt	0	0	0.00000
HETATM	41	Pt	0.28034	1.94268	27.03853	Pt	0	0	0.00000
HETATM	42	Pt	3.03944	1.52193	27.03853	Pt	0	0	0.00000
HETATM	43	Pt	1.30787	8.67381	27.63984	Pt	0	0	0.00000
HETATM	44	Pt	4.06697	8.25305	27.63984	Pt	0	0	0.00000
HETATM	45	Pt	2.33365	6.14962	28.24176	Pt	0	0	0.00000
HETATM	46	Pt	5.09275	5.72886	28.24176	Pt	0	0	0.00000
HETATM	47	Pt	0.60125	4.04555	28.84382	Pt	0	0	0.00000
HETATM	48	Pt	3.36035	3.62479	28.84382	Pt	0	0	0.00000
HETATM	49	Pt	1.62703	1.52123	29.44610	Pt	0	0	0.00000
HETATM	50	Pt	4.38613	1.10047	29.44610	Pt	0	0	0.00000
HETATM	51	Pt	2.65371	8.25268	30.04733	Pt	0	0	0.00000
HETATM	52	Pt	5.41282	7.83192	30.04733	Pt	0	0	0.00000

HETATM	53	Pt	0.92200	6.14855	30.64953	Pt	0	0	0.00000
HETATM	54	Pt	3.68110	5.72779	30.64953	Pt	0	0	0.00000
HETATM	55	Pt	1.94819	3.62381	31.25192	Pt	0	0	0.00000
HETATM	56	Pt	4.70729	3.20305	31.25192	Pt	0	0	0.00000
HETATM	57	Pt	0.21583	1.52012	31.85379	Pt	0	0	0.00000
HETATM	58	Pt	2.97493	1.09937	31.85379	Pt	0	0	0.00000
HETATM	59	Pt	1.24049	8.25129	32.45472	Pt	0	0	0.00000
HETATM	60	Pt	3.99974	7.83004	32.45512	Pt	0	0	0.00000
HETATM	61	Pt	2.26582	5.72591	33.05636	Pt	0	0	0.00000
HETATM	62	Pt	5.02564	5.30459	33.05636	Pt	0	0	0.00000
HETATM	63	Pt	0.53280	3.62057	33.65871	Pt	0	0	0.00000
HETATM	64	Pt	3.29191	3.19964	33.65600	Pt	0	0	0.00000
HETATM	65	Pt	1.55941	1.09593	34.26230	Pt	0	0	0.00000
HETATM	66	Pt	4.31763	0.67252	34.26389	Pt	0	0	0.00000
HETATM	67	Pt	2.58454	7.82842	34.86237	Pt	0	0	0.00000
HETATM	68	Pt	5.34559	7.40435	34.86240	Pt	0	0	0.00000
HETATM	69	Pt	0.85220	5.72247	35.46467	Pt	0	0	0.00000
HETATM	70	Pt	3.60948	5.30155	35.46083	Pt	0	0	0.00000
HETATM	71	Pt	1.88203	3.20010	36.06362	Pt	0	0	0.00000
HETATM	72	Pt	4.63009	2.77207	36.06059	Pt	0	0	0.00000
HETATM	73	Pt	0.14912	1.08613	36.67258	Pt	0	0	0.00000
HETATM	74	Pt	2.89610	0.67718	36.67827	Pt	0	0	0.00000
HETATM	75	Pt	1.17838	7.82986	37.27441	Pt	0	0	0.00000
HETATM	76	Pt	3.92741	7.40044	37.26255	Pt	0	0	0.00000
HETATM	77	Pt	2.19542	5.30712	37.87782	Pt	0	0	0.00000
HETATM	78	Pt	4.95523	4.86949	37.85972	Pt	0	0	0.00000
HETATM	79	Pt	0.46227	3.19724	38.43288	Pt	0	0	0.00000
HETATM	80	Pt	3.22003	2.77192	38.50095	Pt	0	0	0.00000
HETATM	81	Pt	1.48733	0.66648	39.14569	Pt	0	0	0.00000
HETATM	82	Pt	4.23996	0.25365	39.05165	Pt	0	0	0.00000
HETATM	83	Pt	2.53068	7.41853	39.70221	Pt	0	0	0.00000
HETATM	84	Pt	5.27705	6.95072	39.63866	Pt	0	0	0.00000
HETATM	85	Pt	0.78210	5.29503	40.30866	Pt	0	0	0.00000
HETATM	86	Pt	3.54413	4.87363	40.26469	Pt	0	0	0.00000
HETATM	87	Pt	1.82676	2.71954	40.96372	Pt	0	0	0.00000
HETATM	88	Pt	4.52458	2.26241	41.00338	Pt	0	0	0.00000
HETATM	89	Pt	0.02456	0.41720	41.56628	Pt	0	0	0.00000
HETATM	90	Pt	2.65710	0.13234	41.84769	Pt	0	0	0.00000
HETATM	91	O	1.11454	-0.19413	42.86953	O	0	0	0.00000
HETATM	92	O	3.07494	2.13521	42.27028	O	0	0	0.00000
HETATM	93	O	3.55659	3.23495	13.61383	O	0	0	0.00000
HETATM	94	O	1.59572	0.90196	14.21153	O	0	0	0.00000

UNIT ENERGY kcal
 ENERGY -12066.160612
 END

XTLGRF 200
 DESCRP A0150
 REMARK 1x1-fcc-top-{100}-step
 FIXATOMS 18 29
 CRYSTX 2.79100 9.25650 56.48410 90.00000 90.00000 98.67070
 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	1.80808	2.67668	14.38218	Pt	0	0	0.00000
HETATM	2	Pt	0.07445	0.58798	15.48215	Pt	0	0	0.00000
HETATM	3	Pt	1.09078	7.20865	16.28967	Pt	0	0	0.00000
HETATM	4	Pt	2.10204	4.58335	16.39877	Pt	0	0	0.00000
HETATM	5	Pt	0.38658	2.59366	17.32397	Pt	0	0	0.00000
HETATM	6	Pt	1.41247	9.32262	18.06333	Pt	0	0	0.00000
HETATM	7	Pt	2.43728	6.78485	18.64668	Pt	0	0	0.00000
HETATM	8	Pt	0.70441	4.67988	19.16819	Pt	0	0	0.00000
HETATM	9	Pt	1.73278	2.16791	19.78869	Pt	0	0	0.00000
HETATM	10	Pt	2.75840	8.89438	20.44505	Pt	0	0	0.00000
HETATM	11	Pt	1.02470	6.78336	21.03011	Pt	0	0	0.00000

[illegible]